

**EU ACADEMY OF SCIENCES  
EUAS**

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**The President of EUAS**

Professor E.G. Ladopoulos

**& The Board Governors of EUAS**

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# New Aspects of the Energy World by “Universal Mechanics”. Is this the Leading Theory of the Millenium?

by Evangelos Ladopoulos, President & CEO of EUAS

## Short Biography

*Prof. Dr. Civil Engineer, Mechanical (Aerospace) Engineer & Petroleum Engineer, D.Sc.  
Included in the list of 2000 Outstanding Scientists of 20<sup>th</sup> Century by Cambridge Bio  
Centre.*

*Included in the list of 2000 Outstanding Scientists of 21<sup>st</sup> Century by Cambridge Bio  
Centre.*

*Included in the list of 100 Top Scientists of 2007 by Cambridge Bio Centre.*

*Over 500 publications in high quality scientific journals and 5 books.*

*Project Manager for over 500 Projects in Civil Engineering, Mechanical Engineering,  
Aerospace Engineering and Petroleum Engineering.*

*Chairman and Professor by Interpaper Research Organization.*

*Visiting Professor at Universities in Europe and USA.*

*Editor-in-Chief of many SCI Engineering Journals.*

*High Index by Google Scholar.*

*President & CEO of the EU Academy of Sciences.*

*Member by several Academies in USA.*

For the design of the future spacecraft of any speed, even approaching the speed of light, the leading technology of “**Universal Mechanics**” is proposed and investigated. The groundbreaking theory of “*Universal Mechanics*” consists to the combination of the theories of “*Relativistic Elasticity*” and “*Relativistic Thermo-Elasticity*”. Thus, according to the above theories there is a considerable difference between the absolute stress tensor and the stress tensor of the airframe even in the range of speeds of 50,000 km/h. Also, for bigger speeds of the absolute spacecraft, like  $c/3$ ,  $c/2$  or  $3c/4$  ( $c$ =speed of light), then the difference between the two stress tensors is very much increased. Consequently, for the future spacecraft with very high speeds, the relative stress tensor will be therefore very much different than the absolute stress tensor. Also, for velocities near the speed of light, then the values of the relative stress tensor are very much bigger than the corresponding values of the absolute stress tensor. Such future spacecraft will be moving by using laser engines.

When approaching the speed of light an **Energy World** would appear. Is that possible ? Yes of course it is possible. During the past years many people have seen in the sky several lights in the form of spacecraft or flying saucers. So, these might be aliens much more developed than humans with their science very much developed and their spacecraft is in energy form. Hence, if the spacecraft exceeds the speed of light, then it becomes an energy spacecraft. In that case an **Energy World** would be possible.

Another question is what will be next ? Has the energy world to do anything with the life after death ? So, is the soul a kind of energy ? Could be the soul connected to the

energy world ? Also, is the theory of the *Energy World* in connection with “*Universal Mechanics*” the leading theory of the Millenium ?

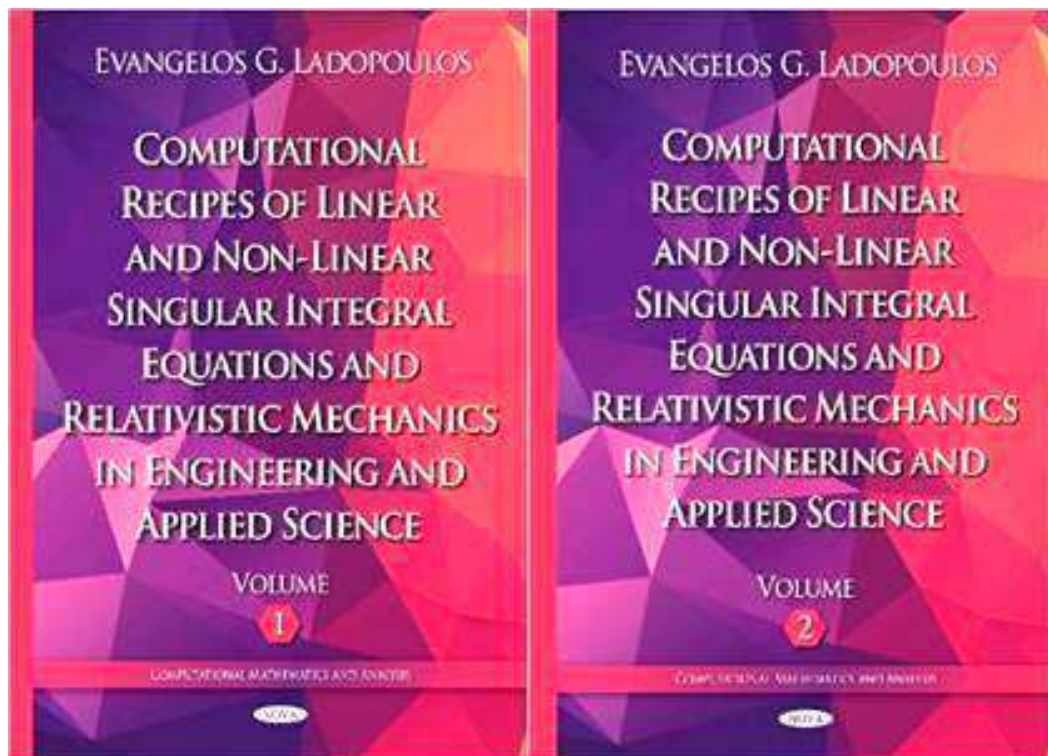
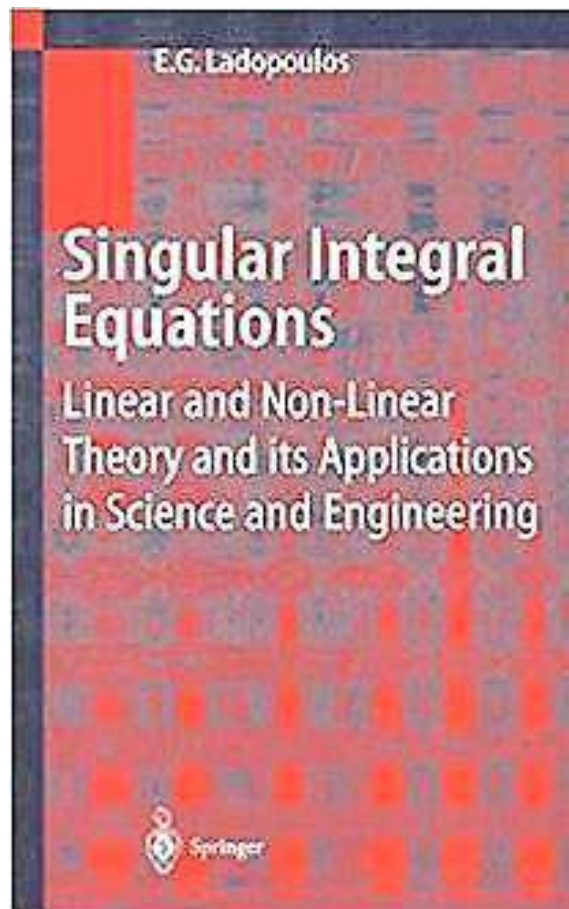
The theory of “*Relativistic Elasticity*” is a combination between the theories of "Classical Elasticity" and "Special Relativity" and results in the “*Universal Equation of Elasticity*”. Furthermore, the theory of “*Relativistic Thermo-Elasticity*” is a combination between the theories of "Classical Thermo-Elasticity" and "Special Relativity" and results in the “*Universal Equation of Thermo-Elasticity*”. The "structural design" of super speed vehicles requires the consideration of mass pulsation and energy-mass interaction at high velocity space-time scale, as the relative stress intensity factors are different than the corresponding absolute stress intensity factors. Such theory results in the “*Universal Stress Intensity Factors*”. Hence, the “*Universal Equation of Elasticity*”, the “*Universal Equation of Thermo-Elasticity*” and the “*Universal Stress Intensity Factors*” are parts of the general theory of “*Universal Mechanics*”.

The scope by the International Space Agencies is to achieve in the future, a new generation spacecraft moving with very high speeds, even approaching the speed of light. How far could be this future ? According to current author’s research such future could be much closer than everybody believes. For the future spacecraft the relative stress tensor will be much different than the absolute stress tensor and so special solid should be used for the construction of the future spacecraft.

Additionally, in order the future spacecraft to achieve very high speed, even approaching the speed of light, then such new generation spacecraft should be moving by using laser engines. Laser is light and so their speed is the speed of light. So, the use of laser engines for the future spacecraft might be the best device. The study of such laser engines is under investigation. Besides, special material should be used for the construction of such spacecraft. Such special material is under study and investigation.

A second question is the following: What happens with our leading theory if somebody in the very future proves that the speed of light is not the maximum speed in the whole universe, but there is another type of energy with higher speed than light ? The answer is that our theory of “*Universal Mechanics*” will valid over the centuries and the milleniums, as the spacecraft when reaching the speed of light then becomes energy and will not be mass any more. Consequently, after the speed of light there is no mass available, but only energy. According to NASA the Large and Small Magellanic clouds were thought to be the closest galaxies to ours, until 1994, when the Sagittarius Dwarf Elliptical Galaxy (SagDEG) was discovered. In 2003, the Canis Major Dwarf Galaxy was discovered - this is now the closest known galaxy to ours. Thus, The Canis Major Dwarf Galaxy is only 25,000 light years from the Sun, and 42,000 light years from the Galactic center. It too, is well-hidden by the dust in the plane of the Milky Way - which is why it wasn't discovered until recently. To get to the closest galaxy to ours, the Canis Major Dwarf, at Voyager's speed, it would take approximately 749,000,000 years to travel the distance of 25,000 light years! If we could travel at the speed of light, it would still take 25,000 years. On the other hand, the galaxy MACS0647-JD appears very young and is only a fraction of the size of our own Milky Way. The galaxy is about 13.3 billion light-years from Earth, the farthest galaxy yet known, and formed 420 million years after the Big Bang. The universe itself is only 13.7 billion years old, so this galaxy's light has been traveling toward us for almost the whole history of space and time.

More details can be seen by the following books:

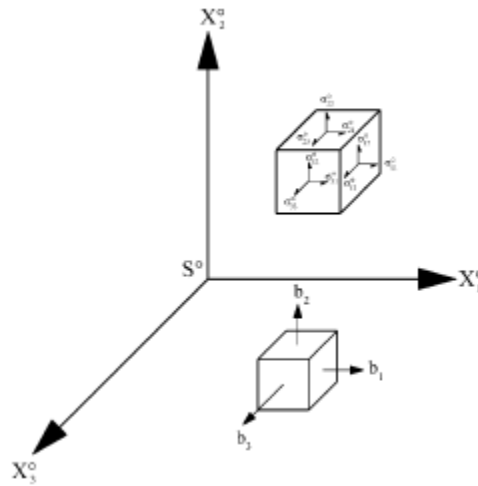


Consider the state of stress at a point in the stationary frame  $S^0$ , defined by the following symmetrical stress tensor: (Fig.1)

$$\sigma^0 = \begin{bmatrix} \sigma_{11}^0 & \sigma_{12}^0 & \sigma_{13}^0 \\ \sigma_{21}^0 & \sigma_{22}^0 & \sigma_{23}^0 \\ \sigma_{31}^0 & \sigma_{32}^0 & \sigma_{33}^0 \end{bmatrix} \quad (1)$$

where:

$$\sigma_{21}^0 = \sigma_{12}^0, \sigma_{31}^0 = \sigma_{13}^0, \sigma_{32}^0 = \sigma_{23}^0 \quad (2)$$



**Fig. 1** The state of stress  $\sigma_{ik}^0$  in the stationary system  $S^0$ .

In addition, we consider an infinitesimal face element  $df$  with a directed normal, defined by a unit vector  $\mathbf{n}$ , at definite point  $p$  in the three-space of a Lorenz system. The matter on either side of this face element experiences a force which is proportional to  $df$ .

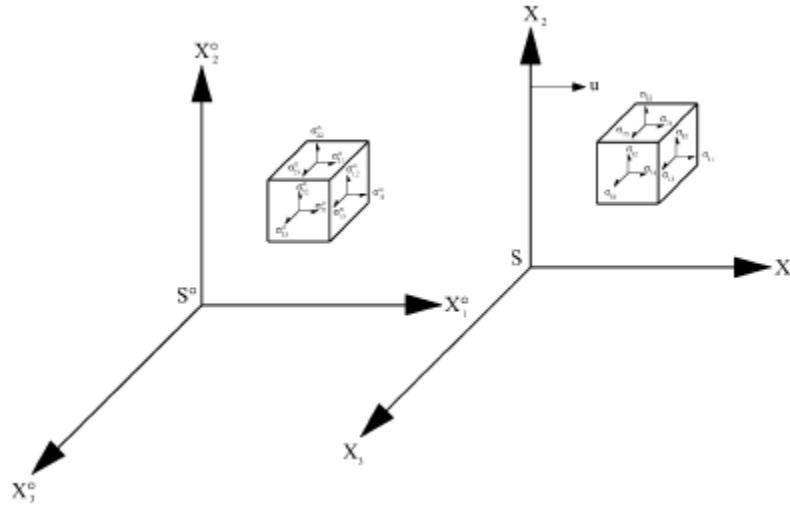
Thus, the force is valid as:

$$d\sigma(\mathbf{n}) = \sigma(\mathbf{n})df \quad (3)$$

The components  $\sigma_i(\mathbf{n})$  of  $\sigma(\mathbf{n})$  are linear functions of the components  $n_k$  of  $\mathbf{n}$ :

$$\sigma_i(\mathbf{n}) = \sigma_{ik} n_k, \quad i, k = 1, 2, 3 \quad (4)$$

where  $\sigma_{ik}$  is the elastic stress tensor, also called as the relative stress tensor, in contrast to the space part  $\sigma_{ik}^0$  of the total energy-momentum tensor  $T_{ik}$ , referred as the absolute stress tensor (Fig. 2).



**Fig. 2** The state of stress  $\sigma_{ik}^0$  in the stationary system  $S^0$  and  $\sigma_{ik}$  in the airframe system with velocity  $u$  parallel to the  $x_1$  - axis.

Also, the connection between the absolute and relative stress tensors is defined as:

$$\sigma_{ik}^0 = \sigma_{ik} + g_i u_k, \quad i, k = 1, 2, 3 \tag{5}$$

where  $g_i$  are the components of the momentum density  $\mathbf{g}$  and  $u_k$  the components of the velocity  $\mathbf{u}$  of the matter.

The relative stress tensor gives the *Universal Equation of Elasticity*:

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} = \begin{bmatrix} \sigma_{11}^0 & \gamma \sigma_{12}^0 & \gamma \sigma_{13}^0 \\ \frac{1}{\gamma} \sigma_{21}^0 & \sigma_{22}^0 & \sigma_{23}^0 \\ \frac{1}{\gamma} \sigma_{31}^0 & \sigma_{32}^0 & \sigma_{33}^0 \end{bmatrix} \tag{6}$$

in which  $\gamma$  is given by:

$$\gamma = 1/(1 - u^2/c^2)^{1/2} \tag{7}$$

with  $c$  the speed of light.

In addition, consider the general system of continuously matter, inside which invisible heat conduction can take place. Then the momentum density  $\mathbf{g}$  of this system is given by the *Universal Equation of Thermo-Elasticity*:

$$\mathbf{g} = m\mathbf{u} + \frac{(\mathbf{u}, \boldsymbol{\sigma})}{c^2} + \frac{\boldsymbol{\xi}}{c^2} \tag{8}$$

where  $\mathbf{u}$  denotes the velocity of the matter at the place and time considered,  $\sigma$  the relative stress tensor,  $m = E/c^2$  is the total mass density and  $\xi$  is given by:

$$\xi = \gamma[\mathbf{V} - \mathbf{u}(\mathbf{V}, \mathbf{u})/c^2] \tag{9}$$

with  $\mathbf{V}$  the four vector.

Beyond the above, “*Universal Mechanics*” gives the complete theory of mechanics for the whole universe. Then the theories of Special and General Relativity, as were proposed by Albert Einstein are completed for the whole universe by “*Universal Mechanics*”, as proposed by the current author. Thus, by the current author is completed the theory of Albert Einstein for the whole universe regarding mechanics engineering behavior. *So, this theory could be the leading Theory of the Millenium ?*

Table 1 shows the values of  $\gamma$  of relativity theory for some arbitrary values of the velocity  $u$  of the moving aerospace structure, where  $c$  is the speed of light (300,000 km/sec):

Table 1

Velocity $u$	$\gamma = 1/\sqrt{1-u^2/c^2}$	Velocity $u$	$\gamma = 1/\sqrt{1-u^2/c^2}$
50,000 km/h	1.000000001	0.800c	1.666666667
100,000 km/h	1.000000004	0.900c	2.294157339
200,000 km/h	1.000000017	0.950c	3.202563076
500,000 km/h	1.000000107	0.990c	7.088812050
10E+06 km/h	1.000000429	0.999c	22.36627204
10E+07 km/h	1.000042870	0.9999c	70.71244596
10E+08 km/h	1.004314456	0.99999c	223.6073568
2x10E+8 km/h	1.017600788	0.999999c	707.1067812
c/3	1.060660172	0.9999999c	2236.067978
c/2	1.154700538	0.99999999c	7071.067812
2c/3	1.341640786	0.999999999c	22360.67978
3c/4	1.511857892	c	$\infty$

From Table 1 follows that for small velocities 50,000 km/h to 200,000 km/h, the absolute and the relative stress tensors are nearly the same. On the other hand, for bigger velocities like  $c/3$ ,  $c/2$  or  $3c/4$  ( $c$  = speed of light), the variable  $\gamma$  takes values more than the unit and thus, relative stress tensor is very different from the absolute one. In addition, for values of the velocity for the moving structure near the speed of light, the variable  $\gamma$  takes bigger values, while when the velocity is equal to the speed of light, then  $\gamma$  tends to the infinity.

For the design of the future spacecraft the “*Universal Stress Intensity Factors*” are further used. So, as was shown by the current author, the relative first and third mode stress intensity factors are the same for both stationary and moving frames, while the relative second mode stress intensity factor is much different in the above frames. All the relative stress intensity factors (first, second and third) are important for the fracture mechanics analysis of the future spacecraft, as for their fracture mechanics analysis a combination of all the three intensity factors should be used.

The **Universal Stress Intensity Factors** are given by the formulas:

$$K_I = \lim_{x_1 \rightarrow 0} \left\{ \sqrt{2\pi x_1} \sigma_{22}^0 \right\} \quad (10)$$

$$K_{II} = \lim_{x_1 \rightarrow 0} \left\{ \sqrt{2\pi x_1} \gamma \sigma_{12}^0 \right\} \quad (11)$$

$$K_{III} = \lim_{x_1 \rightarrow 0} \left\{ \sqrt{2\pi x_1} \sigma_{23}^0 \right\} \quad (12)$$

Hence, from eqs (10) to (12) follows that the relative first and third mode stress intensity factors are the same for both stationary and moving frames, while the relative second mode stress intensity factor is much different in the above frames. Consequently, because of the above difference of the stress intensity factors, follows that the fracture behavior of the future spacecraft would be much different and thus special materials should be used for their construction. The material which can be used is under investigation.

When the relative stress intensity factors are taken into consideration, then the whole theory is known as “*Universal Fracture Mechanics*”.

# Complete Utilization of Food Waste using Innovative Processes and Systems

by Roger Ruan, Member EUAS

## Short Biography

*Dr. Roger Ruan, Professor and Director of Graduate Studies, Department of Bioproducts and Biosystems Engineering, and Director of Center for Biorefining at University of Minnesota, is a Fellow of ASABE, IFT, IAAM, and Vebleo, and have received many other awards, including CAFS Professional Achievement, Scientist of IAAM, etc. Dr. Ruan's research areas include renewable energy and environment technologies for sustainable development and circular economy. Specifically, he has conducted research and published his findings in the areas of biomass and solid wastes such as plastic wastes pyrolysis and gasification for chemicals, materials, fuels and energy production; municipal, agricultural, and industrial wastewater treatment and utilization through novel anaerobic digestion, microalgae cultivation, and hydroponics; airborne and other pathogen disinfection and pollutant control; innovative catalytic non-thermal plasma, low temperature microwave and pulse microwave, photocatalytic intensive pulse light, and NMR/MRI technologies development and applications in nitrogen fixation, food safety assurance, and food quality improvement; and food engineering and various value-added processing.*

*Professor Ruan has published over 600 papers in refereed journals, two books, and 24 book chapters, and holds 20 US patents. He is also a top-cited author with an h-index of 80, i10-index of 393, and over 25,000 citations He has supervised over 75 graduate students, 140 post-doctors, research fellows, and other engineers and scientists, and many of his Ph.D. students and post-doctors hold university faculty positions. He has also been invited to give over 300 keynote lectures, invited symposium presentations, company seminars, and short courses, and has been a consultant for government agencies, and many local, national, and international companies and agencies in bioprocess engineering, food engineering, and renewable energy and environment areas. Professor Ruan has received and managed over 200 projects totaling over \$45 million in various funding for research, including major funding from USDA, DOE, DOT, DOD, LCCMR, and industries. He has served as guest editor or editorial board member of Bioresource Technology, Renewable Energy, Engineering, Applied Catalysis and Chemical Engineering, Journal of Food Process Engineering, The Open Plasma Physics Journal, and Associate Editor of Transactions of ASABE, Engineering Applications in Agriculture, and Transactions of CSAE, and Chairman of Editorial Board and Editor-in-Chief of International Journal of Agricultural and Biological Engineering, etc. He has also organized and chaired multiple international conferences including Conference of Food Engineering (CoFE2018), International Conference on Environmental Pollution and Governance (ICEPG 2021), 2nd International Symposium on Environmental Protection and Chemical Engineering (ISEPCE 2021), International Conference on Energy Engineering, New Energy Materials and Devices (NEMD 2021), etc., and served on many conference organization committees.*

*Professor Ruan has taught many undergraduate and graduate courses, including Renewable energy technologies, Biological process engineering, Managing water in food and biological systems, Instrumentation and control for biological systems, Food process*

*engineering, and Engineering principles and applications, etc.*

America is losing up to 40 percent of its food from farm to fork to landfill. In addition to the fact that 49% of food production is wasted, there are significant environmental impacts associated with that loss. Food accounts for 21% of municipal solid waste that is often disposed of in landfills, and produces 11% of landfill generated methane gas (a powerful greenhouse gas) emissions. Landfills contribute to water quality issues from runoff and leaching of contaminants into the surface and groundwater systems. In our lab, we aim to develop and demonstrate an integrated facility to convert food waste into renewable energy, feeds, foods, and clean water, with the circular economy in mind. The goal is to integrate a series biological/thermochemical processes into a multi-functional system, consisting of the following components: (1) bacteria based fermentation to produce methane and reduce the nutrient levels to a degree suitable for algae cultivation, (2) algae cultivation to further remove nutrients and produce biomass as feeds, (3) black soldier fly larvae culture for feed production, (4) catalytic microwave-assisted pyrolysis/gasification of the remaining solid waste for energy, and (5) aquaponic facility to utilize the water and feeds to produce vegetables and fish.

This biological treatment system (Figure 1) starts with food waste slurry, which may be high in protein and ammonia. Some of this ammonia may need to be removed prior to the downstream processes to protect the microbial communities and enhance biogas production in the anaerobic digester. However, in many cases, general food wastes used for anaerobic digestion (AD) do not need ammonia stripping; in fact, in some cases, ammonia nitrogen is added to enhance anaerobic digestion. In other cases, food waste may need to be mixed with a carbon source, such as ground corn stover, to increase the carbon to nitrogen ratio, which is a key parameter in anaerobic digestion. Higher ratios of carbon to nitrogen favor methane production, while lower ratios (more nitrogen relative to carbon) favor ammonia production. The food waste slurry can then be heated to 53°C for thermophilic AD, or 35°C for mesophilic AD. The food waste slurry can be placed under vacuum conditions, where excess ammonia, if present, and most of the hydrogen sulfide, and some water vapors are evaporated from the solution. These vapors can be pulled by vacuum through a condenser to remove water and ammonia, followed by a sulfuric acid wash to capture the ammonia, as ammonium sulfate, which can be sold as a fertilizer. Finally, the vapors can be pulled through a caustic wash to remove any toxic hydrogen sulfide before the vapor is released into the air. After a few hours under vacuum and heat, any excess ammonia, if present, will be sufficiently removed, and the food waste slurry will be ready to be transferred to an anaerobic digester.

The anaerobic digestion system (Figure 1) can use mesophilic anaerobic digestion to reduce chemical oxygen demand, and break up organic matter to produce biogas, which is rich in renewable methane. Mesophilic means medium heat or about 35°C, and anaerobic means that the reactions take place in an oxygen-free environment. A community of bacteria convert carbon compounds to valuable and renewable methane fuel, mixed with carbon dioxide. The reduction in chemical oxygen demand (COD) is also a key part of treating the waste, and this degradation makes the remaining nutrients in the wastewater more available for algae growth in the next stage. In a typical, 2-Liter laboratory AD reactor, with a 20-day HRT (hydraulic retention time), 4.56 grams of volatile solids (VS) were fed daily, in 100 ml of food waste slurry.

These 4.56 grams/day of VS generated 1.52 grams of methane gas, so the weight-ratio of methane generated per unit of volatile solid in the feed was 0.333 grams of methane/gram of volatile solid. This is close to the theoretical methane production rate estimated, or 0.368 grams methane/gram VS, based on the weighted average of each of the

VS components. Based on the above laboratory food waste biogas results, this potential performance can be scaled up to an industrial food waste, anaerobic digestion process.



**Figure 1.** Lab and pilot AD systems at the UMN.

Such an industrial AD system could slurry 7 tons/hour of food wastes into ~10,100 gallons per hour of industrial wastewater, and yield an AD feed slurry of 196 gallons per minute at an estimated COD load of 57,522 ppm. About 10% of the COD load might come from the wastewater and ~90% from the food wastes. This resulting waste stream is estimated to generate ~ 34,000 cubic feet per hour of methane gas, with an energy content of 30,339,000 BTU's per hour. Assuming 306 operating days/year = 7,344 hours/year, this system is estimated to produce 222.8-billion BTUs/year. On that basis, the gross market value of the above bio-methane is estimated to be \$6,680,000 per year (assuming transportation fuel, valued at \$30/million BTUs). If this bio-methane were to be converted to "CNG" (compressed natural gas) and used internally by a commercial plant, it could potentially displace the purchase of as much as 1,856,747 gallons of petroleum fuel per year.

The solid fraction in the effluent can be separated via filtration and then used to cultivate insects and worms, in consideration of a few advantages: (1) many insects can efficiently utilize a wide variety of organic wastes as a feed source, which demonstrates an important flexibility as a method of waste stream utilization; (2) insects grow rapidly and have high reproductive rates, which leads to high waste-to-food conversion rates; (3) greenhouse gas emissions from insects are significantly lower than traditional livestock; (4) insect farming is easily scalable, and feasible at industrial scales; (5) insect biomass is protein rich, and has a diverse micronutrient profile with high bioavailability; (6) food products made from insects can be a safe and palatable food for human consumption (Addy et al. 2020). The nutrient dense biomass produced by insect rearing practices represents a high-value commodity, as it is rich in protein, oils, and various trace elements, which are ideal for use as food or as animal feed. Also, this biomass frequently contains valuable nutraceutical compounds. We found that maximizing bioconversion efficiencies

of food waste often involves matching the insect/worm with an appropriate feedstock. Fortunately, the immense biodiversity of invertebrates indicates that there are many options when matching invertebrate species with different types of organic wastes. The solid waste, after insects/worms cultivation, can subsequently be injected into our catalytic microwave-assisted pyrolysis system (Figure 2) featuring a SiC mixing ball bed for energy, chemicals, and materials production. For example, energy balance analysis shows that a cold gas efficiency of around 70-80% can be achieved at 800°C gasification, which consumed about 7.2 MJ of electrical energy per kg of biomass at 200 kg/day small scale system (Dai et al. 2017; Zhou et al, 2020; Zhang et al. 2017). Further measures to improve energy efficiency could potentially reduce the electrical consumption to 3.45 MJ/kg biomass, enabling a net electricity production. Furthermore, our analysis shows that the combustion of 85% pyrolytic gas obtained from solid waste pyrolysis/gasification may be able to supply enough energy for catalytic microwave-assisted pyrolysis/gasification system operation, thereby making the process energy self-sufficient. When the capacity of the system increases from 1 ton/day to 10 tons/day, the net annual profit could be enhanced to around \$250,000/year with a return on investment of 8.4%.



**Figure 2.** Prof. Ruan's team has developed a few microwave-assisted pyrolysis/gasification systems over the years, at the UMN.

After the effluent from the anaerobic digester is filtered and diluted, it is ready to be fed to algae. In order to decolorize the effluent to improve algae cultivation, biochar with large surface area, and abundant functional groups, is also developed for further purification. The next stage in the wastewater treatment process is to grow algae in the wastewater medium (Figure 3). During this stage, excess ammonia can inhibit, and even cause algal cell death, which is why ammonia removal pretreatment is essential, to assure that the nutrients in the AD effluent are suitable for microalgae cultivation. The algae are, then, capable of consuming the remaining ammonia, as well as most of the phosphorus and other nutrients, to produce algal biomass at the final concentration of more than 1.0 g/L, and with a productivity of above ca. 30 mg/L/d (Ren et al. 2017; Wang et al. 2010). Along with the significant consumption of total nitrogen and total phosphorus by algal cells after

cultivation in bioreactors, the removal efficiency of chemical oxygen demanding (COD) in the wastewater medium can reach more than 80.0% under optimal conditions. Chemical composition analysis demonstrated that the harvested biomass contained a high content of proteins (35%~60%), saccharides (>10%), and lipids (10%~30%) which can further be utilized as feed, fertilizer, and fuel. Additionally, some of the biogas from the anaerobic digester can be cycled through the algae reactor for biogas upgrading, where much of the carbon dioxide can be absorbed, and consumed by the algae with the biomass yield of ca. 55 %, while the methane passes through and can be collected at the top.



**Figure 3.** Lab and pilot scale algae cultivation systems at the UMN.

After leaving the microalgae reactor, the wastewater still has usable nutrients. This nutrient solution can be transferred to a hydroponic cultivation system where it can be used, and removed, by vegetative plants (Figure 4). Due to higher than preferable salt accumulation in the upstream processes, a salt-tolerant species of Swiss Chard has been chosen. Plants are even more sensitive to ammonia levels than are microalgae, so care must be taken to remove the ammonia nearly fully, prior to hydroponic cultivation. The effluent could further be filtered and conditioned as needed using biochar for recycling or discharge. The use of algae and hydroponic systems can also be combined with a fish production system to help ensure the fish water quality.



**Figure 4.** Fish and vegetable symbiotic systems.

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# Single Atom and Molecule Engineering by Scanning Probe Microscopy

by Nan Yao, Member EUAS



## Short Biography

Professor Nan Yao is the founding director of Princeton's preeminent Imaging and Analysis Center and an Inaugural Professor of the Practice at Princeton University. As a research scholar, Yao has over 300 publications that reflect his significant scientific contributions, including the co-discovery of the first natural quasicrystal, a finding that has revolutionized the science of natural crystal chemistry by identifying the third form of solid in nature besides crystalline and non-crystalline. As a faculty member, Yao is a ten-time recipient of the Excellence in Teaching and Commendation for Outstanding Teaching Award at Princeton where he has taught more than 4000 students, postdocs, and researchers. Yao has been committed to pushing the boundaries of science and engineering to benefit academia, industry and society in myriad ways.

Yao's research has been focused on utilizing advanced imaging, diffraction, spectroscopy and in-situ techniques, in tandem with computer simulation, to conduct fundamental studies of the structure-composition-processing-property relationships in complex materials for applications in nanotechnology, energy, environment and health. Yao has published two books entitled *Handbook of Microscopy for Nanotechnology* (Kluwer/Springer Publishers 2005, Chinese edition: Tsinghua University Press 2006, Russian edition: Springer Publishers 2011) and *Focused Ion Beam System: Basics and Applications* (Cambridge University Press, 2007). He has also authored 18 book chapters and about 300 research publications in scientific journals, including *Science*, *Nature*, and many others. Yao is respected for many contributions to the field including his pioneer work in developing the first 300 keV Environmental-cell Transmission Electron Microscope (1991) and developing a theoretical explanation for the superior imaging resolution of scanning helium-ion microscopy over the scanning electron microscopy (2008).

After searching for more than a decade, in cooperation with L. Bindi, P. J. Steinhardt and P. Lu, Yao obtained the first conclusive evidence of crystallographically forbidden icosahedral symmetry in a naturally occurring phase that led the discovery of natural quasicrystal [*Science* 324 (5932), 1306 (2009)]. This extraordinary breakthrough was cited in the Nobel Prize in Chemistry 2011 press release. Furthermore, in recognition of their achievement, Yao's co-discoverer, Bindi was awarded the "2015 Presidente della Repubblica Prize", the highest national scientific award in Italy. In 2015, Yao's transmission electron microscopy results again provided conclusive evidence for the discovery of the second quasicrystal of any kind found in nature, a novel natural quasicrystal with decagonal symmetry [*Scientific Reports* 5 9111 (2015)]. The discovery of the natural quasicrystals opens a new chapter in the study of mineralogy, forever redefining the conventional classification of mineral forms established in the 19<sup>th</sup> century. This discovery also opens a new way of longitudinally studying metal alloy stability in pressure and temperature conditions not accessible in the laboratory. These discoveries, which came from the study of meteorite samples that formed about 4.5 billion years ago, could answer basic questions about how materials were formed in our universe. In 2010, Yao's work with A. Maloof, et al. resulted in discovering a 650 million-year-old sponge-like organism. The shell-like fossils represent the earliest evidence of such animal forms in the current fossil record. The finding means animals appeared on Earth about 100 million years earlier than first thought, a significant contribution to the study of the development of Earth [*Nature Geoscience* 3 (9), 653 (2010)]. Together with D. Norris, Yao was invited to publish the opening paper in *Nano Letters'* inaugural issue [*Nano Letters* 1 (1), 3 (2001)]. With P. Lu and P. Chaikin, Yao's microscopy work also helped identify the earliest known use of diamond in 4000 BC [*Archaeometry*. 47, 1 (2005)]. In 2018, Yao organized the

inaugural Princeton - Nature Conference, in partner with the scientific publisher - Nature, entitled "Frontiers in Electron Microscopy for the Physical and Life Sciences", which is for the first time brings together scientists from both the physical and the life sciences to explore the new horizons of research now becoming available through electron microscopy.

Yao's primary directive is devoted to teaching in academia, industry, and beyond. He created and directs a teaching curriculum in materials characterization at Princeton. In addition to regular for-credit classes, Yao has also developed an outreach program through short courses and workshops in materials science, which are offered monthly to students from other universities and to industrial scientists, all free of charge. More than 4000 undergraduate and graduate students, postdocs, and researchers have enjoyed their learning experience in Yao's classroom at Princeton. More than 120 teachers and researchers from Africa have studied electron microscopy with Professor Yao and later became the first group of electron microscopists in many Africa countries. Yao is a faculty advisor sought after by many students at Princeton. His students have won many national awards including Fannie and John Hertz Foundation Fellowship, Barry M. Goldwater National Scholarship, Fulbright Scholarship, Rhodes Scholarship, AFCEA National Grand Prize for Science, National Science Foundation Fellowship, National Defense Science and Engineering Fellowship, Materials Research Society Student Award, Microbeam Analysis Society Distinguished Scholar Award, Microscopy Society of America Undergraduate Research Award (5 times), Lawrence Fellowship, Forbes' 30 Under 30, and French Innovators Under 35, etc. Professor Yao has been a mentor in New Jersey Liberty Science Center since 2001. He received the Outstanding Service Award in Preparing Science and Technology Leaders for the Future from the Siemens Foundation in 2011.

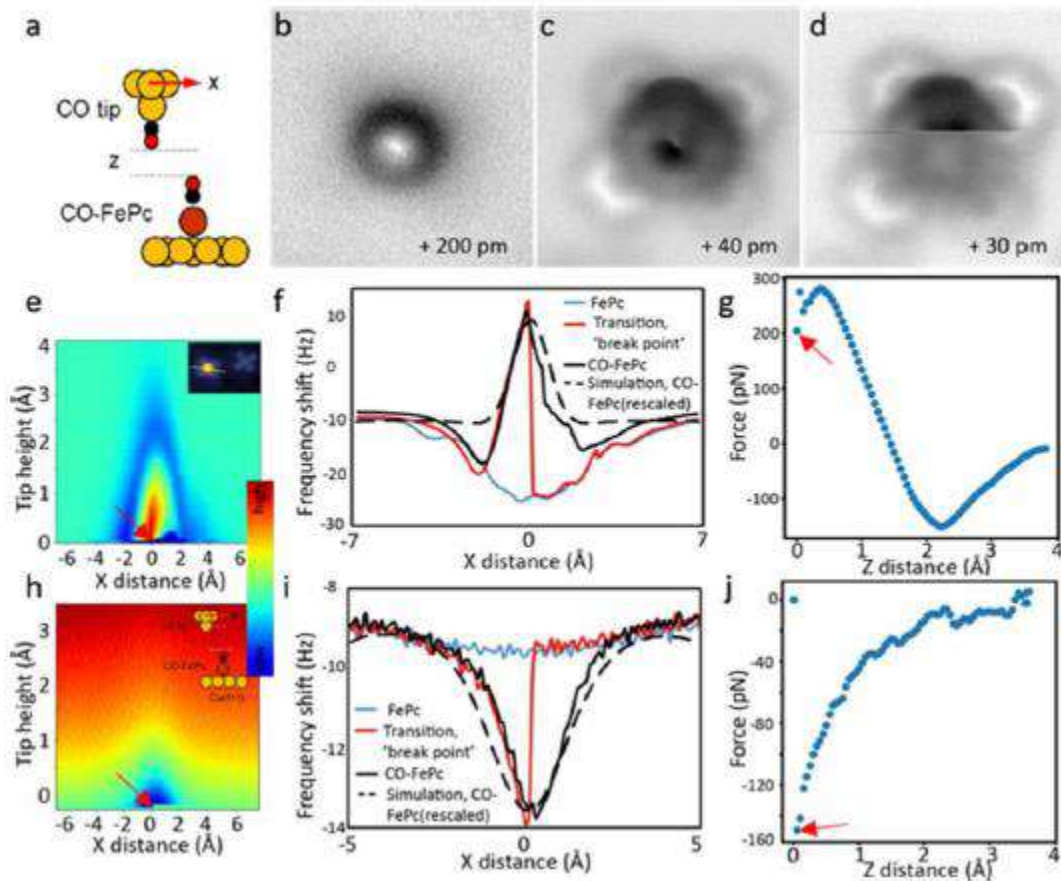
Having started his career as an industrial scientist, Yao has since devoted himself to building stronger bonds between academia and industry, as well as public society. For more than 28 years at Princeton, he has personally educated over 800 industrial scientists from more than 120 companies by providing them with hands-on experience in materials characterization through his short course/workshop program and by facilitating joint collaborative research. Yao's efforts have helped lead these industrial partners to many innovations and new product developments. Companies that have benefited from such collaborative education and research include Bristol Myers Squibb, Colgate-Palmolive, Dow Chemical, DuPont, ExxonMobil, GE, Henkel, Johnson & Johnson, Lockheed Martin, Merck, Shell, Sun Chemical, as well as many new startups. Yao is accomplished at establishing and leading large central facilities under financial constraints and developing them as engines of education, research, and innovation. He carries a strong record for his collaborations and skills at crossing disciplinary to facilitate research at Princeton, and international recognition in the materials and structural analysis.

After receiving a Ph.D. in applied physics and electron microscopy from Arizona State University where John M. Cowley was his dissertation advisor, Yao entered industry, first working at the Shell Development Company, then at the ExxonMobil Research and Engineering Company. He joined Princeton University in 1993 to help build an interdisciplinary imaging and analysis program, which has since become a world-leading materials characterization center at Princeton. Yao is a fellow of the Microscopy Society of America, a fellow of the Royal Microscopical Society of United Kingdom, and a fellow of the American Association for the Advancement of Science.

Science and technology ever seek to build structures of progressively smaller size that has finally reached the point where structures and materials can be imaged and manipulated via atom-by-atom engineering. This ability can enable us to build and characterize model systems that will advance the catalytic material development and the understanding of physics and chemistry.[1-3] By necessity, we must combine both the imaging and manipulation techniques, to affect matter and to real-time monitor the system at atomic level.

Every chemical reaction involves the making and breaking of atomic bonds. Examining the physical nature of these bonds and the forces that alter them is crucial to understanding chemical and catalytic processes. In this article, we report a detailed *in situ* bonding rupture study utilizing a q-Plus type non-contact atomic force microscope (nc-AFM) and scanning tunneling microscope.[4] Using both a metallic tip and a carbon monoxide (CO) functionalized tip, the forces involved in rupturing a dative covalent bond were measured with piconewton (pN) precision. In combination with quantum-based simulations, our results show the bond-breaking process in unprecedented detail. For example, we find that the dative bond between CO and the iron atom in a ferrous phthalocyanine molecule can be ruptured by an attractive

force of  $\sim 150$  pN or by a repulsive force of  $\sim 220$  pN, with a significant contribution of shear forces, accompanied by changes of the spin state of the system. We also find that a FePc molecule can be lifted  $\sim 30$  pm upward from Cu(111) surface by attaching a single CO molecule to the Fe. The breakage of CO and Fe takes place not at the maximum of rupture force and occurred when the tip was  $\sim 30$  picometers above the molecules — a distance that corresponds to about one-sixth the width of a carbon atom.



**Figure 1.** **a** Schematic of a CO-AFM tip interacting with CO-FePc (Cu: yellow; C: black; O: red; Fe: brown). **b–d** Non-contact AFM images obtained at different tip heights ( $z$ ); the final dislodging of CO occurs at  $z = +30$  pm. **e** 3D force map of the frequency shift ( $\Delta f$ ) vs. AFM tip heights ( $z$ ) and horizontal position ( $x$ ), with a CO tip. Step size is 5 pm in  $z$ , and the scan path in  $x$  is across the center of the Fe, as shown in the inset. The tip position at bond rupture is indicated by the breakpoint (arrow). **f** Frequency shift ( $\Delta f$ ) obtained in the horizontal ( $x$ ) direction before, during (indicated by the disjointed curve), and after the bond rupture. **g** The force curve deconvoluted from  $\Delta f$  at the breakpoint in the vertical ( $z$ ) direction. **h** 3D force map of the frequency shift ( $\Delta f$ ) showing quantitative rupture of the dative bond, obtained using a Cu tip; the insert shows schematic of interaction between a Cu tip and CO-FePc. **i** Frequency shift ( $\Delta f$ ) obtained using a Cu tip scanned in the horizontal ( $x$ ) direction. **j** The deconvoluted force curve at the breakpoint in the vertical ( $z$ ) direction using a Cu tip. (Red arrows indicate the bond rupture point. Long-range background forces are subtracted in Figures **g** and **j**).

As demonstrated in Figure 1, the controlled breaking of a single dative bond between a CO molecule and a ferrous phthalocyanine (FePc) complex has been achieved by applying mechanical forces using the scanning probe of AFM. The dative CO-FePc bond is known to be formed via  $\sigma$ -donation from the CO  $5\sigma$  orbital and  $\pi$ -back donation from Fe  $d\pi$ . By decreasing the tip height, the repulsive interactions increased, as indicated by the increased contrast in the images. Upon further reducing the tip height (+30 pm), a sudden change of the image occurred during scanning, as indicated by a line created with a different contrast (Fig. 1d). Subsequent scans showed the repulsion had disappeared, indicating that the CO attached to FePc was dislodged due to the strong repulsion with the tip. Comparison of the contrast in the lower part to the upper part of the same AFM image obtained at the same tip height reveals a downward shift of FePc by  $\sim 30$  pm upon CO removal. This observation confirmed the rupture of the dative bond between CO and FePc induced by the increased interactions during tip scanning and the bonding nature between FePc and the substrate. Our combined experimental and quantum computational studies provide a deeper understanding of the chemical bond breaking process.[5].

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# Applied Research for Geotechnical Structures

by Pedro Pinto, Member EUAS



## Short Biography

**Education:** Licentiate in Civil Engineer (6 years course, 1965-1971) (with honors); from 1971 to 1975 worked with Industry; Master of Engineering (1975 – 1977) (with high honors); 1977-1978 – Fulbright scholarship granted by USA with training periods in MIT (Boston, USA), United States Bureau of Reclamation (Denver), and University of California (Berkeley); Specialist in Geotechnique (Ph.D Degree) 1979 - 1983 (with high honors); from 1992 – Director of Research (Full Professor degree) (with high honors).

ISSMGE Appointed ISSMGE Board member (2017-2022), and before Immediate Past President (2009-2013), President (2005-2009), Vice President for Europe (2001-2005) and Chairman of TC4 “Earthquake Geotechnical Engineer Committee” (1994-2000).

**Positions:** President of Scientific Committee of XVII ECSMGE (2024),

- Member of the European Academy of Sciences
- Fellow of Portuguese Institute of Engineers
- Research Director of LNEC (currently retired)
- Full Professor of Geotechnical Engineering of University of Coimbra (currently retired),
- World Bank Consulting for Dams Safety (2013-2015),
- Invited Professor of Master Courses "Soil Mechanics" and "Engineering Geology" of New University of Lisbon (1983-1995),
- United Nations Consulting for Design and Instrumentation for Dams (1988-1992).
- Invited Guest Lecturer of University of California, USA (1992-1994).
- President of Portuguese Society for Geotechnique (1996- 2000).

**Professional Experience:** Pedro Sêco e Pinto is a Consulting Engineer and has participated in more than 450 major projects in Dams, Power plants, Bridges, Tunnels, Landslides and Quay Walls, in Portugal, Angola, Argelie, Brazil, Cabo Verde, China, Dominican Republic, Ecuador, Guine- Bissau, Guine Ecuatorial, India, Lebanon, Malawi, Morocco, Mozambique, Senegal, Syria, Tunisia, Uganda, Venezuela and Zambia, covering field and laboratory testing, dynamic analyses, earthquake engineering, numerical analyses, ground improvement, slopes, special foundations, instrumentation and safety evaluation.

**Lectures:** He has presented more than 350 State-of-the Art Lectures and Special Lectures in 80 countries of the 5 Continents.

**Awards:** Pedro Sêco e Pinto has received more than 50 international Awards including 3rd Victor de Mello Lecture, 3rd Braja Das Lecture, American Biographical Institute USA, "Special Volume for the Contributors of Earthquake Engineering, Nagadi Lecture by Indian Geotechnical Society, Széchy Lecture by Hungarian S M Society and Hungarian Academy of Sciences, Nonveiller Lecture by Croatia Geotechnical Society, Sukle Lecture by Slovenia Soil Mechanics Society, Chin Lecture by Huanzhou University (China), Qian Jia Huan Lecture by Hohai University (China) and Chin Fung Kee Memorial Lecture by Institute of Engineers of Malasia.

**Journals:** Related his role with Editorial Boards and Reviewer he acted as:

- Associate Editor of International Journal of Earthquake Engineering (since 2017)
- Editor in Chief of International Journal of Case Histories (2011-2017)
- Co-Editor of Geotechnical and Geological Engineering Journal, Springer Publisher (2005-2011)
- Member of Editorial Board of several Journals, namely: "Geotecnia", "Bulletin of Earthquake Engineering", "Acta de Geotecnia", "International Journal of Geotechnical Engineering" and SEAG Journal.
- Editor of Proceedings of 4 International Conferences.

*Author/Co-Author: Pedro Sêco e Pinto is author or co-author of 500 Technical and Scientific Reports, more than 180 papers for national and international conferences and journals and has contributed for 12 books.*

## 1. Introduction

This brief report describes the implemented methodologies for the design of geotechnical structures, namely foundations, dams, tunnelling, landslides and quay walls. This applied research, explored for the different projects that I was involved, a large spectrum covering site investigation, mathematical models, construction issues, instrumentation, monitoring and safety evaluation.

## 2. Foundations Design

The pile foundation design based in ultimate and serviceability limit states was addressed. Foundation system with particular emphasis to soil-structure interaction was analysed.

For the pile foundation each geotechnical design situation shall be verified that no relevant limit state is exceeded. Limit states can occur either in the ground or in the structure or by combined failure in the structure and the ground.

Piles and piers shall be designed to resist the following action effects: (i) inertia forces from the superstructure; and (ii) kinematic forces resulting from the deformation of the surrounding soil due the propagation of seismic waves.

The complete solution is a 3D analysis very time demanding and it is not adequate for design purposes. The decomposition of the problem in steps implies: i) the kinematic interaction involving the response of the base acceleration of the system considering the mass of superstructure equal to zero; (ii) the inertial interaction that involves the computation of the dynamic impedances at the foundation level and the dynamic response of the superstructure.

For the computation of internal forces along the pile, as well as the deflection and rotation at the pile head, both discrete (based in Winkler Spring model) or continuum models were used.

Pile load tests were performed with the following purposes:

- i) to determine the response of a representative pile and the surrounding ground to load, both in terms of settlement and limit load;
- ii) to check the performance of individual piles and to allow judgement of the overall pile foundation;
- iii) to assess the suitability of the construction method.

The results of load tests were used to calibrate the design parameters and to optimize the suggested values for pile lengths, based only on the interpretation of site investigation and laboratory and in situ test results.

For liquefaction evaluation of sandy materials two methods were explored, namely, based in laboratory tests or field tests. The following laboratory tests were used: (i) cyclic triaxial tests; (ii) cyclic simple shear tests; (iii) cyclic torsional shear tests. Due to the difficulties to obtain high quality undisturbed samples field tests were used: SPT tests, CPT tests and seismic cone tests.

For the remedial measures against liquefaction two categories were used: (i) the prevention of liquefaction; and (ii) the reduction of damage to facilities due to liquefaction.

The measures to prevent of occurrence of liquefaction has included the improvement of soil properties or improvement of conditions for stress, deformation and pore water

pressure.

The measures to reduce liquefaction induced damage to facilities have included: (1) to maintain stability by reinforcing structure: reinforcement of pile foundation and reinforcement of soil deformation with sheet pile and underground wall; (2) to relieve external force by softening or modifying structure: adjusting of bulk unit weight, anchorage of buried structures.

### **3. Dam Engineering**

Taking into account the geological and geotechnical interpretative dam model based in situ and laboratory tests, an evaluation of possible solutions for the foundation treatment of the alluvial valley was analysed.

To control dam foundation seepage several methodologies such as: (i) construction of cut-off trenches; (ii) the construction of a diaphragm wall crossing the alluvia material; (iii) and a grouting curtain were explored.

Also, the vibrocompaction treatment to minimize the occurrence of liquefaction of the superficial alluvial sandy materials with low compacity was covered.

To analyse the slope stability of the dam profiles a computer code SLOPE W was used. The construction phase, filling of reservoir and reservoir drawdown were analysed.

Related with the construction phase both upstream and downstream slopes were analysed.

For the filling of the reservoir the most critical situation is related with the downstream slope.

For the drawdown the most critical phase is related with the upstream phase.

Following the recommendations of ICOLD "High embankment dams whose failure may cause loss of life or major damage should be designed by conventional method at first, followed by a dynamic analysis in order to investigate any deficiencies which may exist in the pseudo-static design of the dam", simplified procedures for estimating induced deformations, as well dynamic analyses were explored.

A seepage analysis to calibrate the efficiency of foundation treatment was performed using the SEEP W code.

The construction specifications have covered the testing to asses the quality of the fills.

For the systematic control of dam safety several tasks were included: (i) frequent visual inspection; (ii) periodic visual inspection by a specialist; (iii) regular instrumentation measurements; (iv) data validation; (v) data storage; (vi) safety evaluation; and (vii) corrective actions.

### **4. Tunnelling**

For tunnel design the studies have covered the following ITA guidelines:

- The geological report presenting the results of the geological and geophysical survey.
- The hydrogeological report.
- The geotechnical report on site investigations, including the interpretation of the results of site and laboratory tests with respect to the tunnelling process, soil and rock classification, etc.,
- Information on line, cross-section, drainage, and structural elements affecting later use of the tunnel.

- Plans for and a description of the projected excavation or driving procedure, including the different cross-sections related to different ground conditions.
- Design documents for the types of excavation methods and tunnel supports likely to be applied, considering, e.g., excavation advance and face support (types and number of anchors, shotcrete strength, closure length, etc.).
- The program for the in-situ monitoring of the tunnel by field measurements.
- The analysis of stresses and deformations (for unlined tunnels as well as for single-or double-lined tunnels), and the dimensioning of the tunnel support for intermediate phases and final linings.
- The design has explored empirical methods, analytical methods, NATM methods, TBM method and Observational method.
  - The design for waterproofing or drainage.
- Structural documents for the final design of the tunnel project, including the detailing.
- During and after the excavation, reports on the field measurements and interpretation of their results with respect to the response of the ground and the structural safety of the tunnel.
- Documentation of the problems encountered during the excavation and measures applied, e.g., strengthening the ground or changing the projected type of support, based on monitoring results.

## **5. Landslides**

To assess the slope stability the following methods were used:

- (i) The SMR - Slope Mass Rating rock mass classification
- (ii) The method popular in South America that combines three factors: relative relief, lithologic conditions and soil moisture, with two triggering factors, seismicity and rainfall intensity;
- (iii) The LHEF (landslide hazard evaluation factor) based in the slope instability that integrates the lithology, structure, topography, land relief, cover, and the seepage conditions.

For the seismic analysis the following methodologies were used:

- i) pseudo-static analyses;
- ii) simplified procedures to assess deformations;
- iii) dynamic analysis.

For the prevention and mitigation of rock slopes anchor pull test to verify service load and rock barrier were used.

To prevent landslides disasters the following measures were explored: i) the excavation profile from top towards bottom; (ii) vegetable protection over the slopes; (iii) drainage system including hidden cutting channels to cut infiltration and hidden drainage channels; (iv) slope reinforcement.

For warning systems two approaches were used: direct and indirect monitoring.

For the direct approach a potential sliding area is monitored by simple displacement instrumentation and when a predicted threshold value of displacement is exceeded the people of the valley is evacuated.

For the indirect warning system people were educated to recognize report landslide symptoms (cracking, reactivation of spring lines, surface runoff, etc.).

In general, a combination of the two approaches was used.

## **6. Quay Walls**

The design has integrated an evaluation of the results of the field tests and the laboratory tests for the definition of design parameters.

The static design of the quay wall has followed the Eurocode 7 and so ultimate limit states as well serviceability limit states were analyzed.

The SLOPE W code was used to define the minimum safety factor for different scenarios of water level and pseudo-static methods were used to assess the quay wall safety for different levels of seismic actions.

To verify the serviceability limit states stress-strain analyses were performed by SIGMA code. In these analyses all the steps of construction phases were simulated.

Due to the low degree of compaction of foundations sandy materials and also the risk of liquefaction, a treatment by vibroflotation was performed.

The caissons of the quay wall were monitored to compare the observed displacements with the predicted values by the analyses.

# Energy Sustainability: Activity and Progress

by Marc A. Rosen, Member EUAS

## Short Biography

### **Education**

- *Ph.D., 1987, Univ. of Toronto, Dept. of Mechanical Engineering*
- *M.A.Sc., 1983, Univ. of Toronto, Dept. of Mechanical Engineering*
- *B.A.Sc., 1981, Univ. of Toronto, Div. of Engineering Science, Nuclear and Thermal Power Generation Option*

### **Recent Professional Experience**

- *Professor, Faculty of Engineering and Applied Science, Univ. of Ontario Institute of Technology, Oshawa, Ontario, 2002-pres.*
- *Dean (founding), Faculty of Engineering and Applied Science, Univ. of Ontario Institute of Technology, Oshawa, Ontario, 2002-08.*
- *Chair, Dept. of Mechanical Engineering, Ryerson Polytechnic Univ., Toronto, 1994-99.*
- *Director, School of Aerospace Engineering, Dept. of Mechanical Engineering, Ryerson Polytechnic Univ., Toronto, 1992-94.*

### **Other Significant Professional Positions**

- *Member, Board of Directors, Canadian Academy of Engineering, 2019-pres.*
- *Editor, Energy Conversion and Management, 2013-pres.*
- *Editor-in-Chief, Biofuels, 2014-pres.*
- *Editor-in-Chief, Sustainability, 2009-pres.*
- *Editor-in-Chief, Int. Journal of Energy and Environmental Engineering, 2012-21.*
- *Member, Board of Directors, Oshawa Power and Utilities Corporation, 2010-21.*
- *President, Engineering Institute of Canada, 2008-10.*
- *Director, Durham Strategic Energy Alliance, 2005-07.*
- *President, Canadian Society for Mechanical Engineering, 2002-04.*

### **Honours and Awards**

- *Fellow, Royal Society of Canada*
- *Educational Award of Honour, Minerva Canada*
- *President's Award, Canadian Society for Mechanical Engineering*
- *Engineering Alumni Hall of Distinction, University of Toronto*
- *Andrew H. Wilson History Award, Canadian Society for Mechanical Engineering*
- *C.N. Downing Award, Canadian Society for Mechanical Engineering*
- *Julian C. Smith Medal, Engineering Institute of Canada*
- *Robert W. Angus Medal, Canadian Society for Mechanical Engineering*
- *Fellow, American Society of Mechanical Engineers*
- *Fellow, Engineering Institute of Canada,*
- *Fellow, International Energy Foundation*
- *Fellow, Canadian Society for Mechanical Engineering*
- *Fellow, Canadian Society for Senior Engineers*

### **Principal Areas of Interest**

- *Thermodynamics: Second-Law Analysis. Theoretical development; use in simulation codes; application to improve efficiency and performance of engineering systems.*
- *Energy Sustainability and Energy Systems Analysis. Analysis, design, modelling, simulation and optimization; environmental assessment; energy-environment ties.*

- *Energy Technologies. District energy, thermal energy storage, solar energy, hydrogen energy, nuclear energy, electricity generation and cogeneration, chillers, synthetic fuels production, integrated energy systems.*
- *Heat Transfer. Modelling, simulation and analysis computationally and analytically.*

## **Achievements Related to Energy Sustainability**

Dr. Marc A. Rosen has over his entire career been active in the area of energy, including efficiency, environmental impact and sustainability. He also has taken on key leadership roles for institutions in transformation throughout his career. Many of these achievements have directly and indirectly supported energy sustainability, its applications, and developments of related journals and engineering societies.

As Founding Editor-in-Chief of the journal *Sustainability*, published by MDPI, Dr. Rosen led the journal's development and growth from its launch in 2009 to the point where it now is a leading venue for the publication of research and application articles related to sustainability and sustainable development. This journal has proven transformative in helping advance the field of sustainability while having a global extent and impact. Dr. Rosen also has been heavily involved in the lead conference sponsored by that journal, the World Sustainability Forum. He was the general chair of the first four World Sustainability Forums, and has been heavily involved in subsequent Forums, often delivering keynote presentations.

As Founding Dean of Engineering and Applied Science at Ontario Tech University (University of Ontario Institute of Technology), Dr. Rosen launched a new engineering school, premised on innovative approaches to teaching and learning and on market-oriented research. He also helped build Ontario's first new university in 40 years, one with engineering and technology as its primary area and with energy as one key research and educational focus, and sustainable energy as a theme in much of that activity. There is a strong focus on energy and energy sustainability in many graduate and undergraduate programs that Dr. Rosen helped create. In response to the need for better business and management skills in engineering, Dr. Rosen launched for each engineering program an innovative Engineering and Management version.

Dr. Rosen was instrumental in attaining for his university an institution-defining \$100 million Automotive Centre of Excellence, in collaboration with industry. The Automotive Centre of Excellence supports the development and testing of future vehicles, including sustainable vehicles (e.g., vehicles that operate on alternative fuels like hydrogen, and electric vehicles).

Prior to joining Ontario Tech University, Dr. Rosen was a professor in the Department of Mechanical, Aerospace and Industrial Engineering at Ryerson University. During his tenure there, Dr. Rosen served as department Chair, and Director of the School of Aerospace Engineering. He played a key role in launching graduate programs, expanding research, obtaining accreditation for engineering programs. Dr. Rosen also was a lead developer and player in the university's multidisciplinary program in Environmental Science and Management and he led the creation of thermofluids and energy options within Mechanical Engineering at the undergraduate and graduate levels, and helped ensure sustainability concepts and applications pervade throughout, via such avenues as advanced training in renewable energy sources.

Lately, his teaching of sustainability, and indeed much of his research and other activity, has incorporated and been guided by the new United Nations Sustainable

#### Development Goals.

With over 70 research grants, Dr. Rosen is an active industry collaborator, with much of his research adopted by industry. His innovations have led to increased sustainability and efficiency in energy technologies, improved alternative technologies (like solar, hydrogen and storage technologies), and reduced environmental impact. He was a key player in two projects (valued at over \$10 million) to produce hydrogen from nuclear energy and other renewable thermal forms of energy. He was co-Principal Investigator of the second of these. He also was a theme leader in a \$12 million project on net-zero energy buildings, which advanced the development of buildings that use, on average, zero energy over the year. His noteworthy accomplishments include advancing energy systems to make them more sustainable and less environmentally damaging through research, and collaborating with industry to facilitate the adoption of those innovations.

Some notable examples of Dr. Rosen's research and its impact follow. His research has led to sustainable energy systems, buildings and communities [1-3], and to improvements in the sustainability of transportation technologies of various kinds, especially automobiles, trains and aircraft [4]. Some of his research has led to improvements in the sustainability of manufacturing, production and economic systems. [5-6]. Dr. Rosen's research has also focused on the large scale, including an assessment of the sustainability national energy systems like Canada's [7].

Dr. Rosen has published over 700 journal articles in leading journals, many addressing sustainability, and authored or co-authored over 110 book chapters and 21 books, many directly linked to sustainability [8-12]. These books include the ground-breaking work by Dr. Rosen on the linkages between the thermodynamic quantity "exergy" and sustainability, extending beyond thermodynamics to environment, ecology and economics, challenging convention and leading to new understandings of sustainability. His books on thermal energy storage, exergy, exergy and the environment, and exergy and economics are considered by many to be seminal. In addition, Dr. Rosen has authored or co-authored many books that deal indirectly with sustainability [13-17]. Dr. Rosen has also published extensively on engineering ethics and safety.

As a Director of Oshawa Power for over a decade, a local electrical distribution company that serves a city of about 160,000 people, Dr. Rosen helped that utility's expansion into sustainable energy forms and technologies like solar photovoltaics, wind, and biomass and cogeneration.

During his tenure as President of the Engineering Institute of Canada (EIC), Dr. Rosen assisted in affirming its leadership role and helped in developing a vision statement for EIC that had sustainability at its core, being phrased "Engineering for a prosperous, safe and sustainable Canada." The Engineering Institute of Canada was founded in 1887 and is a federation of leading Canadian engineering societies. Dr. Rosen also helped revitalize the Canadian Society for Mechanical Engineering during his term as President. He chaired that society's Technical Division on Thermofluids Engineering for two decades, focusing on advancements in renewable energy technology and sustainable energy.

Dr. Rosen has been extensively involved in international activities, including the development of a joint distance education course in Pollution Prevention in Brazil, with the support of the Canadian International Development Agency. This project led to a book. He was also his Department's lead contact for five years in the North American Design Institute (NADI), facilitating exchanges between Mexico, the U.S. and Canada. In addition, Dr. Rosen served on several industrial and academic advisory committees, including Canadian Representative on the International Energy Agency Experts Group on Cogeneration/District Cooling.

## **Impact and Significance on Energy Sustainability**

Much of Dr. Rosen's research has been adopted by industry, and helped to improve energy use, mitigate environmental impact, and increase efficiency. He has written over 50 technical reports that attest to this. One project identified efficiency improvements in power plants at Ontario Power Generation. Another project provided compelling evidence of the benefits of cogeneration, convincing large electrical power utilities to implement cogeneration. A third project aims to have Canada's nuclear reactors produce hydrogen for transportation, industry and supporting the oil sands development. Industry benefits resulted from his service as the Canadian Representative on the International Energy Agency Experts Group on Cogeneration/District Cooling. Finally, another aims at reducing the energy use for Canada's building stock, presently responsible for a third of the nation's energy use, to zero. The economic value of the projects he has been involved with directly as a principal or co-investigator exceeds \$30 million.

Dr. Rosen has also carried out work directly on or related to sustainability for a range of national and international companies, such as Imperial Oil Ltd., General Electric, Bell Canada, Apotex Inc., FuelMaker Corporation, and Inst. for Hydrogen Systems. As well, he has carried out projects for various government agencies at the international, national and provincial levels, including International Energy Agency, Natural Resources Canada, Environment Canada, Ontario Ministry of the Environment, and Ontario Ministry of Community and Social Services.

Dr. Rosen has advanced thermodynamic methods, cogeneration, district energy, thermal storage, renewable energy, and environmental stewardship. A significant achievement of Dr. Rosen has been his work to advance the methodology and framework for holistic assessments of sustainability [18-20]. Applications are numerous and include an assessment of the contributions to regional sustainability of the Dead Sea-Red Sea project involving Israel, Jordan and the Palestinian Authority [21]. His work has also led to advanced optimization methods [22]. In addition, Dr. Rosen has carried out technical research on seawater desalination using sustainable energy [23], sustainable transportation via hydrogen energy [24], microgrids for heat and electricity [25], and polygeneration technologies for such products as electricity, cooling and fresh water [26], in addition to broader research on such topics as sustainable cities [27] and the circular economy for industry and business [28].

Dr. Rosen has advanced engineering education, through his many roles in universities. In particular, he helped create a new research intensive university focused on technology. In leading the launch of the Faculty of Engineering and Applied Science at Ontario Tech University, Dr. Rosen created the vision of a new engineering school premised on the use of innovative educational methods and technologies, and value-added research. On the teaching front, Dr. Rosen has been innovative, creating several new courses at the graduate and undergraduate levels. Two examples are graduate courses on Energy and the Environment and Pollution Prevention. In addition, Dr. Rosen helped develop a Faculty-wide course on law, ethics and professionalism for engineers, and has developed innovative options and streams in programs.

Dr. Rosen has also been involved in the American Society of Heating, Refrigerating and Air-Conditioning Engineers, by serving as corresponding member for a technical group on exergy analysis for sustainable buildings. As a member of the Advisory Committee for Sustainable Energy Solutions for the Ontario Centres of Excellence, Dr. Rosen helped advance the sustainability of various earth and environmental technologies. As a director of the Durham Strategic Energy Alliance, Dr. Rosen helped lead development of a regional

energy focus. Finally, as a review committee member on the International Thermonuclear Experimental Reactor, Dr. Rosen advised the Canadian and Ontario governments on fusion energy.

Dr. Rosen has been extensively recognized for his achievements in engineering, education and research, and distinguished service to learned societies. He has received best paper awards (e.g., “Energy and Exergy Analyses of Power Generation via an Integrated Biomass Post-Firing Combined-Cycle” at an IEEE International Conference on Smart Energy Grid Engineering). Dr. Rosen is a fellow of the Canadian Society for Senior Engineers, the Canadian Academy of Engineering, the American Society of Mechanical Engineers, the Engineering Institute of Canada, the International Energy Foundation and the Canadian Society for Mechanical Engineering. He was elected to University of Toronto’s Engineering Alumni Hall of Distinction.

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## Global Health – Major Issues Revealed by COVID-19

by Alain L. Fymat, Member EUAS



### Short Biography

DR. ALAIN L. FYMAT is a medical-physical scientist and an educator. He is the current President/CEO & Institute Professor at the International Institute of Medicine & Science with a previous appointment as Executive Vice President/Chief Operating Officer & Professor at the Weil Institute of Critical Care Medicine, California, U.S.A. He was formerly Professor of Radiology, Radiological Sciences, Radiation Oncology, Critical Care Medicine, and Physics at several U.S. and European Universities. Earlier, he was Deputy Director (Western Region) of the U.S. Department of Veterans' Affairs (Office of Research Oversight). At the Loma Linda Veterans' Affairs Medical Center, he was Scientific Director of Radiology, Director of the Magnetic Resonance Imaging Center and, for a time, Acting Chair of Radiology. Previously, he was Director of the Division of Biomedical & Biobehavioral Research at the University of California at Los Angeles/Drew University of Medicine & Science. He was also Scientific Advisor to the U.S. National Academy of Sciences, National Research Council, for its postdoctoral programs tenable at the California Institute of Technology and Member of the Advisory Group for Research & Development, North Atlantic Treaty Organization (NATO). He is Health Advisor to the American Heart & Stroke Association, Coachella Valley Division, California. He is a frequent Keynote Speaker and Organizing Committee member at several international scientific/medical conferences. He has lectured extensively in the U.S.A, Canada, Europe, Asia, and Africa. He has published in excess of 535 scholarly scientific publications and books. He is also Editor-in-Chief, Honorable Editor or Editor of numerous medical/scientific Journals to which he regularly contributes. He is a member of the New York Academy of Sciences and the European Union Academy of Sciences, a Board member of several institutions, and a reviewer for the prestigious UNESCO Newton Prize, United Kingdom National Commission for UNESCO.

Dr. Fymat's current research interests are focused on neurodegenerative diseases (Alzheimer's, Parkinson's, dementias, epilepsy, and others), oncology (glioblastoma), epigenetics & ecogenetics, and nanomedicine & nanobiotechnology, and emerging infectious diseases. These are represented in part in his latest books: "**The Odyssey of Humanity's Diseases: Epigenetic and ecogenetic modulations from ancestry through inheritance, environment, culture, and behavior**" Volumes 1, 2, and 3; "**From the Heart to the Brain: My collected works in medical science research (2016-2018)**"; "**The Human Brain: Wonders and Disorders**"; "**Alzhei ...Who? Demystifying the disease and what you can do about it**"; "**Parkin...ss..oo..nn: Elucidating the disease and what you can do about it**"; "**Dementia: Fending-off the menacing disease... and what you can do about it**"; "**Epilepsy: The electrical storm in the brain**"; "**Cancer: The pernicious clonally evolving disease braided in our genome**"; "**Lyme disease: The great invader, evader, and imitator**"; and "**Pandemics: Prescription for prediction and prevention**".

## Global Health – Major Issues Revealed by COVID-19

COVID-19 has revealed at least ten (perhaps more) major issues concerning the state of global health. As painfully demonstrated during the pandemic, the health threats devolving therefrom endanger lives, disrupt families and societies, and wreck havoc on economies. Yet, the cost of failing to control outbreaks, ruining and losing lives, destabilizing the social fabric, and decimating economies is considerably greater than the cost of prevention. Now, perhaps more than ever before, we should recognize and seize this moment as the most opportune time to address the prediction, management, and prevention of health crises.

Let us first remember how COVID-19 burst into the scene. In late 2019, a group of patients with a severe acute respiratory syndrome (SARS) of unknown cause appeared in Wuhan, Hubei province, China. Since then, outbreaks of this syndrome had quickly spread across the Chinese territory, resulting in thousands of confirmed cases. On 30 December 2019, the World Health Organization (WHO) notified the world about a pneumonia of unknown cause in Wuhan. Then, the Chinese Center for Disease Control & Prevention organized an intensive outbreak investigation program and attributed the etiology of this disease to a new virus belonging to the coronavirus family. Initially, the new virus was called 2019-nCoV. Subsequently, experts from the International Committee on Taxonomy of Viruses renamed it SARS-CoV2 due to its similarity to the coronavirus responsible for the first epidemic of SARS (SARS-CoV) in 2002. Later, on 11 February 2020, the WHO announced that the disease caused by the new CoV should be called "COVID-19", which stands for "coronavirus disease 2019". It was only on 11 March 2020 that, because of its alarming speed of transmission, the WHO subsequently, *albeit* somewhat belatedly, declared a pandemic state. This delay of approximately three months resulted in many disastrous consequences. Note that SARS-CoV2 is not the most lethal among coronaviruses, however, its speed of propagation makes it one of the deadliest viruses known.

**Problems with global health:** While a full analysis of each such problem would require a separate discussion, very brief remarks are provided below:

1. An unruly world of nearly eight billion people (and growing) who are not easily managed.
2. Glaring inequities among nations, including: the non-availability of medicines and vaccines in many poor or less-developed countries which sport insufficient health infrastructures that preclude them from producing their own medicines and vaccines. Further, these countries are unable to meet the stringent international standards for such productions. Still further, black markets are rampant for fake or sub-standard medicines and vaccines.
3. A plethora of international organizations that constitute a very complex and fragmented legal and institutional landscape under the broad umbrella of the United Nations (UN). These organizations do not operate cooperatively or in synchrony, are focused on their own limited agendas, do not coordinate their respective programs, are subservient to their funders/donors; and have no enforcement power over individual nations.
4. Notwithstanding its otherwise great work, during COVID-19, the WHO was

dilatory in not heeding the early signs of the coming pandemic and taking three or more critical months to declare a pandemic. Further, it issued contradictory recommendations. Still further, it deferred at times to powerful nations (in the present instance, China).

5. National decisions are most often politically driven, international commitments are barely honored, and there are no international consequences for action(s) taken or lack thereof.
6. There is an almost universal short memory regarding the past history of epidemics and pandemics:
7. The early signs of nascent epidemics/pandemics are not heeded despite reports, briefings, warnings about viruses bearing traces of their animal origins and of emerging infectious diseases. In addition, nations and the world remain under-prepared to predict, detect, respond, and even less prevent infectious disease outbreaks and *a fortiori* pandemics.
8. The cardinal socio-economic factors of epidemics/pandemics have not heretofore been fully identified so far.
9. Regarding potential future epidemics/pandemics, the cause(s) are not fully identified and strategies for prediction/prevention have not been devised. Lastly, even
10. Enabling technologies for epidemiological/biological modeling have not been sufficiently developed.

**Facing future health threats and pandemics:** The required measures are listed below:

1. Highlighting global health security.
2. Promoting multidisciplinary engagement.
3. Strengthening multi-sectoral coordination.
4. Emphasizing the importance of financial preparedness.
5. Creating and strengthening necessary mechanisms.
6. Improving early warning and detection.
7. Collecting and sharing data in a timely manner;
8. Conducting laboratory testing;
9. Developing joint outbreak response capacities.
10. Taking appropriate science-based actions.

If implemented, such measures should allow effective detection and response to emerging zoonotic threats and ultimately prevent pandemics.

**Root causes of pandemics:** From the ancestral domestication of plants and animals to the present times, we live on a microbially-unified planet. There are ten intertwined socio-ecological cardinal factors that are the root causes of pandemics. Most (hopefully all) of these factors would need to be simultaneously tackled and remedied:

1. Rapid growth of global human population.
2. Increased globalization.
3. Environmental degradation and destabilization of ecosystems.
4. Creation of new urban or agricultural ecosystems.
5. Economies of scale and monocultures in agriculture and dysfunctional agrifood systems.

6. Loss of land and ocean biodiversity.
7. Water scarcity.
8. Human-induced climate change.
9. Societal inequities.
10. Irrational mass denialism of hard-won facts of science (vaccinations, antimicrobial overuse).

Some of the above factors could be correlated with the UN's Sustainable Development Goals (SDG): factor 4 to SDG # 6; factor 8 to SDG # 13; and factor 9 to SDG # 1, 2, 3, 7, 11, 12, and 16. While important, such SDGs are not the focus of this article.

**A blueprint for strategic pandemic prevention and prevention:** Pandemic prediction and prevention is the organization and management of appropriate measures (scientific, technical, economic, and political) to predict and prevent pandemics. It should not be mistaken for “pandemic preparedness” or “pandemic containment” or “pandemic mitigation”, which largely seek to reduce the severity and negative impacts of pending or established pandemics. Pandemic prediction and prevention seeks to:

1. Reduce causes of new infectious diseases.
2. Prevent outbreaks and epidemics from becoming pandemics.
3. Prepare for potential future pandemics that could not be prevented.
4. Ensure that the causing virus does not re-emerge thereafter (e.g., by sustaining itself in domestic animals).

My blueprint for strategic pandemic prediction and prevention is detailed at length in my book “Pandemics: Prescription for Prediction and Prevention”. It is a multi-level (6 levels) structure with multi-way inter-level communication. These refer to:

1. Creating a new “World Environment Organization” (WEO): With the world on a path to extreme climate change, this new regulatory agency would have the power to censure countries for failing to keep with their commitments and pledges regarding the environment. It would operate in parallel with and complement other similar UN organizations such as the WHO, the World Meteorological Organization, and the World Trade Organization to name some of them. There are plenty of precedents to such a creation. Regretfully, its work may be hampered in several ways including: relying on countries to timely report outbreaks, assuming these countries will heed its advice and recommendations, and countries may not legally commit themselves to take appropriate remedial action when it comes to ill-defined pandemics.
2. Under the auspices of the WHO, establishing a legally-binding “International Pandemic Treaty” (IPT) to better prepare the world for the next pandemic. It would emulate the creation of similar treaties such as the “International Treaty on Ozone Depletion and Climate Change”, “Biodiversity Treaties”, the “Treaty on the Prohibition of Nuclear Weapons”, and others. The treaty would prevent countries who are doing vaccine research (European Union countries, the U.S., China, India, Russia, and others) from maintaining intellectual property on important technologies, bidding each other to find personal protective equipment and coronavirus testing kits, and buying-up most of the stock or restricting exports to other countries. Sadly, however, despite the hoped-for existence of an IPT and a

commitment to the principle of equitable allocations, member countries will regretfully not learn from past history and return to their past behavior (competing with each other for supplies) when the next pandemic strikes ... unless there will not be any new pandemic!

3. Shifting the current health paradigm to the new “One-World/One-*eco*Health” paradigm that will be grounded by the IPT and other international laws. Our context in 2022 encompasses: globalization, climate change, ecological collapse, species extinctions, interconnectedness among humans and animals, human overpopulation, huge economic and political disparities, and unintended consequences of well-meaning interventions. These factors have created a perfect storm for new pandemics. To alleviate/eliminate them, it is imperative to adopt the new paradigm while at the same time developing the needed infrastructures and the national/ regional/ international organizations to pursue this global health agenda.
4. Involving international, intergovernmental, regional, and national health organizations.
5. Incorporating the Global Human Virome Project: It would help identify the bulk of the viruses that threaten us (more than 1.5 million mammalian and waterfowl viruses, spanning across 25 viral families). Of these, between 631,000 and 827,000 (actually one million or more) unknown viruses might be zoonotic (i.e. of animal origin) and, thus, have the potential to infect humans after spillover from host animal populations. It offers a pathway to improve our capacity to detect, diagnose, and discover viruses that potentially pose threats to human populations, particularly in low- and middle-income countries. It could provide an early warning of future threats, data to improve prevention and reduction of these threats, and inputs for advance preparation of responses for unexpected outbreaks of unknown diseases.
6. Actively developing pandemic models (epidemiological, climate-type) with the enabling technologies, and databases.
7. Folding-in the development of vaccines & therapeutics: The following programs are noted such as designing a globally-coordinated vaccine surveillance system for the purpose of monitoring vaccine changes predicated on new SARS-CoV2 virus variants to inform and advise national authorities and vaccine companies, the U.S. National Institutes of Health project “Antiviral Drug Discovery and Development Center, and the COVID R&D Alliance. In addition, public health requires investments in drugs to counter any pathogen with epidemic or pandemic potential, to vaccinate in biodiversity, to develop a new industry-backed coalition, and to create antivirals for more distantly-related pathogens that pose a pandemic risk.
8. Accelerating pandemic research: Research is essential for understanding how pathogens spread and cause disease, and to generate safety and efficacy data to support regulatory decisions on clearance, approval, licensure, and emergency use. Since 2015, global institutions such as the WHO and the World Bank, and public-private partnerships, have been responding to deficiencies in research by ensuring the integration of research into global health security preparedness and response efforts.

**Conclusions:** The following conclusions can be drawn regarding the current state of global health:

1. COVID-19 has evidenced the current poor state of global health. Ten intertwined

cardinal socio-ecological factors that are the root causes of pandemics have been identified. These need to be simultaneously tackled and remedied. Some of these factors could be correlated with the United Nations Sustainable Development Goals. Within this endeavor, the Human Global Virome Project may be of importance.

2. A blueprint has been offered for a 6-level strategic pandemic prevention and prevention. The value and success of the proposed approach will be gauged by four identified measures. Within that blueprint, a stage could be reached wherein future pandemics could be predicted and prevented.
3. A new International Pandemic Treaty was advocated and some of its particulars were discussed.

This would be in addition to current international laws, programs, and agreements that may also help in the creation of the World Environmental Organization. Such an organization may overcome the difficult collaborations between the numerous international, intergovernmental, regional, and national organizations, which do not work well together.

4. The current “One World” paradigm should evolve to the new paradigm “One World-One Health”, or better yet “One World-One *eco*Health”.
5. Taking advantage of several existing enabling technologies and international/national databases, pandemics could be modeled according to two general types (epidemiological; climate/ weather prediction). Such modeling has and could continue to assist in making decisions regarding the management of pandemics. In the meantime, existing programs regarding vaccines and therapeutics and research should be continued and accelerated.

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# **C5a and C5aR1 are Key Drivers of Microvascular Platelet Aggregation in Clinical Entities spanning from aHUS to COVID-19**

**by Giuseppe Remuzzi, Member EUAS**

## Short Biography

*Giuseppe Remuzzi completed his medical training at the University of Pavia in 1974 and then received specialty training in Haematology and Nephrology at the University of Milan in 1977 and 1980, respectively. From 1996 until 2013 he was Director of the public-private Department of Immunology and Transplant Medicine (a collaboration between the Ospedali Riuniti of Bergamo and the Mario Negri Institute) and from 1999 until 2018 he has also been Head of the Division of Nephrology and Dialysis. From 2011 until 2015 he was Director of the Department of Medicine of the Azienda Ospedaliera Papa Giovanni XXIII (formerly the Ospedali Riuniti) of Bergamo. In June 2015 he was nominated Chiara Fama Professor of Nephrology at the University of Milan. Alongside his clinical work in hospital, Prof. Remuzzi has dedicated himself to intense didactic and research activities. Since the Mario Negri Institute for Pharmacological Research opened its branch in Bergamo, Prof. Remuzzi has coordinated all of the research that takes place there, and since 1992 he has done the same for the Aldo e Cele Daccò Clinical Research Centre for Rare Diseases in Ranica, Bergamo. Since July 1st 2018 Professor Remuzzi has also taken on the role of Director of the Mario Negri Institute.*

*His main research interests include the causes of glomerulonephritis and the mechanisms of progression of kidney diseases. He has also conducted many studies in the field of transplant rejection. With an innovative approach (transplanting two kidneys from older donors into one recipient, after carefully evaluating the condition of the organs), his research has facilitated an increase in the number of transplants conducted. His most recent research concerns the possibility of regenerating tissues and creating organs in the laboratory using stem cells.*

*Prof. Remuzzi serves on editorial boards of numerous journals and is member of the International Advisory Board of The Lancet. He served as Editorial Board member of the New England Journal of Medicine from 1998-2013. In recognition of his achievements, he has been awarded in 1998 honorary memberships of the Association of American Physicians and the British Royal College of Physicians. In 2005 during the World Congress of Nephrology in Singapore he received the ISN Jean Hamburger Award. In 2007 he received during the annual American Society of Nephrology Congress in San Francisco the prestigious ASN John P. Peters Award and in 2011 he was awarded with the ISN AMGEN Award (World Congress of Nephrology: WCN 2011, Vancouver). In November 2011 he received the Third Edition of the International Award "Luis Hernando" assigned by the Iñigo Alvarez de Toledo Renal Foundation (FRIAT) in Madrid, Spain.*

*From June 2013 until March 2015 he was President of the International Society of Nephrology (ISN). During his tenure he created and launched the global 0by25 project, the goal of which is that "Nobody should die of preventable and treatable Acute Kidney Injury (AKI) by 2025".*

*In April 2018 he was awarded the "Lennox K. Black International Prize for Excellence in Medicine" at the Thomas Jefferson University in Philadelphia.*

*Prof. Remuzzi is the author of over 1600 publications in International medical journals and has written 24 books. He also regularly writes editorials for the Corriere della Sera newspaper.*

**C5a and C5aR1 are key drivers of microvascular platelet aggregation in clinical entities spanning from aHUS to COVID-19**

Giuseppe Remuzzi et al

*Blood Adv. 2022 Jan 8;6(3):866-881*

### **Abstract**

Unrestrained activation of the complement system till the terminal products, C5a and C5b-9, plays a pathogenetic role in acute and chronic inflammatory diseases. In endothelial cells, complement hyperactivation may translate into cell dysfunction, favoring thrombus formation. The aim of this study was to investigate the role of the C5a/C5aR1 axis as opposed to C5b-9 in inducing endothelial dysfunction and loss of antithrombogenic properties. In vitro and ex vivo assays with serum from patients with atypical hemolytic uremic syndrome (aHUS), a prototype rare disease of complement-mediated microvascular thrombosis due to genetically determined alternative pathway dysregulation, and cultured microvascular endothelial cells, demonstrated that the C5a/C5aR1 axis is a key player in endothelial thromboresistance loss. C5a added to normal human serum fully recapitulated the prothrombotic effects of aHUS serum. Mechanistic studies showed that C5a caused RalA-mediated exocytosis of von Willebrand factor (vWF) and P-selectin from Weibel-Palade bodies, which favored further vWF binding on the endothelium and platelet adhesion and aggregation. In patients with severe COVID-19 who suffered from acute activation of complement triggered by severe acute respiratory syndrome coronavirus 2 infection, we found the same C5a-dependent pathogenic mechanisms. These results highlight C5a/C5aR1 as a common prothrombogenic effector spanning from genetic rare diseases to viral infections, and it may have clinical implications. Selective C5a/C5aR1 blockade could have advantages over C5 inhibition because the former preserves the formation of C5b-9, which is critical for controlling bacterial infections that often develop as comorbidities in severely ill patients. The ACCESS trial registered at [www.clinicaltrials.gov](http://www.clinicaltrials.gov) as [#NCT02464891](https://clinicaltrials.gov/ct2/show/study/NCT02464891) accounts for the results related to aHUS patients treated with CCX168.

### **Effect of Oral Methylprednisolone on Decline in Kidney Function or Kidney Failure in Patients With IgA Nephropathy: The TESTING Randomized Clinical Trial**

Giuseppe Remuzzi et al

*JAMA. 2022 May 17;327(19):1888-1898*

### **Abstract**

**Importance:** The effect of glucocorticoids on major kidney outcomes and adverse events in IgA nephropathy has been uncertain.

**Objective:** To evaluate the efficacy and adverse effects of methylprednisolone in patients with IgA nephropathy at high risk of kidney function decline.

**Design, setting, and participants:** An international, multicenter, double-blind, randomized clinical trial that enrolled 503 participants with IgA nephropathy, proteinuria greater than or equal to 1 g per day, and estimated glomerular filtration rate (eGFR) of 20 to 120 mL/min/1.73 m<sup>2</sup> after at least 3 months of optimized background care from 67 centers in Australia, Canada, China, India, and Malaysia between May 2012 and November 2019, with follow-up until June 2021.

**Interventions:** Participants were randomized in a 1:1 ratio to receive oral methylprednisolone (initially 0.6-0.8 mg/kg/d, maximum 48 mg/d, weaning by 8 mg/d/mo; n = 136) or placebo (n = 126). After 262 participants were randomized, an excess of serious infections was identified, leading to dose reduction (0.4 mg/kg/d, maximum 32

mg/d, weaning by 4 mg/d/mo) and addition of antibiotic prophylaxis for pneumocystis pneumonia for subsequent participants (121 in the oral methylprednisolone group and 120 in the placebo group).

**Main outcomes and measures:** The primary end point was a composite of 40% decline in eGFR, kidney failure (dialysis, transplant), or death due to kidney disease. There were 11 secondary outcomes, including kidney failure.

**Results:** Among 503 randomized patients (mean age, 38 years; 198 [39%] women; mean eGFR, 61.5 mL/min/1.73 m<sup>2</sup>; mean proteinuria, 2.46 g/d), 493 (98%) completed the trial. Over a mean of 4.2 years of follow-up, the primary outcome occurred in 74 participants (28.8%) in the methylprednisolone group compared with 106 (43.1%) in the placebo group (hazard ratio [HR], 0.53 [95% CI, 0.39-0.72];  $P < .001$ ; absolute annual event rate difference, -4.8% per year [95% CI, -8.0% to -1.6%]). The effect on the primary outcome was seen across each dose compared with the relevant participants in the placebo group recruited to each regimen ( $P$  for heterogeneity = .11): full-dose HR, 0.58 (95% CI, 0.41-0.81); reduced-dose HR, 0.27 (95% CI, 0.11-0.65). Of the 11 prespecified secondary end points, 9 showed significant differences in favor of the intervention, including kidney failure (50 [19.5%] vs 67 [27.2%]; HR, 0.59 [95% CI, 0.40-0.87];  $P = .008$ ; annual event rate difference, -2.9% per year [95% CI, -5.4% to -0.3%]). Serious adverse events were more frequent with methylprednisolone vs placebo (28 [10.9%] vs 7 [2.8%] patients with serious adverse events), primarily with full-dose therapy compared with its matching placebo (22 [16.2%] vs 4 [3.2%]).

**Conclusions and relevance:** Among patients with IgA nephropathy at high risk of progression, treatment with oral methylprednisolone for 6 to 9 months, compared with placebo, significantly reduced the risk of the composite outcome of kidney function decline, kidney failure, or death due to kidney disease. However, the incidence of serious adverse events was increased with oral methylprednisolone, mainly with high-dose therapy.

## **Empagliflozin protects glomerular endothelial cell architecture in experimental diabetes through the VEGF-A/caveolin-1/PV-1 signaling pathway**

Giuseppe Remuzzi et al

*J. Pathol* 2022 Apr;256(4):468-479

### **Abstract**

In addition to having blood glucose-lowering effects, inhibitors of sodium glucose cotransporter 2 (SGLT2) afford renoprotection in diabetes. We sought to investigate which components of the glomerular filtration barrier could be involved in the antiproteinuric and renoprotective effects of SGLT2 inhibition in diabetes. BTBR (black and tan, brachyuric) ob/ob mice that develop a type 2 diabetic nephropathy received a standard diet with or without empagliflozin for 10 weeks, starting at 8 weeks of age, when animals had developed albuminuria. Empagliflozin caused marked decreases in blood glucose levels and albuminuria but did not correct glomerular hyperfiltration. The protective effect of empagliflozin against albuminuria was not due to a reduction in podocyte damage as empagliflozin did not affect the larger podocyte filtration slit pore size nor the defective expression of nephrin and nestin. Empagliflozin did not reduce the thickening of the glomerular basement membrane. In BTBR ob/ob mice, the most profound abnormality

seen using electron microscopy was in the endothelial aspect of the glomerular capillary, with significant loss of endothelial fenestrations. Remarkably, empagliflozin ameliorated the subverted microvascular endothelial ultrastructure. Caveolae and bridging diaphragms between adjacent endothelial fenestrae were seen in diabetic mice and associated with increased expression of caveolin-1 and the appearance of PV-1. These endothelial abnormalities were limited by the SGLT2 inhibitor. Although no expression of SGLT2 was found in glomerular endothelial cells, SGLT2 was expressed in the podocytes of diabetic mice. VEGF-A, which is a known stimulus for endothelial caveolin-1 and PV-1, was increased in podocytes of BTBR ob/ob mice and normalized by SGLT2 inhibitor treatment. Thus, empagliflozin's protective effect on the glomerular endothelium of diabetic mice could be due to a limitation of the paracrine signaling of podocyte-derived VEGF-A that resulted in a reduction of the abnormal endothelial caveolin-1 and PV-1, with the consequent preservation of glomerular endothelial function and permeability. © 2022 The Pathological Society of Great Britain and Ireland.

### **Sexual dimorphic response to rituximab treatment: A longitudinal observational study in a large cohort of patients with primary membranous nephropathy and persistent nephrotic syndrome**

Giuseppe Remuzzi et al

*Front Pharmacol 2022 Sep 2;13:958136*

#### **Abstract**

Rituximab is one of the first-line therapies for patients with membranous nephropathy (MN) at high risk of progression towards kidney failure. We investigated whether the response to Rituximab was affected by sex and anti-PLA<sub>2</sub>R antibody levels in 204 consecutive patients (148 males and 56 females) with biopsy-proven MN who were referred to the Nephrology Unit of the Azienda Socio Sanitaria Territoriale Papa Giovanni XXIII from March 2001 to October 2016 and managed conservatively for at least 6 months. The primary outcome was a combined endpoint of complete (proteinuria <0.3 g/24 h) or partial (proteinuria <3.0 g/24 h and >50% reduction vs. baseline) remission. Patients gave written informed consent to Rituximab treatment. The study was internally funded. No pharmaceutical company was involved. Anti-PLA<sub>2</sub>R antibodies were detectable in 125 patients (61.3%). At multivariable analyses, female gender ( $p = 0.0198$ ) and lower serum creatinine levels ( $p = 0.0108$ ) emerged as independent predictors of better outcome ( $p = 0.0198$ ). The predictive value of proteinuria ( $p = 0.054$ ) and anti-PLA<sub>2</sub>R titer ( $p = 0.0766$ ) was borderline significant. Over a median (IQR) of 24.8 (12.0-36.0) months, 40 females (71.4%) progressed to the combined endpoint compared with 73 males (49.3%). Anti-PLA<sub>2</sub>R titers at baseline [127.6 (35.7-310.8) vs. 110.1 (39.9-226.7) RU/ml] and after Rituximab treatment were similar between the sexes. However, the event rate was significantly higher in females than in males [HR (95%): 2.12 (1.44-3.12),  $p = 0.0001$ ]. Forty-five of the 62 patients (72.3%) with anti-PLA<sub>2</sub>R titer below the median progressed to the combined endpoint *versus* 35 of the 63 (55.6%) with higher titer [HR (95%): 1.97 (1.26-3.07),  $p < 0.0029$ ]. The highest probability of progressing to the combined endpoint was observed in females with anti-PLA<sub>2</sub>R antibody titer below the median (86.7%), followed by females with anti-PLA<sub>2</sub>R antibody titer above the median (83.3%), males with titer below the median (68.1%), and males with titer above the median (44.4%). This trend was statistically significant ( $p = 0.0023$ ). Similar findings were observed for complete

remission (proteinuria  $<0.3$  g/24 h) and after analysis adjustments for baseline serum creatinine. Thus, despite similar immunological features, females were more resilient to renal injury following Rituximab therapy. These findings will hopefully open new avenues to identify the molecular pathways underlying sex-related nephroprotective effects.

### **Fresh lemon juice supplementation for the prevention of recurrent stones in calcium oxalate nephrolithiasis: A pragmatic, prospective, randomised, open, blinded endpoint (PROBE) trial**

Giuseppe Remuzzi et al

*EClinicalMedicine 2021 Dec 14;43:101227*

#### **Abstract**

**Background:** Standard diet with normal calcium and reduced animal proteins and salt content reduces stone recurrence in calcium oxalate nephrolithiasis. Whether lemon juice supplementation further reduces recurrence rate is unknown.

**Methods:** In this single-centre, prospective, randomised, open, blinded endpoint trial (Clinical Trials gov [NCT01217372](https://clinicaltrials.gov/ct2/show/study/NCT01217372)) we evaluated the effects of fresh lemon juice supplementation (60 mL twice daily) versus no supplementation, on time to stone recurrence in 203 patients with recurrent idiopathic calcium oxalate nephrolithiasis who were all prescribed a standard diet. Patients were included between July 2009 and March 2017 at the Nephrology Unit of the Papa Giovanni XXIII hospital in Bergamo, Italy. Time to stone recurrence at 2 years of follow-up was the primary outcome. Analyses were by intention-to-treat.

**Findings:** During two years of follow-up 21 of 100 patients randomised to lemon juice supplementation and 32 of 103 controls randomised to no supplementation had stone recurrence [HR (95% CI): 0.62 (0.35-1.07),  $p = 0.089$ ]. Patient adherence to lemon juice supplementation, however, progressively decreased from 68% at one-year to 48% at two-year follow-up. At explorative analyses restricted at one-year follow-up, ten patients with supplementation versus 22 controls had stone recurrence [0.43 (0.20-0.89),  $p = 0.028$ ]. After adjustment by age, sex and normo or hypocitraturia, the HR (95%) was still significant [0.45 (0.20-0.93),  $p = 0.036$ ]. At six months, 24 hour urinary sodium excretion decreased by  $8.60 \pm 65.68$  mEq/24 h in patients receiving lemon juice supplementation and increased by  $3.88 \pm 64.78$  mEq/24 h in controls. Changes significantly differed between groups ( $p = 0.031$ ). This difference was subsequently lost. Treatment was safe. In patients with lemon juice supplementation gastrointestinal disorders were more frequent ( $p < 0.001$ ). Renal and urinary tract disorders were similar between groups ( $p = 0.103$ ).

**Interpretation:** Explorative analyses suggest that fresh lemon juice supplementation to standard diet might prevent stone recurrence in patients with calcium-oxalate nephrolithiasis. However, treatment effect was likely reduced by progressively declining adherence to lemon juice supplementation.

### **SARS-CoV-2 Spike Protein 1 Activates Microvascular Endothelial Cells and Complement System Leading to Platelet Aggregation**

Giuseppe Remuzzi et al

*Front Immunol.2022 Mar 7;13:827146*

**Abstract**

Microvascular thrombosis is associated with multiorgan failure and mortality in coronavirus disease 2019 (COVID-19). Although thrombotic complications may be ascribed to the ability of SARS-CoV-2 to infect and replicate in endothelial cells, it has been poorly investigated whether, in the complexity of viral infection in the human host, specific viral elements alone can induce endothelial damage. Detection of circulating spike protein in the sera of severe COVID-19 patients was evaluated by ELISA. *In vitro* experiments were performed on human microvascular endothelial cells from the derma and lung exposed to SARS-CoV-2-derived spike protein 1 (S1). The expression of adhesive molecules was studied by immunofluorescence and leukocyte adhesion and platelet aggregation were assessed under flow conditions. Angiotensin converting enzyme 2 (ACE2) and AMPK expression were investigated by Western Blot analysis. In addition, S1-treated endothelial cells were incubated with anti-ACE2 blocking antibody, AMPK agonist, or complement inhibitors. Our results show that significant levels of spike protein were found in the 30.4% of severe COVID-19 patients. *In vitro*, the activation of endothelial cells with S1 protein, *via* ACE2, impaired AMPK signalling, leading to robust leukocyte recruitment due to increased adhesive molecule expression and thrombomodulin loss. This S1-induced pro-inflammatory phenotype led to exuberant C3 and C5b-9 deposition on endothelial cells, along with C3a and C5a generation that further amplified S1-induced complement activation. Functional blockade of ACE2 or complement inhibition halted S1-induced platelet aggregates by limiting von Willebrand factor and P-selectin exocytosis and expression on endothelial cells. Overall, we demonstrate that SARS-CoV-2-derived S1 is sufficient in itself to propagate inflammatory and thrombogenic processes in the microvasculature, amplified by the complement system, recapitulating the thromboembolic complications of COVID-19.

**Shiga Toxin 2 Triggers C3a-Dependent Glomerular and Tubular Injury through Mitochondrial Dysfunction in Hemolytic Uremic Syndrome**

Giuseppe Remuzzi et al

*Cells. 2022 May 26;11(11):1755***Abstract**

Shiga toxin (Stx)-producing *Escherichia coli* is the predominant offending agent of post-diarrheal hemolytic uremic syndrome (HUS), a rare disorder of microvascular thrombosis and acute kidney injury possibly leading to long-term renal sequelae. We previously showed that C3a has a critical role in the development of glomerular damage in experimental HUS. Based on the evidence that activation of C3a/C3a receptor (C3aR) signaling induces mitochondrial dysregulation and cell injury, here we investigated whether C3a caused podocyte and tubular injury through induction of mitochondrial dysfunction in a mouse model of HUS. Mice coinjected with Stx2/LPS exhibited glomerular podocyte and tubular C3 deposits and C3aR overexpression associated with cell damage, which were limited by C3aR antagonist treatment. C3a promoted renal injury by affecting mitochondrial wellness as demonstrated by data showing that C3aR blockade reduced mitochondrial ultrastructural abnormalities and preserved mitochondrial mass and energy production. In cultured podocytes and tubular cells, C3a caused altered mitochondrial fragmentation and distribution, and reduced anti-oxidant SOD2 activity. Stx2 potentiated the responsiveness of renal cells to the detrimental effects of C3a through increased C3aR protein expression. These results indicate that C3aR may represent a novel

target in Stx-associated HUS for the preservation of renal cell integrity through the maintenance of mitochondrial function.

## **A Home-Treatment Algorithm Based on Anti-inflammatory Drugs to Prevent Hospitalization of Patients With Early COVID-19: A Matched-Cohort Study (COVER 2)**

Giuseppe Remuzzi et al

### **Abstract**

**Background and aim:** While considerable success has been achieved in the management of patients hospitalized with severe coronavirus disease 2019 (COVID-19), far less progress has been made with early outpatient treatment. We assessed whether the implementation of a home treatment algorithm-designed based on a pathophysiologic and pharmacologic rationale-and including non-steroidal anti-inflammatory drugs, especially relatively selective cyclooxygenase-2 inhibitors and, when needed, corticosteroids, anticoagulants, oxygen therapy and antibiotics-at the very onset of mild COVID-19 symptoms could effectively reduce hospital admissions.

**Methods:** This fully academic, matched-cohort study evaluated outcomes in 108 consecutive consenting patients with mild COVID-19, managed at home by their family doctors between January 2021 and May 2021, according to the proposed treatment algorithm and in 108 age-, sex-, and comorbidities-matched patients on other therapeutic schedules (ClinicalTrials.gov: [NCT04854824](https://clinicaltrials.gov/ct2/show/study/NCT04854824)). The primary outcome was COVID-19-related hospitalization. Analyses were by intention-to-treat.

**Results:** One (0.9%) patient in the "recommended" cohort and 12 (11.1%) in the "control" cohort were admitted to hospital ( $P = 0.0136$ ). The proposed algorithm reduced the cumulative length of hospital stays by 85% (from 141 to 19 days) as well as related costs (from €60.316 to €9.058). Only 9.8 patients needed to be treated with the recommended algorithm to prevent one hospitalization event. The rate of resolution of major symptoms was numerically-but not significantly-higher in the "recommended" than in the "control" cohort (97.2 vs. 93.5%, respectively;  $P = 0.322$ ). Other symptoms lingered in a smaller proportion of patients in the "recommended" than in the "control" cohort (20.4 vs. 63.9%, respectively;  $P < 0.001$ ), and for a shorter period.

**Conclusion:** The adoption of the proposed outpatient treatment algorithm during the early, mild phase of COVID-19 reduced the incidence of subsequent hospitalization and related costs.

# Experimental Investigation on Intermittent Spray Cooling and Toxic Hazards of Lithium-Ion Battery Thermal Runaway

by Jinhua Sun, Member EUAS



## Short Biography

### **Education and Positions**

- 2022~ Chair Professor, University of Science and Technology of China  
 2019~ Chairman, Sub-Academic Advisory Committee of USTC  
 2004~2019 Vice Director of State Key Laboratory of Fire Science of China, CHINA  
 2014~ Director of Energy Fire Safety Institute, SKLFS, CHINA  
 2002~ Professor, University of Science & Technology of China, CHINA  
 1999~2002 Research Professor, Japan Science and Technology Agency, JAPAN  
 1996~1999 Ph.D., The University of Tokyo, JAPAN  
 1988~1996 Associate Professor, Anhui University of Science & Technology, CHINA  
 1986~1988 M. Sc., Nanjing University of Science and Technology, CHINA  
 1983~1986 Assistant Professor, Anhui University of Science & Technology, CHINA  
 1979~1983 B. Sc., Nanjing University of Science and Technology, CHINA

### **Professional Activities**

- Vice-Presidents of Asia-Oceania Association for Fire Science and Technology (2007~2020)  
 Committee Member of the International Association for Fire Safety Science (2008~2017)  
 Committee Member of the National Science and Technology Award (2010~)  
 Vice-chairman of Chemical Safety Committee, CIESC (2017~)  
 Vice-chairman of Building Fire Protection Committee, CFPA (2008~2022)  
 Experts of the first national emergency response expert group for work safety (2015~)  
 Experts of the fifth national work safety expert group (2014~)  
 Academic Committee Member of University of Science and Technology of China (2009~)  
 Safety expert committee Anhui Province, Civil blasting group leader (2009~)  
 Member of Science and Technology Award Committee, Ministry of Public Security (2007~)  
 Member of Academic Committee of urban safety and disaster prevention, Urban Planning Society of China (2005~2015)  
 Evaluation expert in international scientific and technological cooperation program, Ministry of Science and Technology of China (2005~)  
 Executive director of Anhui Fire Protection Association (2005~)  
 Associate Editorial or Editorial Board of five International Journals (2010~)  
 Editorial Board of nine national Journals (2003~)  
 Academic Committee Member of China Fire Protection Association (2003~)

### **Honors and Awards**

- Model Research Worker Award, Anhui Province, China (2022)  
 Moral Model of Teacher Award, Anhui Province, China (2021)

*Lifetime Contribution Award, Asia-Oceania Association for Fire Science and Technology (2021)*  
*Science and Technology Progress Award, First-class Award, the China Association for Public Safety (2021)*  
*Special government allowance of the State Council, The State Council of the P. R. China (2019)*  
*Science and Technology Innovation Award, First-class Award, CFPA (2018)*  
*Science and Technology Progress Award, First-class Award, China Highway and Transportation Society (2018)*  
*Zhu Li Yuehua excellent teacher Award, Chinese Academy of Sciences (2017)*  
*Excellent graduate student supervisor Award, Chinese Academy of Sciences (2017)*  
*Zhu Li Yuehua excellent teacher Award, Chinese Academy of Sciences (2014)*  
*Excellent graduate student supervisor Award, Chinese Academy of Sciences (2014)*  
*Teaching Award of Anhui Province, First-class Award, Anhui Province (2010)*  
*Beijing Science and Technology Award, Third-class Award, Beijing (2008)*  
*Science and Technology Award for Young Scientist, Anhui Province (2006)*  
*Safety Science and Technology Award of State Administration of Work Safety, Second-class Award (2006)*  
*National Science and Technology Progress Award, Second-class Award, China (2006)*  
*Outstanding Member Hundred Talent Program, Chinese Academy of Sciences (2005)*  
*Member of Hundred Talent Program, Chinese Academy of Sciences (2001)*  
*National Science and Technology Progress Award, First-class Award, China (1993)*

Professor Sun Jinhua has long been devoted to academic research and education in the area of fire science and fire protection. He has made substantial accomplishments in a number of fields in fire safety science and engineering, including fire risk assessment, performance-based fire protection design, building fire safety, industrial fire safety, fire safety in new energies. He led as a PI more than 20 important national research projects, such as the National “973 Program”, key projects funded by National Natural Science Foundation of China (NSFC), the “11th Five-Year plan” and the “13th Five-Year Plan” national key R&D program, the sixth Framework Project of the EU International Cooperation Program in Science and Technology, general projects of NSFC, and “Outstanding Talents” project funded by the Chinese Academy of Sciences.

Prof. Sun has published more than 400 papers in peer-reviewed journals, including Progress in Energy and Combustion Science, Combustion and Flame, Renewable and Sustainable Energy Reviews, et al, which have been cited more than 11,000 times (Web of Science). Contributions have also been recorded in 11 academic books or book chapters and over 40 keynote or invited talks at national or international conferences. In addition, Prof. Sun has supervised more than 50 PhD students.

### **Major Research Areas**

1. Theories and methods of fire prevention for new energies.
2. Methods for fire risk assessment and safety design of buildings and urban areas.
3. Theory of fire dynamics, fire prevention and control for buildings.
4. Industry fire dynamics and fire prevention.

### **Selected Publications in 2022**

1. Zesen Wei, Chen Liang, Lihua Jiang, Linjun Wang, Siyuan Cheng, Qingkui Peng, Lei Feng, Wenhua Zhang, Jinhua Sun\* , Qingsong Wang\*, n-depth study

**on diffusion of oxygen vacancies in  $\text{Li}(\text{Ni}_x\text{Co}_y\text{Mn}_z)\text{O}_2$  cathode materials under thermal induction, *Energy Storage Materials*, 47(2022) 51-60**

It is generally believed that an increase in Ni content will severely reduce the lattice structure stability of the cathode material, causing it to release more oxygen during thermal induction. However, the thermal degradation mechanism at the microscopic level remains unclear, which hinders the safety design of cathodes. In this work, we focus on the secondary particles of different  $\text{Li}(\text{Ni}_x\text{Co}_y\text{Mn}_z)\text{O}_2$  cathodes, report the formation and condensation of oxygen vacancies on the surface in detail, and quantitatively analyze the oxygen vacancy concentration distribution inside the particles after thermal failure. The results reveal that the increase of Ni content promotes the oxygen vacancies to diffuse deeply from the surface of the secondary particles to the bulk under thermal induction, resulting in an increase of oxygen vacancy concentration in the bulk of the secondary particles and the release of more oxygen. When the Ni content  $x$  in  $\text{Li}(\text{Ni}_x\text{Co}_y\text{Mn}_z)\text{O}_2$  increases to 0.8, both the surface layer and bulk exhibit high oxygen vacancy concentrations, leading to an overall failure of the secondary particles. Furthermore, we suggest that the formation and evolution of intergranular cracks inside the secondary particles depend on the oxygen vacancy concentration gradient. Our work provides a new idea for future research on the thermal stability of cathode and the thermal safety design of Ni-rich cathode materials.

**2. Lin Zhang, Qiangling Duan, Xiangdong Meng, Kaiqiang Jin, Jiajia Xu, Jinhua Sun\*, Qingsong Wang\*, Experimental investigation on intermittent spray cooling and toxic hazards of lithium-ion battery thermal runaway, *Energy Conversion and Management*, 252(2022)115091**

The fire extinguishing and cooling of lithium-ion battery thermal runaway have attracted significant research attention. In this study, an intermittent spray method for cooling lithium-ion battery during thermal runaway is proposed. The internal temperature and voltage of the battery, as well as the gases generated during thermal runaway are investigated. In addition, the extinguishing and cooling ability of the intermittent spray method at different intermittent periods (cycle consisting of a spray time and an interval time) and duty cycles (the percentage of the pulse duration occupied in a cycle) are compared and discussed. Furthermore, the toxic effects of the generated gases are evaluated. Experimental results reveal that the internal temperature of the battery is significantly higher than the surface temperature during the thermal runaway. Particularly, the internal temperature of the cell with 100% state of charge was as high as approximately 1000°C. In addition, the surface temperature of the cell may rebound after cooling owing to the insufficient heat transfer and a large radial temperature gradient of the battery. Furthermore, intermittent spray with more spray pulses of shorter duration performs better cooling effect. Particularly, the cooling effect initially increases, and then decreases with decreasing duty cycle. The major toxic gases produced during thermal runaway are CO and HF, whose yield increases with an increase in the state of charge, and the toxicity of these gases increases after the water spray. The findings of this study indicate that strict safety protection is needed when water spray is used to extinguish LIB fires.

**3. Qiangling Duan, Qian Zeng, Kaiqiang Jin, Qingsong Wang, Jinhua Sun\*, Mechanism of self-ignition and flame propagation during high-pressure hydrogen release through a rectangular tube, *Process Safety and Environmental Protection*,**

164(2022)283-290

The dynamic mechanisms of self-ignition and flame propagation during high-pressure hydrogen release through a rectangular tube were experimentally investigated using pressure records, flame detection and high-speed photographs. Experimental results show that the minimum burst pressure for self-ignition decreases with an increase in axial distance to the diaphragm and then remains at an almost constant value. The self-ignition onset at the same location of the tube exhibits certain randomness even if the intensity of the shock wave produced in the tube is similar. Multiple ignitions were observed at the early stage of hydrogen release. They usually had difficulty to sustainably develop and were extinguished owing to oxygen deficiency. At a subsequent stage, the ignition kernel appears again and grows rapidly in the axial and radial directions, finally converging to a complete flame across the tube width. It was found that the radial growth rate of the flame was lower than the axial growth rate.

**4. Mi Li, Yu Wang\*, Lin Jiang, Fuhai Gou, Jinhua Sun\*, Mass loss prediction of inclined fuel combustion using variable B-number theory, Fuel, 310(2022)122446**

Predictions of combustion behavior over solid fuel have long been goals for researchers in fuel science. This study theoretically and experimentally investigated the free buoyancy flame spread over translucent fuel (polymethyl methacrylate, PMMA) with different widths and inclinations, through developing global and effective mass loss rate prediction models based on the variable B-number theory. A total of 90 tests were performed: five inclinations (30° to 90° from the horizontal) were selected to investigate inclined flame spread; In each inclination, six sample widths ranging from 2 to 7 cm were tested. The flame length, pyrolysis length, flame spread rate, and the mass loss rate of experimental data were investigated. Based on the reasonable approximations and assumptions for the free-convective laminar burning of inclined fuel sheet, theoretical and numerical relationships on flame standoff distance, global mass loss rate, and the lateral diffusion mass loss rate were obtained from the transform of the conservation equations. Then a methodology for calculating the experimental B-number was developed by processing the flame image sequences in the stable stage of the inclined flame spread. From the calculated B-number, a prediction model of the global mass loss rate was developed and validated. Moreover, with the consideration of the lateral diffusion mass loss rate, the global effective mass loss rate, the heat release rate, and the heat loss rate at the fuel surface were obtained and analyzed. The study provided an insight into the inclined laminar burning of solid fuel with free buoyancy in the aspect of heat and mass transfer, which may be applied in the prediction and assessment of the usage and recycling of energy sources in reality.

# New Aspects of Liquid Crystal Displays & Photonic Devices

by Vladimir Chigrinov, Member EUAS



## Short Biography

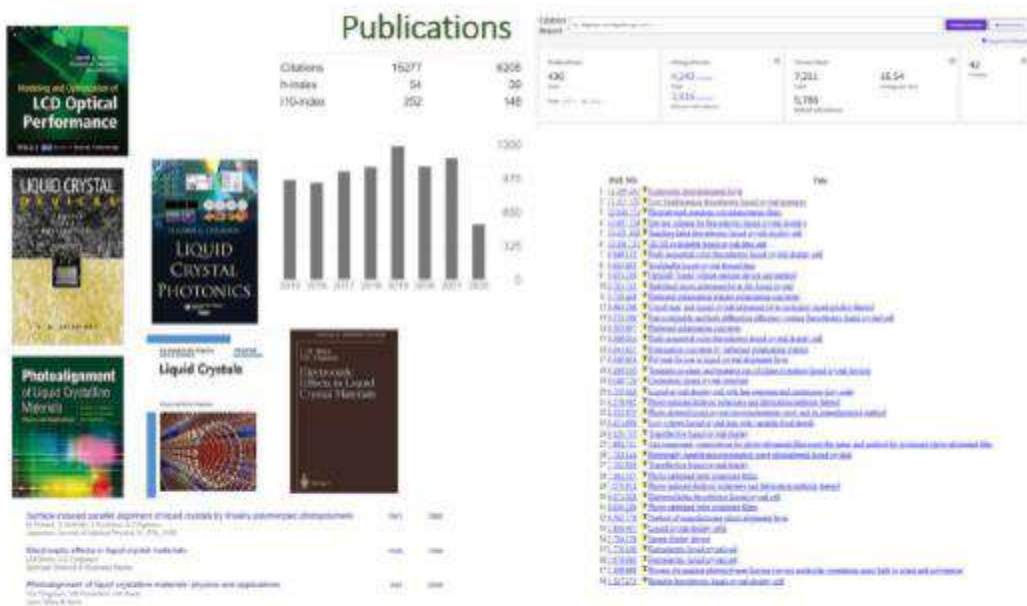
*Professor Vladimir G. Chigrinov is Professor of Hong Kong University of Science and Technology since 1999. He is an Expert in Flat Panel Technology in Russia, recognized by the World Technology Evaluation Centre, 1994, and SID Fellow since 2008. He is an author of 6 books, 31 reviews and book chapters, about 322 journal papers, more than 677 Conference presentations, and 121 patents and patent applications including 38 US patents in the field of liquid crystals since 1974. He got Excellent Research Award of HKUST School of Engineering in 2012. He obtained Gold Medal and The Best Award in the Invention & Innovation Awards 2014 held at the Malaysia Technology Expo (MTE) 2014, which was hosted in Kuala Lumpur, Malaysia, on 20-22 Feb 2014. He is a Member of EU Academy of Sciences (EUAS) since July 2017. He got A Slottow Owaki Prize of SID in 2018 <http://www.ee.ust.hk/ece.php/enews/detail/660>. He is 2019 Distinguished Fellow of IETI (International Engineering and Technology Institute). <http://www.ieti.net/news/detail.aspx?id=184> <http://www.ieti.net/memberships/Fellows.aspx> Since 2018 he works as Professor in the School of Physics and Optoelectronics Engineering in Foshan University, Foshan, China. 2020-2024 Vice President of Fellow of Institute of Data Science and Artificial Intelligence (IDSAI) Since 2021 distinguished Fellow of Institute of Data Science and Artificial Intelligence. Since March 2022 he is A Fellow of National Academy of Technology for his contributions to Information Electrical and Electronic Research : <http://www.usnat.org/fellows.html>*

## RESEARCH INTERESTS

- Computer modeling of various electrooptical effects in Liquid Crystals (LC).
- Liquid crystals: physics and applications.
- 3. Photo-aligning and photo-patterning by azodye nanolayers technique for LC application in displays and photonics such as: (i) fast high resolution LC display

devices, such as field sequential color ferroelectric LCD; (ii) LC sensors; (iii) LC lenses with a variable focal distance; (iv) LC E-paper devices, including electrically and optically rewritable LC E-paper, fast bi and multistable ferroelectric LC devices; (v) photo induced semiconductor quantum rods alignment for new LC display applications; (vi) 100% polarizers based on photoalignment; (vii) LC smart windows based on photopatterned diffraction structures; (viii) LC antenna elements with a voltage controllable frequency; (ix) security films.

- 3. LC devices in fiber optics: LC based bandgap fibers, Spectral filters, Tunable waveplates, Tunable gratings, Polarimeter, beam steering devices



NAT certifies that

**Vladimir G. Chigrinov**

has been elected to the

**Fellow of NAT (FNAT)**

for contributions to Information, Electrical and Electronic Technology research

Url: <http://www.usnat.org/fellows.html>

NAT Secretary-General:

**Otilia Mantz**

March 15, 2022

Scientific Committee Member of Euro-Global Conference on Biotechnology and Bioengineering, June 2022, Rome, Italy, <https://biotechnology-conferences.magnusgroup.org/scientific-committee/2022>

Honorary Chair of Information Management and Computer Science Conference, 2022 5th International Conference on E-Business, Information Management and Computer Science (EBIMCS 2022) Committees, Hong Kong, December 2022

3rd Global Webinar on Laser, Optics and Photonics, Member of Organizing Committee, India, September 2022, <http://www.globalscientificguild.com/laser-optics-photonics/organizing-committee.php>

Since March 2022 he is A Fellow of National Academy of Technology for his contributions to Information Electrical and Electronic Research (<http://www.usnat.org/fellows.html>)

The following research has been done recently (year 2022):

### Papers

1. Chigrinov, VG, Kudreyko, AA, Kozenkov, VM, Kinetics of photoinduced phase retardation in azo dye layer, *Liquid Crystals*, 10.1080/02678292.2022.2037766 (2022).
2. DONG XU, HUIJIE ZHAO, TIAN LIU, QI GUO, VLADIMIR G CHIGRINOV, AND HOI-SING KWOK, Flexible and wide-range tuning of liquid crystal polarization grating period based on single and interference-free exposure, *Optics Express*, Vol. 30, No. 13/20, pp. 23115-23123 (2022).
3. Vladimir Chigrinov, Aleksey Kudreyko Photosensitive Alignment: Advanced Electronic Paper-Based Devices, *Crystals*, , 2022, 12, 364. <https://doi.org/10.3390/cryst12030364>
4. Aleksey Kudreyko, Vladimir Chigrinov, and Jiatong Sun, Structural and Optical Characteristics of Flexible Optically Rewritable Electronic Paper, *Crystals*, 2022, 12, 1149, <https://doi.org/10.3390/cryst12081149>

### Tutorials

Vladimir Chigrinov, *Liquid crystal applications in displays and photonics: new possibilities*, ICDT 2022, Tutorials, Fuzhou, China, July 2022.

### Conference

1. Vladimir Chigrinov, Key Note: Liquid Crystal Photoaligned by Azodye Nano Layers: Physics and Applications, Nanoforum 2022, Auragen Group, March 07, 2022.
2. Vladimir Chigrinov, Plenary Talk: Photoaligning and Photopatterning of Liquid Crystals: Physics and Application, Global Summit on Semiconductors, Optoelectronics and Nanostructures (GSSON2022), March 23, 2022.
3. Vladimir Chigrinov, Key Note: Azodye nanolayers: applications in E-paper and security films, Electronics and Electrical Engineering meeting V-EEE, 2022 March 25, 2022.
4. Vladimir Chigrinov, A Liquid crystal photoaligned by azodye nano layers: Physics and applications in photonics, Herald Meetings, USA, "5th Online International Conference on Nanomaterials and Nanotechnology" held from April 2022.
5. Vladimir G. Chigrinov, Key Note: Liquid crystal photoaligned by azodye nano layers: Physics and applications in displays and photonics, 4<sup>th</sup> World Nanotechnology Conference, Magnus Group USA, April 2022.
6. Vladimir G. Chigrinov, Key Note: Liquid crystal photoaligned by azodye nano layers:

physics and applications in displays and photonics, Euro Global Conference Biotechnology and Bioengineering, ECBB22, Magnus Group USA, June 2022.

7. Vladimir G. Chigrinov, Plenary Talk: Liquid crystal photoaligning and photopatterning by azodye nano layers: physics and applications in displays and photonics, Global Experts Meet on Condensed Matter Physics, CMP22, Rome, Italy, June 2022.

8. Vladimir G. Chigrinov, Photoalignment and photopatterning by nanosize azodye layers: New LC display and photonics technology, 28th International Conference on Advanced Materials, Toronto, Canada, June 2022.

9. Vladimir G. Chigrinov, Photoaligning and photopatterning of liquid crystals: physics and Applications, International Liquid Crystal Conference 2022, Lisbon, Portugal, July 2022.

10. Vladimir G. Chigrinov, Key Note: Liquid Crystal Photoaligned by Azodye Nano Layers: Physics and Applications in Displays and Photonics, Global Web Forum on APPLIED SCIENCE, MECHANICAL AND ENGINEERING, Aurageng Group, August 2022.

11. Vladimir G. Chigrinov, Key Note: Photoalignment and photopatterning: New LC display and photonics technology, European Lasers, Photonics and Optics Technologies Summit, ELOS 202, September 2022.

12. Vladimir G. Chigrinov, Key Note: Liquid crystal photoaligned by azodye nano layers: physics and applications in photonics, Euro Global Climate Change Conference, Virtual Event, September 2022.

13. Aleksey Kudreyko, Vladimir Chigrinov, Olga Bachurina, Characteristics of ORW E- Paper with Small Azo Dye Exposure Time, AIP Conference Proceedings 2533, 020016 (2022); <https://doi.org/10.1063/5.0098847> Published Online: 14 September 2022

14. Vladimir G. Chigrinov, Plenary Talk: Photo alignment and Photo patterning by Nano size Azodye Layers: New Liquid Crystal Devices, Global Webinar on Material Science and Engineering, Nanoscience and Nanotechnology GWMSE-2022, GWNANO-2022, October 2022.

15. Vladimir G. Chigrinov, Liquid Crystal Photoaligning and Photopatterning by Nanosize Azodye Layers: Bright Future, OPTICS, PHOTONICS AND LASERS, OPL 2022, Nov 9-11 virtual, United Scientific group.

17. Vladimir G. Chigrinov, Key Note: Liquid crystal photoaligning and photopatterning by nanosize azodye layers: new trends, NanoTech 2022: 2nd Global Virtual Summit on Nanoscience & Nanotechnology, Nov 10-11 virtual.

18. Vladimir G. Chigrinov, Photoalignment and Photopatterning of Liquid Crystals by Azodye Nanolayers: New Trend, AstronomyForum2022 November 14-15, 2022 Sercotel Sorolla Palace, Valencia, Spain 2nd International Forum on Physics and Astronomy.

## Patents

Tseng Man Chun , Srivastava Abhishek Kumar , Meng Cuiling , Chigrinov; Vladimir Grigorievich , Kwok; Hoi Sing , Shi Yue , Ho Yeuk Lung Jacob , Zhao Chenxiang , **Composite photoalignment layer**, US Patent, 11,294,241, April 5, 2022.

# Updated Investigations in Atmospheric Propagation & Microwave Biophysics

by André Vander Vorst, Member EUAS

## Short Biography

*André Vander Vorst was born in Brussels in 1935. At high school, he studied classical humanities, including Latin and Greek. He graduated in 1958 as an electrical and mechanical engineer at the UC Louvain (UCL), Belgium, from which he received his Doctoral degree in 1965. During his thesis he spent two times six weeks working at Philips Natuurkundig Laboratorium, Eindhoven, The Netherlands. As a research associate, he was at M.I.T 1964-1965 where he earned a M.Sc. degree in microwaves, and at Stanford University 1965-1966, both years in radioastronomy. Back in Belgium in 1966, he founded the Microwave Laboratory at UCL, which he headed for 35 years. His research interests were successively loaded waveguides and cavities, atmospheric propagation up to 300 GHz, opto-microwaves, humanitarian demining, and bio-microwaves. He has been teaching in four Belgian Universities on electromagnetics, transmission lines, and microwaves. He also taught analogue and hybrid computation, antennas, and microwave satellite communications. He supervised 27 doctoral theses and about 200 engineer's theses.*

*Prof. Vander Vorst has authored and co-authored seven books, a number of book chapters, and 400 papers in peer-reviewed journals and conference proceedings. His last book, RF/Microwave Interaction with Biological Tissues, with A. Rosen and Y. Kotsuka as co-authors was published in 2006 by Wiley, U.S.A. He recently co-authored papers on various websites on the 5G and the effect of electromagnetics on viral infections. He has written chapters on bioelectromagnetics in a collective book investigating electro-hypersensitivity and papers on the same subject.*

*Through his academic career at UCL, Prof. Vander Vorst has been Head of EE Department 1970-1971, Dean of Engineering 1972-1975, Vice-President of the Academic Council 1973-1975, and President of the Open School in Economic and Social Politics 1973-1987.*

*Over the last 60 years, Prof. Vander Vorst has been actively involved in developing the international microwave community. In 1967-2001 he was chairing Student Activities Committee and Educational Activities Committee and setting up Chapter Coordination Committee in I.E.E.E. Region 8. He was a corresponding member of the Organizing Committee of the first European Microwave Conference (EuMC) in London 1969, Chair EuMC Technical Program Committee in Brussels 1973, and Chair EuMC in Liège 1984. He has been a reviewer for every EuMC since 1969. He is a founder member of the European Microwave Association (EuMA) and has been EuMA Secretary General for 18 years. In the latter function he has set up and developed EuMA Headquarters. He is now appointed Secretary Emeritus and Data Protection Officer and is still active with EuMA.*

*Prof. Vander Vorst has offered his service to the microwave community also under the umbrella of I.E.E.E. MTT Society, in which he has been active in 1985-2006. He is a Life fellow of the I.E.E.E. He obtained a number of awards including the Microwave Career Award 2004 from I.E.E.E. MTT-S, the Distinguished Service Award 2016 from EuMA and the Propagation Award 2019 from the European Association for Antennas and Propagation (EurAAP).*

*He is an emeritus member of Belgian Academia of Letters and Science, a member of Academia Europaea, the Electromagnetics Academy, and the EU Academy of Sciences. He is an Honorary Member of Belgian National Committee or URSI and of a number of international committees. He has been a member of National Health Council in both Belgium and The Netherlands.*

*He has been cited in a number of Who'sWho.*

*He loves music and has conducted choirs for more than 40 years.*

*He has five children, twelve grandchildren and two great granddaughters.*

From 1960 to 1964, André Vander Vorst investigated **fast switching of magnetic cores** for his doctoral thesis. As a research associate with a post-doctoral fellowship, he spent two years in the USA: 1964-1965 at M.I.T. and 1965-1966 at Stanford University in both Laboratories of Radio-astronomy. In 1966, back in Belgium he founded the Microwave Laboratory at the Université catholique de Louvain (UCL). Some typical publications are mentioned in what follows for each research topic mentioned.

He started research on propagation in lossless closed structures at X-band like loaded waveguides and cavities. The first doctoral thesis he supervised in the Laboratory was by F. Gardiol, 1966-1969, who analytically investigated the impact of a one-dimensional inhomogeneity on waveguide propagation [1].

Simultaneously, A. Vander Vorst started developing **numerical analysis for propagation** in diverse inhomogeneously loaded microwave transmission lines by means of variational principles [2]. He produced a numerical version of the variation-iteration method presented by Morse and Feshbach, *Methods of Theoretical Physics*, Part 1 and 2, McGraw-Hill, 1953. In 1969, he obtained the first numerical solution of a second-order partial derivative eigenvalue equation, describing the propagation in a rectangular waveguide loaded by inserts.

A number of doctoral students then investigated the impact of inhomogeneity on miscellaneous propagating structures, like microstrips, fin lines, and p-i-n transmission lines, as well as opto-induced effects on transmission lines [3]-[8].

This research ended up with propagation on lossy distributed structures at frequencies up to 100 GHz. In 2002, he co-authored with a research book on variational principles and distributed circuits [9].

**Atmospheric propagation** has been a research interest of A. Vander Vorst from 1968 [10] until about 2000. In 1970, he set up two horizontal links at 11.6 and 35 GHz, respectively, operating for a five-year period [11]. This has been the subject of the first of his five consecutive COST projects on atmospheric propagation, covering both horizontal links and slant paths.

He was the Belgian participant to the Orbital Test Satellite (OTS) of the European Space Agency (ESA), 1978-1983. For this, he obtained significant funding from the Belgian State (equivalent to 5 million EUR at today's value) to obtain one transmitting-receiving fixed television station at 14 GHz (up, 2 kW) and 11 GHz (down), as well as two receiving stations at 11 GHz, one fixed and one mobile [12]-[14].

He has been the Belgian participant to the ESA Olympus experiment, 1988-1993, and obtained significant funding from the Belgian State and PTT Department, respectively, to set up two receiving stations at 12.5 and 30 GHz and 12.5 and 20 GHz in both polarisations at both frequencies, respectively. Measurements made at Louvain-la-Neuve included attenuation, depolarisation and scintillation at 12.5 and 30 GHz and radiometry in two polarisations at 12 and 35 GHz [15]. Fast measurements were available, every 34 ms, especially in view of investigating the time scale of the scintillation effects.

These experimental tools stimulated original atmospheric propagation investigations in theory, experiment, and simulation as well. With the OTS stations, the Laboratory has been one of the three research centres to experimentally point out the microwave scintillation phenomena, extensively investigated by several PhD students in their doctoral thesis and later.

**Site-shielding**, in particular by a knife-edge obstacle, has been investigated with measurements from 8 to 94 GHz [16]. The research then evaluated the bit-error rate prediction of atmospheric communications links [17]. It continued until the year 2000 with the evaluation of some special effects related to the structure of linearly tapered slot

antennas including the Vivaldi antenna, up to some tens of GHz [18].

A. Vander Vorst conducted research on atmospheric propagation of EM waves at frequencies up to 300 GHz [19]. He has been involved in EM wave propagation since 1960, start of his doctoral thesis, until the end of his active professional career.

**Microwave biophysics** has been another subject of interest of A. Vander Vorst. The project started at the end of the 70s by designing and implementing a system for eliminating bacteria in air by microwave heating, to proceed to open air medical surgeries. This system was patented and commercialized.

**Experimental work has been going on with rabbits** from 1987 through 1994, for a doctoral thesis in three experimental steps.

The first was devoted to developing a microwave acupuncture method by inserting a miniature cable into acupuncture points and exciting these by injecting microwaves in the cable, offering a quantitative method for measuring analgesia. The purpose was to excite the nervous system in some specific points for detecting an analgesic effect. Results were positive [20].

The second consisted of the development of a method to measure the effect of analgesia in the cervical centre of pain [Fig. 1]. This showed that by doing so the composition of the cervical liquid in the pain centre was modified similarly to what is obtained when ingesting analgesic products [21].

In the third step, a method was developed for measuring in the cervical centre of pain the effect of an electric impulse applied to a rabbit's foot in both the absence and presence of analgesia produced by microwave acupuncture. Simultaneously, the deformation of the impulse was measured on the nervous system and in particular the spinal cord, by inserting a microwave micro-antenna inside of the backbone [22], looking for a non-thermal microwave effect. The result was negative [23].



**Fig. 1.** Measuring pain threshold on a rabbit as a function of antalgic microwave acupuncture

A cooperation went on with colleagues of the UCL School of Medicine in the years 1993-1997 to evaluate the effect of magnetic induction produced by a coil to implant on a mouse for obtaining a muscular reinforcement. The result was positive [24].

Dielectric parameters and blood absorption have been measured from 2 to 110 GHz [25] and a review of microwave effects on nervous system and nervous fibre has been performed [26].

Research has then been more oriented toward biological effects and medical applications [27] and more specifically to **biological effects on living systems and especially human beings** [28]. Face heating at the occasion of a telephone conversation has been measured in direct view of a base station, on stairs and in the basement of a building, respectively, with the measurement of an increase of 0.7°C after 10 minutes in the basement [29].

Specific very low frequency magnetic field measurements have been made on spontaneous bioelectric activity of neurons [30] while dielectric absorption microwave power has been evaluated at the scale of nucleic acids [31].

**Microwave exposure of rats** has been prepared, performed and evaluated from 1998 through 2009, for another doctoral thesis. Rats were submitted to a microwave level corresponding to the calculation by WHO of the limit for the human being, taking into account however a factor 10 for difference of length between the human being and the rat. The exposure duration has been long: 2 hours per calendar day of 70% of the rat lifetime which was 30 months. There were four groups of 31 rats, including three groups exposed to three different microwave schemes, respectively, and one sham-exposed group, with in particular exposure to 970 MHz CW. Fifteen blood parameters were analysed 6 times on the 124 rats, yielding more than 10.000 biological data, together with behavioural effects and mortality. A combination of positive and negative results has been obtained on monocytes, behavioural effects, and mortality, respectively [32][33].

**Planar antennas** have been designed and evaluated in view of medical applications, from 2005 through 2013, being mainly the subject of the doctoral thesis of H. Halheit. This necessitated the evaluation of a radiating structure, the operating frequencies, the influence of the substrate on the resonance frequencies of the antenna and their bandpass, the power necessary for medical applications, and mutual coupling between the elements [34].

A number of presentations have been made in medical symposia [35]. At the request of Wiley, a research book was written on the subject of *RF/Microwave interaction with biological tissues* and published by Wiley U.S. in 2006, with PhD students as a prime target [36]. During the last three years, A. Vander Vorst co-authored papers on various websites on 5G and on the effect of electromagnetics on viral infections. He wrote chapters on bioelectromagnetics (em) and bioelectromagnetic interaction with the human body in a collective book investigating **electro-hypersensitivity** (EHS) [37]. He is a co-author of a review paper on the importance of molecular biomarkers and imaging in the study of EHS [38]. Over the last years, he co-authored about ten letters concerning em in hospitals on one hand [39] and on em interaction with the human body on the other [40].

### Selected Publications

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- [2] Vander Vorst A., Govaerts R., "Application of a Variation-Iteration method to inhomogeneously loaded waveguides", *IEEE Trans. Microwave Theory Tech.*, vol. 19, March 1971, pp. 322-331
- [3] Decreton M., Loute E., Vander Vorst A., Gardiol F., "Computer optimization of E-plane resonance isolators", *IEEE Trans. Microwave Theory Tech.*, vol. MTT-19, March 1971, pp. 322-331
- [4] Cermak I., Getsinger W., Leake B., Vander Vorst A., Varon D. "The status of computer-oriented microwave practices", *IEEE Trans. Microwave Theory Tech.*, vol. 22, March 1974, pp. 229-237 (invited)

paper)

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- [6] Aksas R., Vander Vorst A., "Transverse conduction current and radiation pattern of an arbitrary shaped symmetrical patch antenna coupled with a director", *Microwave Optical Technology Lett.*, November 1994, vol. 7, n° 16, pp. 737-739
- [7] Zhu Z., Vander Vorst A., "Microwave propagation in p-i-n transmission lines", *Microwave and Guided Waves Letters*, MTT-IEEE, vol. 7, n° 6, June 1997, pp. 159-161
- [8] Serres M., Huynen I., Vander Vorst A., "Wideband photo-induced carriers at the end of an open-ended microstrip line", *IEEE J. Sel. Topics Quantum Electr.*, vol. 4, n° 6, November-December 1998, pp. 948-952
- [9] Vander Vorst A., Huynen I., *Variational Principles and Distributed Circuits*, Research Studies Press, Baldock, United Kingdom, 2002, 318 p.
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- [13] Vanhoenacker D., Vander Vorst A., "Experimental evidence of a correlation between scintillations and radiometry at centimeter and millimeter wavelength", *IEEE Trans. Antennas Propagation*, vol. AP-33, January 1985, pp. 40-47
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- [15] Vanhoenacker D., Vasseur H., Vander Vorst A., « Limitations de la largeur de bande dues aux phénomènes atmosphériques sur des liaisons spatiales de 10 à 300 GHz », *L'Onde Electrique*, vol. 72, mai-juin 1992, n° 3, pp. 35-38
- [16] Vyncke C., Vander Vorst A., "A new approximate formula for site-shielding by a knife-edge obstacle, based on measurements from 8 to 94 GHz", *Microwave Optical Technology Lett.*, June 1995, vol. 9, n° 4, pp. 210-214
- [17] Vander Vorst A., Vasseur H., Vyncke C., Amaya-Byrne C., Vanhoenacker-Janvier D., "From electromagnetics to system performance: a new method for the error rate prediction of atmospheric communications links", *IEEE J. Selected Areas in Communications*, Vol. 15, N° 4, May 1997, pp. 656-666
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- [19] Vander Vorst A., Vanhoenacker D., "Propagation limitations for transionospheric systems from 10 to 300 GHz", *AGARD*, Paris, Rome, Boston, LSP-172, June 1990, pp. 3.1-19 (*invited paper*)
- [20] Teng J., Vanhoenacker D., Vander Vorst A., "Biological effects of microwaves in acupuncture", *Proc. Eur. Microwave Conf.*, London, September 1989, pp. 918-923
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# Electrochemical Biosensing of Glucose Based on the Enzymatic Reduction of Glucose

**by Pankaj Vadgama, Member EUAS**

## Short Biography

### **CURRENT APPOINTMENTS**

2000-                    *Director IRC in Biomedical Materials, Queen Mary University of London*  
 2000 -                    *Professor of Clinical Biochemistry, Queen Mary University of London*  
 2000 - 15                *Honorary consultant Chemical Pathologist Barts Health NHS Trust*  
 2003 - 15                *Head of NHS Clinical Service (Appointed NHS Consultant 1983)*  
 2015-                    *Visiting Professor Southern Medical University Guangzhou, China*  
 2017 -                    *Visiting Professor University of Grenoble Alps*

### **ACADEMIC QUALIFICATIONS**

1971                    *MB, BS Newcastle University*  
 1976                    *BSc Chemistry (1<sup>st</sup> Class Hon) Newcastle University*  
 1977                    *Member (later Fellow) Royal College of Pathologists*  
 1984                    *PhD Newcastle University*  
 1994                    *Fellow Royal Society of Chemistry*  
 2001                    *Fellow Institute of Materials Minerals and Mining*  
 2002                    *Fellow Institute of Physics*  
 2006                    *Fellow Royal Society of Medicine*  
 2008                    *Chartered Scientist (Institute of Materials, Minerals and Mining)*  
 2010                    *Fellow Royal Society of Biology*

### **ACADEMIC APPOINTMENTS**

1977-1980              *MRC Training Fellow Newcastle University*  
 1983-1988              *Director Biosensor Research Group Newcastle University*  
 1988-2000              *Professor of Clinical Biochemistry, Manchester University*  
 1998-2000              *Professor of Biomedical Materials, Manchester University*  
 1991-1997              *Head of Department of Medicine, Manchester University (Salford)*  
 1993-1996              *Postgraduate Dean, Faculty of Medicine, Manchester University*  
 1996-1998              *Research Dean, Faculty of Medicine, Manchester University*  
 1998-2000              *Head of Division of Biomedical Engineering, Manchester University*

### **Editorial Board Positions**

*Editorial Board: Physiological Measurement, Medical Engineering and Physics, Bioanalytical Reviews, Functional Biomaterials, Medical Devices and Sensors, 3D Printed Systems and Materials, Journal of Biochemistry and Molecular Biology Research, Chinese Chemical Letters. Guest Editor for Analytical and Bioanalytical Chemistry: (i) Thin film characterisation (ii) Membrane based sensors. Sub-Editor Biomaterials Series (RSC). Editor for (i) Bioelectrochemistry for the Encyclopedia of Interfacial Chemistry, Surface Science and Electrochemistry (ii) Bioinstrumentation and Bioinformatics for the Encyclopedia of Biomedical Engineering (Elsevier).*

### **National/International Committees**

*Member EPSRC (Engineering and Physical Science Research Council): Materials Strategic Advisory Team (SAT) (2004/5/7/8); Healthcare (2005). Member, Institute of Materials Minerals and Mining Smart Materials Committee, Nanotechnology Committee, Biomedical Applications Division and External Advisory Committee. National Measurement Systems (NMS) Grants Committees for Materials and Modelling (2002 – 15) and Innovation R&D (2012-15); NPL(National Physical Laboratory)/LGC (Laboratory of the Government Chemist) projects. Past EPSRC grants panel memberships (includes as chair of some panels) from 1986: Materials, Structural Materials,*

Chemistry, Multidisciplinary (Engineering), Health Care, Analytical Science, Mechanical and Medical Engineering, Follow-on Funding, DTCs (Doctoral Training Centres), Master's Training Packages, Sensors' Policy Group, SMART Technologies, Basic Sciences, Life Science Interface, Engineering Fellowships (Senior/Advanced). Nanotechnology Strategy Working Group (co-author, section on nanomedicine) (2005). ROPA (Realising our Potential) Panels EPSRC, MRC (Medical Research Council) (1995-96). MRC Joint Research Equipment Initiative Panel (JREI, 1996-7). Royal Society of Chemistry, Industrially-Sponsored Award in Electroanalytical Chemistry (1997, 2000). Member of Organisation and Delivery of Healthcare Task Force (Foresight Healthcare, 1999-2000). Member Academy of Medical Sciences/Foresight Working Group on the Detection and Identification of Infectious Disease (2004). Member Institution of Electrical Engineers Professional Group S9 (Biomedical Engineering, 1990-93). Chair (i) R&D (ii) Point of Care Testing committees, Division of Pathology Barts Health NHS Trust (2002-2011). Member BBSRC Strategic Research Studentships Panel 2004, LINK Program Medical Technologies and Molecular Sensors (1994-2001), Foresight LINK awards (2001). European Space Agency Advisory Panel on bioassay under microgravity (2000). Various EU FP IV & V Panels: Biotechnology, Biomedical and Health Research, Cell Factory, Growth, Standards, Measurements and Testing (1993-2000). Chair DTI Building up Biomaterials (BuB) Materials Healthcare Advisory Group (2001-2003). Member UK delegations (x3) to Japan (Biomaterials) and Singapore (x1) (Materials). Roadmap Champion for Diagnostics for human health, RSC (2010). Member Manchester Commonwealth Games 2002 Scientific Congress Committee.

RAE (Research Assessment Exercise, UK) Panel member Materials (2008). External Assessor Faculty of Engineering, University of Coimbra, Portugal (2013), Founder member biennial international conference series: Biomaterials Interfaces (2007-). Chair RSC Chemistry in Medicine Panel (2010). Chair, Steering Committee EPSRC IRColl Interdisciplinary Research Collaboration) in Bionanotechnology, University of Oxford (2003-5), Member 4th Generation Light Source (4GLS) Advisory Group, Daresbury. Member, international task force on environmental carcinogens (Halifax Project, 2014). Advisor, UK Biobank Project (2004). Member Special Inquiry into Regenerative Medicine Research at UCL.

RAE Advisor University of Manchester, REF Advisor University of Central Lancashire. Academic promotions advisor (Rutgers, Cranfield, Ulster, Manchester, Leeds, Flanders). Advisor, Engineering – Materials Faculty research quality, Limerick (2011). Cranfield University Senate committee panel member on Biomedicine MScs (2013). External advisor on the reorganization of the Chemistry Department, University of Surrey (2001). Scrutineer for Fellowship/Membership applications to the Institute of Materials Minerals and Mining. External assessor for staff appointments, PhD applications for Nazarbayev University (2014). Advisor to University of Ege (Turkey) on summer school biotechnology rolling Programme. International advisory member (vice-chair) of Uganda based research training foundation; advice on training needs and external funding, eg secured for geological sciences MScs. Co-Chair UK – China Biomaterials Partnership (2006-9). Global Initiative of Academic Networks (GIAN, India) lecture course at University of Tezpur (2016). Host to Commonwealth Fellows India (Tezpur, 2015; Aligarh Muslim University, 2003), PhD Fellow (Government of Pakistan, 2017). NMS research project advisor, LGC (2005-07).

Chair UK Foresight Panel on Biomaterials and member of Materials, Smart Materials panel (2004) (co-author, strategy documents). Member, DTI Innovation and Growth Team (2006), Member UK Standards Group on ISO TC 229; nanotechnology nomenclature (2006 -). Chair of ISO Working Group on Nanomedicine and member Working Group on Nanobiotechnology (2006 – 2010). Member BSI Committees on Nanotechnology, Botechnology and Cell Therapies.

Member DFG Review Panel for German Excellence Initiative: Materials 2005,2007). Member Finland Research Council panel on Bioscience and Engineering (2008). Grants reviewing national funding councils: Australia, Qatar, Hong Kong, Portugal, Austria, Netherlands, Italy, Ukraine, Kazakhstan, Netherlands, Romania.

## **Electrochemical Biosensing of Glucose Based on the Enzymatic Reduction of Glucose**

Ben Tahar, A Chmayssem, M Zelsmann, P Vadgama, J-L Lenormand, P Cinquin, D K Martin and A Zebda.

Sensors 2022, 22, 7105.

### **Abstract**

In this work, the enzyme aldehyde reductase, also known as aldose reductase, was synthesized and cloned from a human gene. Spectrophotometric measurements show that in presence of the nicotinamide adenine dinucleotide phosphate cofactor (NADPH), the aldehyde reductase catalyzed the reduction of glucose to sorbitol. Electrochemical measurements performed on an electrodeposited poly(methylene green)-modified gold electrode showed that in the presence of the enzyme aldehyde reductase, the electrocatalytic oxidation current of NADPH decreased drastically after the addition of glucose. These results demonstrate that aldehyde reductase is an enzyme that allows the construction of an efficient electrochemical glucose biosensor based on glucose reduction.

## **A biocompatible iron doped graphene based cathode for an implantable glucose biofuel cell**

G Menassol, L Dubois, M Nadolska, P Vadgama, D K Martin and A Zebda.

Electrochimica Acta 2022, 141627.

### **Abstract**

In this study we propose the use of an iron/nitrogen co-doped reduced graphene oxide (Fe/N-rGO) based electrode as a cathode for a future glucose biofuel cell application. We used a mechanical compression process to fabricate cathodes in the form of pellets. We studied electrocatalytic activity toward oxygen reduction of the cathode under physiological solution conditions. Our results demonstrated the capacity of these cathodes to operate under these conditions with long-term stability exceeding two years with only 8% loss of activity. Cytotoxicity tests performed under standard in vitro cell-culture conditions showed that cathodes did not exhibit any toxic effect and thereby are promising for in vivo applications.

## **A naringin-derived bioink enhances the shape fidelity of 3D bioprinting and efficiency of cartilage defect repair**

Y Huang, X Meng, Z Zhou, W Zhu, X Chen, Y He, N He, X Han, D Zhou, X Duan, P M Vadgama and H Liu.

Journal of Materials Chemistry B 2022 10, 7030-7044.

### **Abstract**

3D bioprinting is a major area of interest in health sciences for customized manufacturing, but lacks specific bioinks to enhance the shape fidelity of 3D bioprinting and efficiency of tissue repair for particular clinical purposes. A naringin derived bioink, which contains 1.5 mM methylacryloyl naringin and 0.15 mM methylacryloyl gelatin, improves the fidelity of 3D bioprinting due to 405 nm light absorption of methylacryloyl naringin. The naringin derived bioink promotes the growth of chondrocytes due to preserving bioactivities of naringin and functions as a medical ingredient from which it has been described as a medical bioink in this study. It facilitates cartilage regeneration by upregulating the transcription of chondrogenesis-related genes like SOX9 and genes against oxidative stress like SOD1 and SOD2 and maintains chondrocytes active resulting from the significantly enhanced COL II/COL I ratio. According to a rabbit cartilage defect model, the proposed naringin derived medical bioink significantly improves the efficiency and quality of cartilage defect repair, suggesting that the bioink is suitable for cartilage defect repair applications and a feasible strategy is provided for the formulation of medical bioinks for specific clinical purposes.

# Contributions on Digitization Drives Energy Efficiency

by Zhangxing (John) Chen, Member EUAS



## Short Biography

### **Education:**

- *Post-doctoral Fellow, University of Minnesota, USA, 1991-1993.*
- *Ph.D., Purdue University, USA, 1986-1991.*
- *M.S., Xi'an Jiaotong University, China, 1983-1985.*
- *B.S., Nanchang University (formerly, University of Jiangxi), China, 1979-1983.*

### **Academic Experience:**

- *Killam Professor in Engineering, University of Calgary, Canada, 2020-present.*
- *Founding Director, Global Initiative for Research in Unconventional Oil and Gas: The Beijing Site, University of Calgary, 2014-2020.*
- *Founding Director, Foundation CMG/Frank-Sarah Meyer Collaboration Centre, University of Calgary, Canada, 2012-present.*
- *Director, Schlumberger iCentre for Simulation and Visualization, University of Calgary, Canada, 2009-present.*
- *AITF (Alberta Innovates - Technology Futures, formerly iCORE) Industrial Research Chair in Reservoir Modeling, University of Calgary, Canada, 2009-present.*
- *NSERC (Natural Sciences and Engineering Research Council of Canada) / AIEES (Alberta Innovates: Energy and Environment Solutions) / Energi Simulation Industrial Research Chair in Reservoir Simulation, University of Calgary, Canada, 2008-present.*
- *Professor, Department of Chemical and Petroleum Engineering, University of Calgary, Canada, 2007-present.*
- *Professor, Southern Methodist University, Dallas, USA, 2001-2006.*
- *Associate Professor, Southern Methodist University, Dallas, USA, 1998-2001.*
- *Assistant Professor, Southern Methodist University, Dallas, USA, 1995-1998.*
- *Visiting Assistant Professor, Texas A&M University, College Station, Texas, USA, 1993-1995.*

### **Selected Academic Awards and Honors:**

- *Member, European Union Academy of Sciences (EUAS), Elected in 2022.*
- *Academician, Chinese Academy of Engineering, China, 2021.*
- *Fellow, The Parex Resources Innovation Fellowship Program, Canada, 2021.*
- *The Friendship Medal of The People's Republic of China, China, 2020.*
- *Fellow, Royal Society of Canada, Canada, 2020.*
- *Killam Professor Award, Killam Trust, Canada, 2020.*
- *Fellow, Engineering Institute of Canada, Canada, 2019.*
- *Fellow, Canadian Academy of Engineering, Canada, 2017.*
- *The Fields-CAIMS Industrial Mathematics Prize, Canadian Applied and Industrial Mathematics Society and the Fields Institute, Canada, 2017.*

- *Peak Scholar in Entrepreneurship, Innovation, and Knowledge Engagement, University of Calgary, Calgary, Canada, 2017.*
- *NSERC's Synergy Award for Innovation, NSERC (Natural Sciences and Engineering Research Council of Canada), Canada, 2016.*
- *The President's Award, CWLS (Canadian Well Logging Society), Canada, 2015.*
- *NSERC (Natural Sciences and Engineering Research Council of Canada) Discovery Grant Accelerator Supplement Award, Canada, 2013.*
- *Outstanding Leadership in Alberta Technology Award (ASTech Award), Canada, 2012.*
- *IBM Faculty Award, IBM T.J. Watson Research Center, USA, 2012.*
- *Gerald J. Ford Research Award, The Gerald J. Ford Foundation, Dallas, USA, 2004.*

### Highlighted Scholarship Contributions

Dr. Chen has authored/co-authored 650 journal articles in the most prominent journals in his research field, including *Progress in Materials Science, Advanced Energy Materials, NanoToday, Applied Catalyst B: Environmental, Small Methods, Angewandte Chemie, Chemical Engineering Journal, Advances in Colloid and Interface Science, and PNAS*, and 400 conference proceedings articles. His publications have received 23,000 citations and an *H-index* of 66 (Google Scholar), ranking the most in reservoir simulation in the world in the past ten years. He has authored/co-authored 13 monographs and edited eight books with such publishers as Springer-Verlag and Elsevier. These monographs and books have been downloaded online over 650,000 times, and five of them have been used as undergraduate and graduate textbooks worldwide. Particularly, his text *Computational Methods for Multiphase Flows in Porous Media*, published in 2006 and cited 1,600 times, has been adopted extensively by many universities globally. Dr. Chen owns 30 patents and have delivered 460 invited/keynote/plenary talks. These articles, books, patents, and public talks have profoundly helped to advance many disciplines including Chemical, Petroleum, Energy, and Environmental Engineering, and engaged the public in the people and ideas shaping the future of the world. His research funding of over \$100M from private and public sponsors over the past 30 years has made him one of the highest-funded engineers and scientists worldwide.

Dr. Chen has made exceptional contributions to the fields of Chemical and Petroleum Engineering, Energy and Environmental Engineering, and particularly to the field of multidisciplinary studies in fluid flow and its applications to various industries. His original and novel research is of a fundamental and applied nature, reflected in his most significant contributions to research and practical applications in the globe. On the fundamental side, his ground-breaking research on multiphase flows in porous media has advanced the fields of *reservoir modeling, computational methods, and fluid flow in nanopores*. His comprehensive scientific models of fluid flows in porous media were the world's first in reservoir modeling in that they represent reservoirs from pore- to kilometer-scale, reflecting their real physics in terms of mass, heat, composition, kinetics and geomechanics. His models have significantly increased the energy industry's confidence in reservoir simulations, been foundational in the development of reservoir simulators, and set the stage for new directions in energy and environmental stewardship. They were foundational for the top energy company Shell's simulators to design their oil recovery projects and the world's largest independent reservoir simulator developer Computer Modelling Group (CMG) Ltd. to develop their commercial reservoir simulation

software.

Dr. Chen is an international expert on the development of computational methods for fluid flows. This extraordinary research has made numerous wide-ranging contributions in multiple areas, such as solid and fluid mechanics, groundwater modeling, and environment science. He invented a set of mixed and nonconforming finite element spaces and a suite of control volume methods for flow simulations. These novel methods generate highly accurate attributes (pressure, temperature, composition, and velocity) in complex reservoirs, and provide a three-fold improvement in accuracy and a two-fold increase in stability over earlier methods. Recognizing these outstanding achievements, the global computational method community named these spaces after him: the Chen-Douglas (his former PhD supervisor) mixed finite element spaces and Chen-rotated spaces.

Dr. Chen's fundamental research on fluid flow has significantly advanced the development and application of fluid flow mechanisms in nanopores. Unlike traditional fluid flow in porous media, fluid flow in nanopores involves more challenging mechanisms including continuum flow, slip flow, surface diffusion and adsorption. His breakthrough was a new theory that captures all these important mechanisms while detailing the variable contribution of each in nanofluid flow. This theory has significantly impacted gas production and separation, carbon capture and storage, carbon nanotube membranes, catalysis, and methane storage in vehicles. While collaborating with top service and energy companies such as CMG Ltd., ExxonMobil, and China National Petroleum Corporation (CNPC), Dr. Chen has applied this theory to studies of numerous gas production wells worldwide and guided production in nanoporous petroleum reservoirs.

Dr. Chen has developed innovative fast linear solvers and parallel simulators for reservoirs. These novel solvers and simulators have shown a thousand-fold improvement in speed over previous commercial reservoir software while their accuracy is preserved. They allow for simulations of giga-cell (billion) sizes and play a key role in increasing oil and gas recovery through a better resolution of vast disparate seismic, geologic, and field data. Moreover, they have assisted history matching methods and increased the effectiveness of field optimization. In turn, these advancements have significantly improved the modeling and simulation processes of enhanced oil recovery for conventional (light oil and natural gas), unconventional oil and gas (tight and shale oil and gas, and coalbed methane), heavy oil, and oil sands reservoirs and led to tremendous capital and operational savings for the energy industry.

In 2008, Dr. Chen created Canada's most prominent reservoir simulation consortium, which includes 15 companies who have collectively provided \$15M over 15 years to address urgent knowledge gaps in the energy industry. This consortium led to 11 patents and the spin-off technology company, ISUT Ltd. One of the most notable technologies arising from his research was the world's first patented nano-catalytic in situ upgrading technology; field tests demonstrated a 25% reduction in greenhouse gas emissions for each barrel of oil produced compared to other recovery technologies. The energy industry recognized this technology as one of 15 most promising oil and gas exploration and production technologies in the next ten years (Economics & Technology Research Institute, CNPC, 2018). Moreover, it was recognized as one of 10 most advanced technologies in petroleum in the world in 2020. In addition, Dr. Chen was a Co-founder and the Chairman of the oil production company RockEast Corp., a global leader in the provision of innovative cost-effective and environmentally friendly recovery processes for

extraction and refinement of petroleum resources. These companies and initiatives have contributed to the diversification and growth of Canada's economy and quality of life through the technologies and jobs created. His multifaceted career and ability to transfer technology have garnered national recognitions, including the NSERC Synergy Award for Innovation (2017) and two Alberta Science & Technology Foundation (ASTech) Awards (2010, 2012). The University of Calgary named Dr. Chen a Peak Scholar (2017) for his exceptional record of innovation, collaboration, knowledge engagement and technology transfer.

### **Training of Highly Qualified Personnel (HQP)**

Since joining the University of Calgary in 2007, Dr. Chen has successfully established a creative world-class research program, the largest multidisciplinary program on campus, composed of about 70 research associates, post-doctoral fellows (PDFs) and graduate students annually. He has trained 48 PDFs and graduated 77 PhD and 76 MSc students in his career; remarkably, 45 of these trainees are now faculty members at first-class universities in 16 countries, such as University of Calgary, University of Wyoming, University of Aberdeen, and China University of Petroleum. Some PhD students have won the most prestigious scholarships during their study including the NSERC Vanier Scholarship, Killam Laureate, and Alberta Innovates Scholarship. Furthermore, some students have won prestigious awards in their organizations, such as the SPE Reservoir Description and Dynamics Awards, Distinguished Achievement Awards, and Outstanding Young Professional Awards. Dr. Chen has twice been recognized as a top Graduate Educator in the Schulich School of Engineering, University of Calgary (2011-12 and 2014-15). Institutional equity, diversity, and inclusion (EDI) principles have been explicitly implemented in his HQP training; over 70% of his HQP are women and underrepresented people.

### **Representative Books**

- J. Li, X. Lin and Z. Chen, *Finite Volume Methods for the Incompressible Navier-Stokes Equations*, Springer Briefs in Mathematical Methods, Volume 11219, Springer-Verlag, 2022.
- X. Dong, H. Liu and Z. Chen, *Hybrid Enhanced Oil Recovery Processes for Heavy Oil Reservoirs*, Developments in Petroleum Science, Volume 73, Elsevier, 2021.
- L. Zhang, Z. Chen and Y. Zhao, *Well Production Performance Analysis in Shale Gas Reservoirs*. Developments in Petroleum Science, Volume 66, Elsevier, 2019.
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1. B. Tian, D. Ho, J. Hu, Z. Chen, D. Voiry, Q. Wang and Z. Zeng, Framework structure engineering of polymeric carbon nitride and its recent applications, *Progress in Materials Science*, November 2022, Article 101056.
2. L. Jiang, Z. Chen, SM F. Ali and J. Zhang, Storing Carbon Dioxide in Deep Unmineable Coal Seams for Centuries Following Underground Coal Gasification, *Journal of Cleaner Production*, Volume 378, December 2022, Article 134565.
3. M. Chai, H. Nourozieh, M. Yang and Z. Chen, A Semi-Compositional Approach to Model Asphaltene Precipitation and Deposition in Solvent-Based Bitumen Recovery Processes, *Applied Energy*, Volume 328, December 2022, Article 120197.
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# Directed Graph Clustering Algorithms, Topology and Weak Links

by Frank Lewis, Member EUAS



## Short Biography

*Dr. Frank L. Lewis was born in Würzburg, Germany, subsequently studying in Chile and Gordonstoun School in Scotland. He obtained the Bachelor's Degree in Physics/Electrical Engineering and the Master's of Electrical Engineering Degree at Rice University in 1971. He spent six years in the U.S. Navy, serving as Navigator aboard the frigate USS Trippe (FF-1075), and Executive Officer and Acting Commanding Officer aboard USS Salinan (ATF-161). In 1977 he received the Master's of Science in Aeronautical Engineering from the University of West Florida. In 1981 he obtained the Ph.D. degree at The Georgia Institute of Technology in Atlanta, where he was employed as a professor from 1981 to 1990. He is Moncrief-O'Donnell Endowed Chair Professor of Electrical Engineering at The University of Texas at Arlington.*

*Lewis is Ranked as number 19 in the world of all scientists in Electronics and Electrical Engineering by Research.com. Ranked number 5 in the world in the subfield of Industrial Engineering and Automation according to a Stanford University Research Study in 2021. Recognized as a Top 1% Highly Top Cited Researcher by Clarivate Web of Science every year since 2019. Fellow, National Academy of Inventors. Fellow of the IEEE, Fellow of IFAC, Fellow of the U.K. Institute of Measurement & Control, Fellow European Union Academy of Sciences, Fellow American Association for the Advancement of Sciences, Member of the New York Academy of Sciences. Registered Professional Engineer in the State of Texas and Chartered Engineer, U.K. Engineering Council. Published 500 Refereed Journal Papers. 80,800 google citations, h-index 123. Charter Member (2004) of the UTA Academy of Distinguished Scholars. UTA Academy of Distinguished Teachers 2012. IEEE Control Systems Society Distinguished Lecturer 2012-1014. Founding Member of the Board of Governors of the Mediterranean Control Association. Served as Visiting Professor at Democritus University in Greece, Hong Kong University of Science and Technology, Bristol University UK, Chinese University of Hong Kong, City University of Hong Kong, National University of Singapore, Nanyang Technological University Singapore.*

*Received IEEE Computational Intelligence Society Neural Networks Pioneer Award 2012, AIAA Intelligent Systems Award 2016, John Ragazzini Education Award 2018 from American Automatic Control Council. Received Fulbright Research Award 1988, American Society of Engineering Education F.E. Terman Award 1989, Int. Neural Network Soc. Gabor Award 2009, U.K. Inst Measurement & Control Honeywell Field Engineering Medal 2009, three Sigma Xi Research Awards, UTA Halliburton Engineering Research Award, UTA Distinguished Research Award, ARRI Patent Awards, various Best Paper Awards, IEEE Control Systems Society Best Chapter Award (as Founding Chairman of DFW Chapter), and National Sigma Xi Award for Outstanding Chapter (as President of UTA Chapter). Received Outstanding Service Award from the Dallas IEEE Section and selected as Engineer of the year by Ft. Worth IEEE Section. Listed in Ft. Worth Business Press Top 200 Leaders in Manufacturing. Appointed to NAE Committee on Space Station in 1995 and IEEE Control Systems*

*Society Board of Governors in 1996. Received the 2010 IEEE Region 5 Outstanding Engineering Educator Award and the 2010 UTA Graduate Dean's Excellence in Doctoral Mentoring Award. Texas Regents Outstanding Teaching Award 2013.*

*Current interests include autonomous systems, unmanned aerial vehicles, distributed cooperative control on graphs, reinforcement learning, nonlinear systems, intelligent control, process control, and neurobiological systems. Author of 7 U.S. patents, 472 journal papers, 52 chapters and encyclopedia articles, 420 refereed conference papers, and 20 books including Optimal Control, Optimal Estimation, Applied Optimal Control and Estimation, Aircraft Control and Simulation, Control of Robot Manipulators, Neural Network Control, High-Level Feedback Control with Neural Networks and the IEEE reprint volume Robot Control. Editor of Taylor & Francis Book Series on Automation & Control Engineering. Served as Editor for the flagship journal Automatica. Served/serves on many Editorial Boards including International Journal of Control, Neural Computing and Applications, Optimal Control & Methods, and Int. J. Intelligent Control Systems. Recipient of NSF Research Initiation Grant and continuously funded by NSF since 1982. He has received \$12 million in funding from NSF, ARO, ONR, AFOSR and other government agencies, including significant DoD SBIR and industry funding. His SBIR program was instrumental in ARRI's receipt of the US SBA Tibbets Award in 1996.*

## **Directed Graph Clustering Algorithms, Topology and Weak Links**

Xiao Zhang, Bosen Lian, Frank L. Lewis

IEEE TRANSACTIONS ON SYSTEMS, MAN, AND CYBERNETICS:  
SYSTEMS, VOL. 52, NO. 6, JUNE 2022

### **Abstract**

In this article, a general approach for directed graph clustering and two new density-based clustering objectives are presented. First, using an equivalence between the clustering objective functions and a trace maximization expression, the directed graph clustering objectives are converted into the corresponding weighted kernel  $k$ -means problems. Then, a nonspectral algorithm, which covers both the direction and weight information of the directed graphs, is thus proposed. Next, with Rayleigh's quotient, the upper and lower bounds of clustering objectives are obtained. After that, we introduce a new definition of weak links to characterize the effectiveness of clustering. Finally, illustrative examples are given to demonstrate effectiveness of the results. This article provides a glance at the potential connection between density-based and pattern-based clustering. Compared with other approaches for directed graph clustering, the method proposed in this article naturally avoids the loss of the nonsymmetric edge data because there is no need for any additional symmetrization.

## **Robustness Analysis of Distributed Kalman Filter for Estimation in Sensor Networks**

Bosen Lian, Frank L. Lewis, Gary A. Hewer, Katia Estabridis

IEEE TRANSACTIONS ON CYBERNETICS, VOL. 52, NO. 11, NOVEMBER 2022

**Abstract**

Motivated by the guaranteed stability margins of linear quadratic regulators (LQRs) and standard Kalman filter (KF) in the frequency domain, this article extends these results to the distributed Kalman-consensus filter (DKCF) for distributed estimation in sensor networks. In particular, we study the robustness margins of DKCF in two cases, one of which is based on the direct target observation while the other uses estimates from neighbor sensors in the network. The loop transfer functions of the two cases are established, and gain and phase margin robustness results are derived for both. The robustness margins of DKCF are improved compared to the single-agent KF. Furthermore, as communication topology varies in sensor networks, graph overall coupling strengths change. We also analyze the correlation between overall coupling strengths and the robustness margins of DKCF.

## Progresses on Structural Safety and Control

by Hong-Nan Li, Member EUAS



### Short Biography

*Dr. Hong-Nan Li received his bachelor's degree from Shenyang Jianzhu University in 1982, his master's and PhD degrees from the China Earthquake Administration in 1987 and 1990, respectively. He had conducted his postdoctoral research at Virginia Polytechnic Institute and State University from 1992-1994. He has been a Distinguished Professor (professor of Cheung Kong Scholars Program) of School of Civil Engineering at Dalian University of Technology (DUT), China since Sept. 2001. He is the founding director of the Research Center for Structural Health Monitoring and Control at DUT.*

*He is a Fellow of American Society of Civil Engineers (ASCE). His research interests are primarily in safety and security of civil infrastructure systems, focusing on development of innovative and interdisciplinary science and technology for sensors, health monitoring, damage assessment, structural control and disaster prevention. He is the author/co-author of 8 books and more than 450 refereed journal papers. He is also an inventor or co-inventor of more than 70 invention patents and 10 computer software certificates. He has delivered over 80 keynote and invited lecture at international conferences and universities in different countries.*

*He ever edited the first standard in the area of SHM in China “Design Standard for Structural Health Monitoring Systems (CECS 333: 2012)” and other 15 standards. His related achievements have been applied to more than 70 major infrastructures, such as the Zhoushan Transmission Tower (The World's the Tallest Transmission Tower), Dalian gymnasium (The World's Largest Span Suspended Dome Structure), the long span suspension dome structure NB35-2 (Ultra Large Offshore Oil Platform), Shenyang Boguan bridge (Complicated Long-Span Arch Bridge), Dalian World Trade Center. He received various prizes in recognition of his innovative achievements in research, such as played a leading role in the 2015 National Technology Invention Award, 2010 & 2007 National Science and Technology Progress Awards, and more than 10 provincial Science & Technology awards in China. He was also awarded as the “Outstanding Technical Contribution Award” by ASCE Aerospace Division (2014)*

*With a long-term commitment to serving society, He is currently the Editor-in-Chief of Structural Monitoring and Maintenance, An international Journal, Associate Editor of Journal of Aerospace Engineering-ASCE and an editorial board member of more than 30 other journals. He also has held many extensive academic and professional leadership positions related to: vice chair of the Advanced Materials and Structures committee & vice chair Dynamics and Controls Committee, American Society of Civil Engineers (ASCE); vice chair of China Panel, International Association for Structural Control and Monitoring (IASHM); council member of The International Society for Structural Health Monitoring of Intelligent Infrastructure (ISHMII), etc.*

*Dr. Li promoted the education of undergraduate students and graduate students in Civil Engineering. He has supervised more than 60 Ph.D. students and 75 Master students. Some thesis from his students were awarded for the provincial excellent theses.*

## **New Progress on Research Activities**

### **1. Wind-induced fragility analysis of a transmission tower based on multisource monitoring data and deep learning theory**

To predict the performance of transmission towers under strong wind disasters, a wind-induced fragility assessment framework for transmission towers based on multisource monitoring data and deep learning is proposed in this study. The transmission tower installed structural health monitoring system is taken as an example. First, a monitoring data preprocessing framework that integrates multiple data processing methods is proposed to carry out missing data processing, outlier data processing, and denoising processing. Then, multisource monitoring data are fused to reconstruct displacement responses, which are taken as the dataset to build the surrogate model of wind field data input and structural response output by deep learning. The optimal hyperparameters of the model are obtained by the Bayesian optimization method. The wind field data with uniform disaster intensity are generated by numerical simulation, and the surrogate model predicts the displacement response at the top of the tower. Finally, the fragility curves of the transmission tower at different damage states are fitted. The results show that the surrogate model can cover all uncertainties existing in practical engineering and effectively predict the dynamic response of the transmission tower in the complex wind field. Instead of preparing many dynamic response data by the numerical model, the proposed framework can more efficiently evaluate the wind-induced fragility of transmission towers.

### **2. Generalized Discrete Estimating Method for Moving Force Identification on a Simply Supported Beam Bridge**

Moving forces are one of the main types of loads acting on a bridge deck. Moving force identification is very important for the bridge safety, and it based on a sparse expression of a force space consisting of a set of basis functions performs outstandingly in solving the ill-posed problems. Because the form of an authentic moving force is complex and unknown, the basis function with a fixed frequency and single type cannot express the moving force sparsely enough. Additionally, the discrete sampling will aggravate the ill-posed structure inversion matrix, resulting in difficulty in identifying forces. In this study, a trigonometric function and variable frequency rectangular function are used to sparsely express the force, and the Duhamel integral is used to avoid the ill-posed reduction of discrete sampling. A generalized discrete estimating method is proposed to identify moving forces. The

L1 regularization method in a sparse solution is introduced to transform the force identification problem into an L1 regularization solution problem. The fast-iterative shrinkage threshold method is used to solve the L1 regularization problem, and the coefficient of basis functions is obtained by combining the Bayesian criteria to identify the force. To validate the method, the single and double time-varying force on a simply supported beam are identified by the numerical simulation. The results show that the method can accurately identify the time-varying force and is strongly robust. Then, the proposed method is compared with the current methods, and the response combinations of moving force identification are discussed.

Through the generalized discretization of force, the generalized discrete force is convoluted with the unit impact response, the response space is obtained by using the integrity of the Duhamel integration, and the moving force is identified by the response space. Some numerical simulations are carried out to verify the effectiveness of the method and reached the following conclusions:

(1) The GDEM can identify motion force with high accuracy and strong noise robustness. The static component of the moving force is also identified. The GDEM identifies the varying component of multiple moving forces very well.

(2) The static and varying component forces are significantly affected by the response combination. Moving force identification is preferable using both the bending moment and acceleration response.

(3) For multiple moving force identification, the number of bending moment responses is equal to the number of moving forces, and the number of accelerations is greater than or equal to the number of moving forces.

### **3. Optimal vibration control design of antenna mast on super-tall buildings against multi-hazards of earthquake and wind**

Antenna mast structures are usually set on the top of modern super-tall buildings to meet the requirements of communication and aesthetics, and such buildings are highly sensitive to horizontal loads that can greatly increase the acceleration and displacement responses during their life-cycles owing to the inherent high flexibility and low damping. As a result, the antenna masts with small mass and stiffness may suffer serious whiplash effect under the earthquake or wind excitations. In this paper, a multi-hazard protective system with hybrid isolated and energy-dissipated devices of isolation bearing, viscous damper, and mild steel damper is presented for the typical inserted antenna mast structures on super-tall buildings. To determine the optimum parameters of the hybrid system that maximize the structural control efficiency under a single hazard of earthquake or wind load, as well as the coupled conditions of these two hazards, an optimization method based on the genetic algorithm is developed for the presented hybrid control system to resist various hazard scenarios. Objective functions are further proposed to penalize the relative

accelerations and displacements at the top of the antenna mast structure. Taking a super-tall TV tower as an example, the OpenSeesPy platform is employed to establish the finite element (FE) model. The numerical results show that the optimization scheme for the hybrid energy-dissipated antenna mast system under a single hazard is not suitable for the other hazard condition, while the optimized results for the multi-hazard condition can give consideration to the effects of both earthquake and wind. Moreover, the sensitive analysis is performed to investigate the effect of each parameter of the hybrid system on the objective functions. It can be concluded that the proposed hybrid system performs well under earthquake, wind and coupled multi-hazard, which is of practical significance for the vibration control of antenna masts on super-tall buildings as follows:

(1) The developed simplified MFS model of the super-tall TV tower can yield compatible modal periods, vibration modes and dynamic response time histories with the refined FE model, and is efficiency in the optimal design of the presented antenna system.

(2) The hybrid control antenna system achieves the best performance for the external excitations it was designed for, and when used for the different external excitations, the control efficiency will reduce to a certain extent. All the optimal design cases can achieve good performance under different kinds of hazard loads. (i.e., for the DBW case, the vibration-reduction rates of displacement for three optimal design cases are 20.59%, 18.19%, 20.49%, respectively.)

(3) The influences of the all the design parameters on the objective functions of three external excitations are biased, but the trends of the objective functions with the same parameter are roughly the same. (i.e., both  $F_E$ ,  $F_W$  and  $F_C$  increase as  $\alpha$  increase, but  $F_W$  decreased at  $\alpha$  larger than 0.6 while increased at  $\alpha$  less than 0.6)

(4) It is demonstrated that the viscous damping coefficient  $C$  and velocity index  $\alpha$  have the greatest influence on the performance of the hybrid control system under all of the three kinds of external excitations, while the pre-yield stiffness of IB  $K_b$  and ratio between post-yield stiffness and initial elastic stiffness of MSD  $\alpha_m$  play negligible role in the hybrid system.

The results of the present study show that seismic load is the dominant external load when the hybrid control antenna system is subjected to coupled multi-hazard of earthquake and wind. It is suggested that the effect of multi-hazard should be taken into account in the seismic design of the hybrid control antenna system to balance the vibration control effect under various hazard conditions.

# Advanced Wastewater Treatment in Moving Bed Biofilm Reactors

by Jan A. Oleszkiewicz, Member EUAS

## Short Biography

*Dr Oleszkiewicz is a Distinguished Professor Emeritus in Environmental Engineering at the University of Manitoba, in Winnipeg, Canada and President of JAAO Environmental Engineering Ltd. His expertise is in municipal wastewater treatment and biosolids processing, specializing in biological and chemical nutrient removal and recovery, anaerobic processes for sludge wastewater treatment. He has graduated over 60 Master's and Doctoral candidates, publishing 580 refereed journal and conference papers and has 10 recent patents. Wrote several handbooks, including the seminal co-authored Manual for Wastewater Treatment Plant Operators, which received a Gold Medal from the Minister of Environment in Poland. Published by PZITS and Poznan University of Technology, the hugely popular book in its 3<sup>rd</sup> edition, at 1152 pages, is currently used at every wastewater treatment plant in Poland. He has served as scientific and technical advisor to governments and to over forty municipalities for a variety of wastewater treatment plants such as Winnipeg North MB, Kitchener ON, Alexandria VA, Boston MA, Warsaw PL, Gdansk PL. He has been teaching advanced wastewater treatment processes and solid waste management at University of Manitoba and was a visiting professor at several universities in Poland, Australia, USA and Canada. He has served as scientific advisor to variety of companies such as BCR Environmental in Jacksonville FL, Nexom in Canada, ICI Australia or Lemtech Konsulting in Krakow PL.*

*Dr Oleszkiewicz received his MSc in Sanitary Engineering from Wroclaw University of Technology and MSc in Water Quality Management and PhD in Environmental Engineering from Vanderbilt University. He served as Scientific Secretary of Environmental Protection Institute in Wroclaw PL; as Research Project Manager at DLA Inc in Pittsburgh USA, before becoming Associate Professor of Environmental Engineering in School of Engineering and Adjunct Professor in Department of Microbiology at the University of Manitoba in 1983. Active in Water Environment Federation (WEF) and International Water Association (IWA) he has been inducted as Fellow of WEF and Fellow of IWA. The Nutrient Removal and Recovery Specialist Group of IWA has organized an International Conference honoring Professor Oleszkiewicz in April 2022 (<https://wwrr.put.poznan.pl/>). He is a Fellow of Canadian Academy of Engineering (CAE) and Diplomate of American Academy of Environmental Engineers and Scientists (AAEES), Fellow of Canadian Society of Civil Engineers (CSCE). Poznan University of Technology awarded him Doctorate Honoris Causa in 2014 for contributions to science of water pollution control. His numerous awards include, among other Gordon M Fair Medal from WEF for Engineering Education; the Rh Institute Foundation Medal and Prize (\$25,000) for Research Excellence; Medal of Merit from Gdansk University of Technology, Aquarina Award and Prize; and Albert E Berry Medal from CSCE.*

Dr Oleszkiewicz recently led an interdisciplinary research team to develop a continuous flow aerobic granular sludge process for wastewater treatment. The invention represents a paradigm shift in wastewater treatment technology. The process, which typically is used in

a batch mode, can be run in a continuous mode and requires inexpensive upgrades to existing facilities, which will make it possible for municipalities to significantly improve effluent quality from their existing treatment facilities.

Dr. Oleszkiewicz's ground-breaking cold-temperature wastewater research showed for the first time that ammonia-nitrogen removal is possible at water temperatures as low as 0.5°C. This led to a major policy shift in Canadian wastewater treatment. With almost 1000 lagoon treatment systems throughout Canada treating wastewater from smaller communities, the regulators and municipalities across Canada and USA started to demand that ammonia be removed from lagoon effluent even in winter, which would be a tremendous boost to sustainability of year-around treatment. This spawned an entirely new approach to treatment of cold lagoon effluents using novel biofilm reactors for ammonia removal. Research was performed on application of moving bed biofilm reactors (MBBR) which are beginning to dominate cold-wastewater treatment due to documented efficiency of ammonia nitrogen removal.

Another invention developed and patented included a system to remove ammonia and nitrates from mainstream cold wastewater using a novel anammox bacterial process. The main stream anammox treatment is a holy grail of wastewater treatment as it does not require supplying carbon to complete the denitrification process. Anammox bacteria remove total nitrogen autotrophically offering the lowest cost of treatment for dilute municipal wastewater streams. Use of moving bed biofilm reactors (MBBR) in pre-nitrification/anammox configuration (PN/A) and ingenious inhibition of rapid conversion of nitrite to nitrate using un-ionized ammonia, proved a resilient process to temperature and wastewater quality variations.

**Di Biase A, T Devlin, M Kowalski, J A Oleszkiewicz (2019) Moving bed biofilm reactor technology in municipal wastewater treatment: A review. *Jour. Environmental Management.* 247:849-866**

The review encompasses the development of municipal wastewater treatment process using MBBR from early stages, established application, and recent advancements. An overview of main drivers leading to the MBBR technology development over its early stage is discussed. Biocarriers types and features together with biofilm development and role of extracellular polymeric substances (EPS) are presented, ultimately, addressing the challenge in decreasing startup time required for full time operation. Furthermore, the review investigates the state of

the art of MBBR technology for nutrient removal (i.e., COD and BOD, nitrogen and phosphorus) through process functionality and configuration of established (e.g. IFAS) and under development (e.g. PN/A) applications. Reactor operational characteristics such as media filling fractions, mixing properties, dissolved oxygen requirements, and loading rates are presented and related to full scale examples. Current literature discussing the most recent studies on MBBR capability in reduction and removal of chemicals of emerging concern (CEC) released is presented. Ultimately, high-rate carbon and nitrogen removal

through A/B stage process are examined in its main operational parameters and its application towards energy neutrality suggesting novel MBBR application to further reduce energy requirements and plant footprint.

**Di Biase A, T Devlin, M Kowalski, JA Oleszkiewicz (2022) Physicochemical methods for biofilm removal allow for control of biofilm retention time in a high-rate MBBR. *Environ.Techn.* 43:10, 1593-1602**

Controlling biofilm retention time in moving bed biofilm reactor (MBBR) and maintaining its performance for A-stage carbon redirection requires a reliable method to use as side stream biocarriers treatment. This paper investigates biofilm detachment and residual biofilm activity under multiple physicochemical treatment scenarios aiming to provide an applicable technique for control of biofilm retention time. Different mixing intensities (i.e. 30–120 rpm), filling fractions (i.e. 20%–100%), and pH (i.e. 2–12) were evaluated. Two continuously operating MBBRs were subjected to pH shocks of 2 and 12 to evaluate the impact of residual acidic or alkaline compounds on performance. The highest solids detachment (i.e.  $70 \pm 5\%$ ) was found in alkaline conditions and independent of mixing intensity and filling fraction. Biofilm detachment test revealed that alkaline shock produced higher detachment levels in a longer exposure time when compared to acidic conditions. The kinetic tests revealed 60% and 90% of the residual biofilm activity was lost at pH 12 and 2. The continuously operating MBBRs subjected to pH shocks of 2 and 12 demonstrated a 50% loss of soluble COD removal capability within one hydraulic retention time. Extracellular polymeric substances changes in its structure and surface properties influencing the degree of biofilm detachment and its solubilization properties leading to differences in biofilm resilience. The findings have shown that by applying a side stream alkali treatment it could be possible to control biofilm retention time ensuring its detachment up to 70% and a reduced impact on the residual biofilm activity returning to the reactor.

**Di Biase A, T Devlin, D Flores-Orozco, R Patidar, M Kowalski, P Jabari, A Kumar, JA Oleszkiewicz (2022) Performance and recovery of nitrifying biofilm after exposure to prolonged starvation *Chemosphere* 290: 133323**

Achieving consistent ammonia removal in post-lagoon processes faces two major challenges impacting nitrifiers due to the unique seasonal variation of lagoon-based systems: summer to winter temperature drop and summer to fall ammonia starvation period while lagoon is removing ammonia. The objective of this study was to follow microbial diversity and define conditions that could overcome these challenges in a post-lagoon moving bed biofilm reactor (MBBR) operated at an initial surface area loading rate (SALR) of  $0.3 \text{ g NH}_4\text{-N/m}^2\text{d}$  from mesophilic (20 °C) to psychrophilic (4 °C). Initially the

temperature was maintained at 20 °C and decreased to 10°C until steady state was achieved. During starvation conditions (i.e., continuous, intermittent and no aeration without inflow; decanted media; and intermittent and continuous ammonia supplement) the temperature was decreased by 2°C per week until 4 °C. The results indicated that operational procedures, such as intermittent ammonia supplement with SALR of 0.15 g NH<sub>4</sub>-N/m<sup>2</sup>d could improve performance with 80% ammonia removal achieved immediately after starvation period. Intermittent ammonia supplement had produced the greatest biofilm preservation comparable to the initial load with the highest specific and surface area removal rates. In the recovery phase (initial load restoration) 10 days were required to reestablish performance above 95% ammonia removal. When temperature was decreased from mesophilic to psychrophilic, the microbial diversity was found higher when starving biofilm compared to the control operated at the initial load while it converged to a similar population over recovery. The main actors associated to nitrification enriched at psychrophilic conditions were *Proteobacteria* and *Bacteroidetes* at phyla level. Ammonia oxidation to nitrite was mainly driven by the order *Burkholderiales* and nitrite oxidation to nitrate by *Pseudomonadales*. This procedure should be considered in the implementation of full-scale post-lagoon MBBR technologies to ensure reliable, robust, and consistent performance despite the inherent seasonal variability of lagoon-based processes.

**Kowalski M, T R Devlin, A di Biase, J A Oleszkiewicz (2019) Controlling cold temperature partial nitrification in moving bed biofilm reactor. *Chemosphere* 227: 216-224**

Mainstream partial nitrification was studied at 10°C in a moving bed biofilm reactor treating synthetic wastewater containing both nitrogen (40 mg/L) and organic carbon at COD/N ratio ranging from 1.3 to 2.2. Three different control strategies were investigated to achieve partial nitrification. Initially, biofilm age was controlled by incorporating a media replacement strategy. Next, separately from the media replacement, oxygen limited conditions were investigated and finally pH control was incorporated together with oxygen limitation. Successful partial nitrification was achieved only by combining oxygen limitation with pH control. The average NH<sub>4</sub>-N concentration was equal to 16.0 ± 1.6 mg/L and average NO<sub>2</sub>-N concentration was equal to 15.7 ± 2.4 mg/L during steady state partial nitrification. The average residual NO<sub>3</sub>-N concentration was equal to 2.6 ± 2.2 mg/L. The results obtained from this study prove for the first time that partial nitrification can be successfully controlled in a biofilm reactor treating wastewater with low nitrogen concentration, relatively high COD/N ratio and at low temperature. An algorithm for dynamic process control of partial nitrification has been also developed.

**Kowalski M, T R Devlin, A di Biase, JA Oleszkiewicz (2019) Effective nitrogen removal in a two-stage partial nitrification-anammox reactor treating municipal wastewater - piloting PN-MBBR/AMX-IFAS. *Bioresource Technology*. 289: October 2019, 121742**

A novel partial nitrification-anammox (PNA) reactor configuration was piloted for 250 days. Primary effluent from full-scale municipal wastewater treatment plant was treated in a two-stage biofilm system incorporating innovative process control for cold partial nitrification. Partial nitrification was combined with carbon removal in a moving bed biofilm reactor (MBBR) to achieve high-rate treatment and nitrification was obtained with dissolved oxygen to total ammonium nitrogen (DO/TAN) ratio control and free ammonia (FA) for inhibition of nitrification.

Effluent from MBBR was directed to an integrated fixed-film activated sludge (IFAS) reactor where nitrogen was removed via anammox. MBBR achieved partial nitrification at  $2.0 \pm 0.3$  g N/m<sup>2</sup>d and nitrogen removal in the IFAS reactor reached  $0.45 \pm 0.1$  g N/m<sup>2</sup>d ( $55$  g N/m<sup>3</sup>d). The process performed well at  $19 \pm 3$  °C with an average effluent total inorganic nitrogen (TIN) concentration of  $11 \pm 4$  mg/L.

## Health Inequity, Disease Biology, and Prostate Cancer

by William Nelson, Member EUAS



### Short Biography

*Dr. Nelson serves as the Marion I. Knott Professor of Oncology and Director of the Sidney Kimmel Comprehensive Cancer Center at Johns Hopkins. He is also a Professor of Medicine, Pharmacology, Pathology, Radiation Oncology, Urology, and Environmental Health Sciences. He arrived at Johns Hopkins after securing an undergraduate degree in Chemistry at Yale University, and went on to earn doctoral degrees in Pharmacology and in Medicine at the Hopkins School of Medicine. He also completed Internship and Residency training in Internal Medicine and a Fellowship in Medical Oncology at the Johns Hopkins Hospital. .*

*Dr. Nelson's research has focused on cancer epigenetics and on prostate cancer development. He has now authored some 328 articles and book chapters, attracting >40,000 citations with an h-index of 106. He also has secured 12 issued patents from the US Patent and Trade Office, and has conducted some 95 podcast interviews. He currently serves on the Board of the V Foundation, as a Scientific Co-Chair for Stand Up 2 Cancer, as Chair of the Board for Break Through Cancer, and on the Scientific Advisory Board for the Prostate Cancer Foundation. He is also the Executive Editor of Cancer Today and a Senior Editor of Cancer Research.*

### **Health Inequity and Disparities in Prostate Cancer Outcomes between African American Men and European Men in the United States**

Despite the high incidence and prevalence of the prostate cancer among aging men in the United States (US), outcomes from the disease remain undermined by health inequities: Black men show a 1.78-fold higher incidence and a 2.2-fold higher mortality for prostate cancer than non-Hispanic White men. This difference, comprising the largest disparity for any common cancer in the US, has been variously attributed to inheritance, to diet and lifestyle, and to unequal access to high-quality treatment<sup>1,2</sup>.

Inherited susceptibility to prostate cancer is supported by classic twin

studies<sup>3</sup>. *HOXB13*, encoding a homeobox transcription factor that interacts with the androgen receptor, affects prostate cancer risk<sup>4,5</sup>. Different *HOXB13* founder mutations are associated with prostate cancer in men with different ancestries: *G84E* for men with European ancestry, *G132E* for Japanese men<sup>6</sup>, *G135E* for Chinese men<sup>7</sup>, and *HOXB13 X285K* for men of African descent in Martinique<sup>8</sup>. Aberrations at the DNA repair genes *BRCA1*, *BRCA2*, and *ATM* appear in as many as 19.3% of metastatic castration-resistant prostate cancers (CRPCs), more frequently in Black men than in White men<sup>9,10</sup>. Finally, a high-risk prostate cancer allele at chromosome 8q24 near a *MYC* enhancer appears present in 30% of Black men but only 13% of White men; the population-attributable risk (PAR) of this allele for Black men has been estimated to be 16%<sup>11</sup>.

Diet and lifestyle together exert a dominant influence on prostatic carcinogenesis, historically demonstrated by migrant studies showing adoption of risk upon moving to high-risk regions in the world<sup>12</sup>. Fat intake, particularly animal fat from red meats, increases prostate cancer risk, while consumption of tomatoes, soy, and other vegetables likely protects against the disease<sup>13-16</sup>. Food preparation, such as overcooking of meats leading to heterocyclic aromatic amine (HAA) carcinogen formation, may also drive prostatic carcinogenesis<sup>17</sup>. In the US, Black men in low-income urban neighborhoods have limited access to healthy foods and are prone to overconsume food that is less nutritious and of higher caloric density<sup>18</sup>. Physical activity, which could offset the high caloric intake, is difficult in urban areas with high poverty rates<sup>19</sup>.

The critical driver of prostate cancer is chronic prostatic inflammation, spawning proliferative inflammatory atrophy (PIA), a precursor to prostatic intraepithelial neoplasia (PIN) and prostate cancer. PIA lesions, which exhibit molecular features of cell and genome damage stress, appear before prostate cancer in nearly all rodent models of the disease induced by exposures, including estrogens and dietary carcinogens<sup>20</sup>. PIA lesions characteristically elaborate inflammatory cytokines, like IL-1, IL-6, and IL-8<sup>21,22</sup>. Mice engineered to produce IL-1 in the prostate manifest epithelial changes reminiscent of human PIA<sup>22</sup>.

Prostate cancers accumulate many somatic genome and epigenome alterations as the disease progresses to threaten life<sup>23,24</sup>. The most consistent changes are (i) *MYC* activation, (ii) telomere shortening, (iii) increased DNA methylation at critical genes such as *GSPT1*, (iv) rearrangements involving ETS family transcription factors, (v) loss of *PTEN*, (vi) *SPOP* mutations, and (vii) *TP53* mutations. Most of these defects are shared between prostate cancers from Black versus White men<sup>25</sup>. Nonetheless, many reports highlight potential differences segregating with self-reported race. The most striking discordance may be the lower frequencies of *TMPRSS2-ERG* rearrangements,

*PTEN* deletions, and *SPOP* mutations in prostate cancers from Black men<sup>26-28</sup>. More recently, differences in hypermethylation at the *GSTP1* promoter causing loss of *GSTP1* expression, the earliest and most frequent gene function defect in prostate cancer<sup>29</sup>, were reported, with retained *GSTP1* expression seen in a greater number of cases from Black men (9.5%) versus White men (3.2%)<sup>30</sup>.

Insights into the impact of inheritance, the environment, and sociology on prostate cancer incidence and mortality have converged on a unified mechanism: diet and lifestyle promote prostate inflammation, generating PIA lesions that can give rise to prostatic adenocarcinomas. Genetic predisposition, particularly variants in genes for genome damage and repair or for cell and tissue damage and regeneration, further amplifies these stresses. The resultant gene-environment interactions, fueled by inequities resulting from poverty and a history of racism, drives prostatic carcinogenesis disproportionately among men of color. Remarkably, when prostate cancers are treated at a Veterans Health Administration facility or as part of a clinical trial, Black men and White men exhibit similar outcomes when receiving the same treatment for the same stage of disease<sup>31-33</sup>. Also, though Black men suffered worse prostate cancer-specific survival than White men in a study in Detroit, MI, adjustment for socioeconomic status (SES) eliminated the survival differences<sup>34</sup>.

All of what is now known about prostate cancer suggests that disparities in prostate cancer incidence and mortality for Black versus White men in the US likely reflect social determinants of health and health equity, which must be better addressed to improve disease outcomes<sup>35</sup>. Prostate cancer risk reduction through healthier dietary practices, and improvements in prostate cancer screening, detection, diagnosis, and treatment via incorporation of new technologies like germline gene testing and risk stratification, should all be implemented in such a way as to reduce inequities associated with race/ethnicity and socioeconomic status.

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# Stunted Children Display Ectopic Small Intestinal Colonization by Oral Bacteria

by B. Brett Finlay, Member EUAS



## Short Biography

*Dr. B. Brett Finlay is a Professor in the Michael Smith Laboratories, and the Departments of Biochemistry and Molecular Biology, and Microbiology and Immunology at the University of British Columbia. He obtained a B.Sc. (Honors) in Biochemistry at the University of Alberta, where he also did his Ph.D. (1986) in Biochemistry under Dr. William Paranchych, studying F-like plasmid conjugation. His post-doctoral studies were performed with Dr. Stanley Falkow at the Department of Medical Microbiology and Immunology at Stanford University School of Medicine, where he studied Salmonella invasion into host cells. In 1989, he joined UBC as an Assistant Professor in the Biotechnology Laboratory. Dr. Finlay's research interests are focussed on host-microbe interactions, at the molecular level. By combining cell biology with microbiology, he has been at the forefront of the field called Cellular Microbiology, making several fundamental discoveries in this area, and publishing over 525 papers (h index=140). His laboratory studies several pathogenic bacteria, including Salmonella and pathogenic E. coli, and more recently microbiota. He is well recognized internationally for his work, and has won several prestigious awards including the E.W.R. Steacie Prize, the CSM Fisher Scientific Award, CSM Roche Award, a MRC Scientist, five Howard Hughes International Research Scholar Awards, a CIHR Distinguished Investigator, BC Biotech Innovation Award, the Michael Smith Health Research Prize, the IDSA Squibb award, the Jacob Biely Prize, the prestigious Canadian Killam Health Sciences Prize, the Flavelle Medal of the Royal Society, the Queen Elizabeth II Diamond Jubilee Medal, the Prix Galien, is a Fellow of the Royal Society of Canada and the Canadian Academy of Health Sciences, is a Member of the German National Academy of Sciences, the European Union Academy of Sciences, the American Academy of Microbiology, Chair d'État, Collège de France and is the UBC Peter Wall Distinguished Professor. He is an Officer of the Order of Canada and Order of British Columbia, and inducted into the Canadian Medical Hall of Fame. He is a cofounder of Inimex Pharmaceuticals, Inc. and Microbiome Insights, scientific cofounder of Vedanta Pharmaceuticals and CommenSe, Director of the SARS Accelerated Vaccine Initiative, and Founding Director and Senior Fellow of CIFAR's Microbes and Humans. He is also the co-author of the books Let Them Eat Dirt and The Whole Body Microbiome.*

## **Contributions to Science**

1. Role of the microbiota in brain diseases. We have begun studies to look at the effect of microbes on healthy brain function, and in the context of Parkinson's Disease, Alzheimer's, dementia, depression, anxiety and stress. We are using a combination of testing microbiota in clinical cohorts of patients and controls to look for dysbiosis. We are also developing in vitro model systems (such as blood-brain barriers) to probe the effects

of microbes on brain health.

2. Role of the microbiota in malnutrition and environmental enteropathy (EE). We developed the first animal model for malnutrition and associated EE and have been using this model to explore the mechanisms behind these problems. We have shown that particular fecal microbiota species, as well as diet, are critical for these events. We have also found that these symptoms affect brain development and cognitive functions. We are continuing to explore this model, including testing various preventative and therapeutic treatments to improve these problems.

3. Role of the microbiota in allergic diseases. We have been probing the role of the microbiota in immune development, and how it affects allergic responses, especially in asthma. By using antibiotics and a murine model, we showed that the microbiota can have profound effects on asthma development, and which microbial species are responsible for this, as well as the host immune responses. We have extended this work to a pediatric clinical cohort study, monitoring the fecal microbiota in several thousand children from birth to age 5, and showed that specific microbes early in life influence asthma susceptibility. By comparing cohorts in Canada and Ecuador, we have shown that different microbes in different geographical areas mediate this, and that fungi also play a key role in these interactions.

4. Role of microbiota in enteric infectious diseases. We have been addressing the interplay between the microbiota and the bacterial pathogens *Salmonella* and *E. coli* during enteric infectious diseases. We have made seminal findings in this area to indicate that the microbiota composition plays a significant role in susceptibility and resistance to enteric diseases. We are currently characterizing the interactions between pathogens and the microbiota and establishing microbiota compositions that increase and decrease resistance to disease as well as studying the shifts of population that occur during inflammatory diseases including inflammatory bowel disease. This work will further help us to understand the interplay between the host, the pathogen and the microbiota during infectious diseases.

5. Enteropathogenic and enterohemorrhagic *E. coli*. Enteropathogenic and enterohemorrhagic *E. coli* (EPEC and EHEC) belong to a family of pathogens that adhere to intestinal cells, causing effacement of microvilli, and a pedestal to form beneath adherent bacteria. We have been studying the molecular events associated with this process and examining its role in disease. Some of the areas of study include defining the signals that are activated in epithelial cells that are necessary for infection. We have shown that a small number of secreted bacterial proteins are key to forming pedestals, and that these proteins are secreted by a type III secretion system. We are studying these secreted proteins and defining how they are inserted into the host cell, and how they interface with host cell signaling, immune responses, and mitochondrial effects. This includes extensive use of proteomics and other systems biology tools. We use murine infection models to study the events associated with disease to determine if the events characterized in vitro actually occur in vivo. Finally, we are trying to relate the role of these events to production of disease, and identify methods (inhibitors, vaccines) to combat disease.

### **Stunted children display ectopic small intestinal colonization by oral bacteria which cause lipid malabsorption in experimental models.**

Vonaesch P, Araújo JR, Gody JC, Mbecko JR, Sanke H, Andrianonimiadana L, Naharimanananirina T, Ningatoloum SN, Vondo SS, Gondje PB, Rodriguez-Pozo A,

Rakotondrainipiana M, Kandou KJE, Nestoret A, Kapel N, Djorie SG, **Finlay BB**, Wegener Parfrey L, Collard JM, Randremanana RV, Sansonetti PJ; Afribiota Investigators. *Proc Natl Acad Sci U.S.A.* 2022 Oct 11;119(41)

### **Abstract**

Environmental enteric dysfunction (EED) is an inflammatory syndrome postulated to contribute to stunted child growth and to be associated with intestinal dysbiosis and nutrient malabsorption. However, the small intestinal contributions to EED remain poorly understood. This study aimed to assess changes in the proximal and distal intestinal microbiota in the context of stunting and EED and to test for a causal role of these bacterial isolates in the underlying pathophysiology. We performed a cross-sectional study in two African countries recruiting roughly 1,000 children aged 2 to 5 years and assessed the microbiota in the stomach, duodenum, and feces. Upper gastrointestinal samples were obtained from stunted children and stratified according to stunting severity. Fecal samples were collected. We then investigated the role of clinical isolates in EED pathophysiology using tissue culture and animal models. We find that small intestinal bacterial overgrowth (SIBO) is extremely common (>80%) in stunted children. SIBO is frequently characterized by an overgrowth of oral bacteria, leading to increased permeability and inflammation and to replacement of classical small intestinal strains. These duodenal bacterial isolates decrease lipid absorption in both cultured enterocytes and mice, providing a mechanism by which they may exacerbate EED and stunting. Further, we find a specific fecal signature associated with the EED markers fecal calprotectin and alpha-antitrypsin. Our study shows a causal implication of ectopic colonization of oral bacterial isolated from the small intestine in nutrient malabsorption and gut leakiness in vitro. These findings have important therapeutic implications for modulating the microbiota through microbiota-targeted interventions.

### **Gastric acid and escape to systemic circulation represent major bottlenecks to host infection by *Citrobacter rodentium*.**

Woodward SE, Vogt SL, Peña-Díaz J, Melnyk RA, Cirstea M, Serapio-Palacios A, Neufeld LMP, Huus KE, Wang MA, Haney CH, **Finlay BB**. *ISME J.* 2022 Sep 24

### **Abstract**

The gastrointestinal (GI) environment plays a critical role in shaping enteric infections. Host environmental factors create bottlenecks, restrictive events that reduce the genetic diversity of invading bacterial populations. However, the identity and impact of bottleneck events on bacterial infection are largely unknown. We used *Citrobacter rodentium* infection of mice, a model of human pathogenic *Escherichia coli* infections, to examine bacterial population dynamics and quantify bottlenecks to host colonization. Using Sequence Tag-based Analysis of Microbial Populations (STAMP) we characterized the founding population size ( $N_b'$ ) and relatedness of *C. rodentium* populations at relevant tissue sites during early- and peak-infection. We demonstrate that the GI environment severely restricts the colonizing population, with an average  $N_b'$  of only 12-43 lineages (of 2,000+ inoculated) identified regardless of time or biogeographic location. Passage through gastric acid and escape to the systemic circulation were identified as major bottlenecks during *C. rodentium* colonization. Manipulating such events by increasing gastric pH

dramatically increased intestinal Nb'. Importantly, removal of the stomach acid barrier had downstream consequences on host systemic colonization, morbidity, and mortality. These findings highlight the capability of the host GI environment to limit early pathogen colonization, controlling the population of initial founders with consequences for downstream infection outcomes.

### **Longitudinal Body Mass Index Trajectories at Preschool Age: Children with Rapid Growth have Differential Composition of the Gut Microbiota in the First Year of Life.**

Reyna M, Petersen C, Dai D, Dai R, Becker A, Azad M, Miliku K, Lefebvre D, Moraes T, Mandhane P, Boutin R, **Finlay BB**, Simons E, Kozyrskyj A, Lou W, Turvey S, Subbarao P. *Int J Obes (Lond)*. 2022 Jul

#### **Abstract**

**Background/objective:** The steep rise in childhood obesity has emerged as a worldwide public health problem. The first 4 years of life are a critical window where long-term developmental patterns of body mass index (BMI) are established and a critical period for microbiota maturation. Understanding how the early-life microbiota relate to preschool growth may be useful for identifying preventive interventions for childhood obesity. We aim to investigate whether longitudinal shifts within the bacterial community between 3 months and 1 year of life are associated with preschool BMI z-score trajectories.

**Methods:** BMI trajectories from birth to 5 years of age were identified using group-based trajectory modeling in 3059 children. Their association with familial and environmental factors were analyzed. Infant gut microbiota at 3 months and 1 year was defined by 16S RNA sequencing and changes in diversity and composition within each BMIz trajectory were analyzed.

**Results:** Four BMIz trajectories were identified: low stable, normative, high stable, and rapid growth. Infants in the rapid growth trajectory were less likely to have been breastfed, and gained less microbiota diversity in the first year of life. Relative abundance of Akkermansia increased with age in children with stable growth, but decreased in those with rapid growth, abundance of Ruminococcus and Clostridium at 1 year were elevated in children with rapid growth. Children who were breastfed at 6 months had increased levels of Sutterella, and decreased levels of Ruminococcus and Clostridium.

**Conclusion:** This study provides new insights into the relationship between the gut microbiota in infancy and patterns of growth in a cohort of preschool Canadian children. We highlight that rapid growth since birth is associated with bacteria shown in animal models to have a causative role in weight gain. Our findings support a novel avenue of research targeted on tangible interventions to reduce childhood obesity.

### **Effects of gut microbiota alterations on motor, gastrointestinal, and behavioral phenotype in a mouse model of Parkinson's disease.**

Radisavljevic N, Cirstea M, Bauer K, Lo C, Metcalfe-Roach A, Bozorgmehr T, Bar-Yoseph H, **Finlay BB**. *J Parkinsons Dis*. 2022 Mar 10;12(5):1479-1495.

#### **Abstract**

**Background:** Parkinson's disease (PD) is a multi-system disorder consisting of not only classic motor symptoms but also a variety of non-motor symptoms including gastrointestinal (GI) dysfunction and mood disorders. The gut microbiota has been suggested to play a role in modulating PD motor and non-motor features, although the causality and mechanisms behind these proposed interactions remains largely understudied.

**Objective:** In this study, we aimed to provide in-depth characterization of an established mouse model of PD (transgenic (TG) SNCA A53T) and experimentally address how changes to the gut microbiota impact the PD-like phenotype.

**Methods:** We profiled the PD-like phenotype of transgenic mice through a panel of motor, GI, and behavioral tests. We then investigated how antibiotic treatment or gut microbial community transfer (via cohousing with wild-type mice) impacted the PD-like phenotype.

**Results:** We found that this mouse model demonstrated early (6 weeks of age) motor symptoms when compared to a wild-type control mouse strain. Transgenic mice also exhibited early GI dysfunction, as well as behavioral alterations, including reduced anxiety-like behavior, and increased depression-like and apathy-like behavior. Compared to wild-type mice, the transgenic fecal microbiota was less diverse and compositionally distinct. Interestingly, drastic alterations to the gut microbiota, through antibiotic treatment or cohousing with wild-type mice, had a minimal effect on the motor, GI, and behavioral phenotype of transgenic mice.

**Conclusion:** We concluded that this mouse model effectively recapitulates motor and non-motor features of PD; however, the gut microbiota appears to exhibit a minor impact on the pathophysiology of this PD model.

## **The Oral and Fecal Microbiota in a Canadian Cohort of Alzheimer's Disease.**

Cirstea M, Kliger D, MacLellan A, Yu A, Langlois J, Fan M, Boroomand S, Kharazyan F, Hsiung R, MacVicar B, Chertkow H, Whitehead V, **Finlay B**, Appel-Cresswell S. **J Alzheimers Dis.** 2022 Mar 7.

### **Abstract**

**Background:** Despite decades of research, our understanding of Alzheimer's disease (AD) etiology remains incomplete. In recent years, appreciation has grown for potential roles for the microbiota in shaping neurological health.

**Objective:** This study aimed to examine associations between the microbiota and AD in a human cross-sectional cohort.

**Methods:** Forty-five AD patients and 54 matched controls were recruited in Vancouver, Canada. Fecal and oral samples underwent 16S microbiota sequencing. A wide array of demographic and clinical data were collected. Differences between participant groups were assessed, and associations between microbes and clinical variables were examined within the AD population.

**Results:** The gut microbiota of AD patients displayed lower diversity relative to controls, although taxonomic differences were sparse. In contrast, the AD oral microbiota displayed higher diversity, with several taxonomic differences relative to controls, including a lower abundance of the families Streptococcaceae and Actinomycetaceae, and a higher abundance of Weeksellaceae, among others. The periodontitis-associated oral microbe *Porphyromonas gingivalis* was 5 times more prevalent among patients. No significant

associations between gut or oral microbes and cognition were detected, but several correlations existed between microbes and mood disorders and BMI among patients, including a strong positive correlation between Alphaproteobacteria and depression score. Conclusion: The gut microbiota of AD patients was not overtly different from controls, although it displayed lower diversity, an overall marker of microbiota health. The oral microbiota did display marked differences. Cognition was not associated with a microbial signature, but other relevant AD factors including mood and BMI did demonstrate an association.

### **Gut Microbiome in Parkinson's Disease: New Insights from Meta-Analysis.**

Toh TS, Chong CW, Lim SY, Bowman J, Cirstea M, Lin CH, Chen CC, Appel-Cresswell S, Finlay BB, Tan AH. *Parkinsonism Relat Disord.* 2022 Jan;94:1-9.

#### **Abstract**

Background: Gut microbiome alterations have been reported in Parkinson's disease (PD), but with heterogeneous findings, likely due to differences in study methodology and population. We investigated the main microbiome alterations in PD, their correlations with disease severity, and the impact of study and geographical differences. Methods: After systematic screening, raw 16S rRNA gene sequences were obtained from ten case-control studies totaling 1703 subjects (969 PD, 734 non-PD controls; seven predominantly Caucasian and three predominantly non-Caucasian cohorts). Quality-filtered gene sequences were analyzed using a phylogenetic placement approach, which precludes the need for the sequences to be sourced from similar regions in the 16S rRNA gene, thus allowing a direct comparison between studies. Differences in microbiome composition and correlations with clinical variables were analyzed using multivariate statistics. Results: Study and geography accounted for the largest variations in gut microbiome composition. Microbiome composition was more similar for subjects from the same study than those from different studies with the same disease status. Microbiome composition significantly differed between Caucasian and non-Caucasian populations. After accounting for study differences, microbiome composition was significantly different in PD vs. controls (albeit with a marginal effect size), with several distinctive features including increased abundances of *Megasphaera* and *Akkermansia*, and reduced *Roseburia*. Several bacterial genera correlated with PD motor severity, motor response complications and cognitive function. Conclusion: Consistent microbial features in PD merit further investigation. The large variations in microbiome findings of PD patients underscore the need for greater harmonization of future research, and personalized approaches in designing microbial-directed therapeutics.

# Plastic Strain-Induced Phase Transformations Under High Pressure: Four-Scale Theory, Experiments and Phenomena

by Valery I. Levitas, Member EUAS



## Short Biography

### **Valery I. Levitas**

*Anson Marston Distinguished Professor in Engineering*

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### **Education and Training:**

*Kiev Polytechnic Institute, Kiev, USSR Mechanical Engineering M.S. (Honors), 1978*

*Institute for Superhard Materials, Kiev, USSR Materials Science Ph.D., 1981*

*Ins. Electronic Machinebuilding, Moscow, USSR Continuum Mechanics Dr. of Sci., 1988*

*University of Hannover, Germany Continuum Mechanics Doctor-Engineer habil., 1995*

### **Appointments**

*08.08-present Anson Marston Distinguished Professor in Engineering (2018, permanent); Vance Coffman Faculty Chair Professor (17-), Schafer 2050 Challenge Professor (08-17), Dept. Aerospace Engineering, Dept. Mechanical Engineering; Dept. Material Science and Engineering, Iowa State University; Faculty Scientist, Ames Labor.*

*08.02-present Associate Professor (99-02), Professor (02-08)*

*Lubbock, TX, Department of Mechanical Engineering.*

*08.14-12.14 Visiting Scholar, NIST and Geophysical Lab., Carnegie Institution of Washington.*

*01.05-05.05 Visiting Scholar, Los Alamos National Labs, Los Alamos, NM.*

*08.93 -08.99 Humboldt–Research Fellow (93-95), Visiting & Research Professor (95-99),*

*University of Hannover, Inst. Structural & Computational Mechanics, Hannover, Germany.*

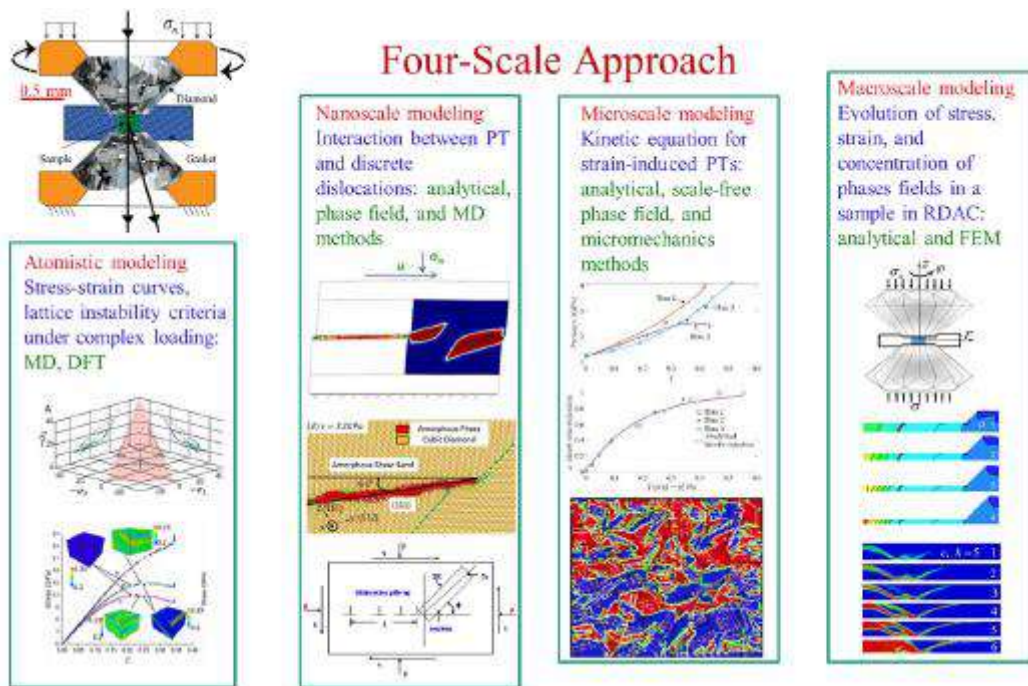
*04.78–08.94 Engineer (78-81), Junior Researcher (81-84), Senior Researcher (84–88), Leading Researcher (89–94); Leader of research group (82–94), Ins. for Superhard Materials of the Ukrainian Academy of Sciences, Kiev, Ukraine.*

*Consultant: Los Alamos National Labs; NIST; Geophysical Laboratory, Carnegie Institution of Washington; Ins. for Superhard Materials (Kiev); Seyeon E&S corporation (Daejeon, South Korea).*

**Products:** *461 publications, including 291 refereed journal papers, 3 books, 11 book chapters and 11 patents; more than 11,000 citations, H-index - 62.*

**Plastic Strain-Induced Phase Transformations Under High Pressure: Four-Scale Theory, Experiments and Phenomena**

High-pressure phase transformations (PTs) are usually studied in a diamond anvil cell (DAC) within or without hydrostatic media (gas or liquid). While without hydrostatic media, PTs occur during the plastic deformation of materials, they were characterized in terms of pressure only. We introduced a new concept of plastic strain-induced PTs under high pressure rather than pressure-induced PTs [1-3]. Pressure- and stress-induced PTs start at crystal defects that naturally exist in material and when stresses do not reach the yield limit. These defects (e.g., various dislocation structures or grain boundaries) produce stress concentrators and serve as nucleation sites for a phase transformation. First, nucleation occurs at defects with the strongest stress concentration; pressure should then be increased to cause nucleation at defects with decreasing levels of generated stresses. An overview for analysis and characterization of the pressure-induced and stress-tensor-induced PTs can be found in [2].



**Fig. 1** Schematic of RDAC (top left) and four-scale approaches to modeling the plastic strain-induced phase transformations under high pressure.

Plastic strain-induced PTs take place by nucleation and limited growth at defects produced in the course of plastic straining. The largest stress concentration can be produced at the tip of the dislocation pileups. Indeed, all stress components (and, consequently, pressure) are proportional to the number N of dislocations in a pileup. Since N=10-100, local stresses could be huge and can be increased by growing

plastic deformation at relatively low pressure, thus driving phase transformations. The important point is that the deviatoric (nonhydrostatic) stresses near the defect tip are not bounded by the engineering yield strength but rather by the ideal strength in shear for a defect-free lattice, which may be larger by a factor of 10 to 100. Local stresses of such magnitude may result in the nucleation of the high-pressure phase at an applied pressure that is not only significantly lower than that under hydrostatic loading but also below the phase-equilibrium pressure. In addition, such highly-deviatoric stress states with large stress magnitudes cannot be realized in bulk. Such unique stresses may lead to PTs into stable or metastable phases that were not or could not be attained in bulk under hydrostatic or quasi-hydrostatic conditions. It was concluded [1-3] that plastic strain-induced transformations require very different thermodynamic, kinetic, and experimental treatments than pressure- and stress-induced transformations.

The most direct way to study plastic strain-induced PTs is under compression and shear in rotational DAC (RDAC), in which, after compression, one of the anvils rotates with respect to another. The superposition of plastic shear leads to numerous mechanochemical phenomena, including reducing PT pressure by one to two orders of magnitude and the appearance of new phases [1-7]. Thus, plastic straining reduced PT pressure from graphite-like boron nitride to superhard diamond-like boron nitride by order of magnitude [4,5] and from graphite to diamond from 70 GPa to 0.7 GPa, i.e., by two orders of magnitude [6]. These could be precursors of new defect-induced technologies of synthesis of superhard materials, at room temperature, without catalyst, and at low pressure. The new high-density amorphous phase of SiC was revealed under pressure and shear [8]. It is important since amorphization is the main damage mechanism of armor ceramics. Since this PT is reversible, the only way to detect it is to perform in situ study.

In situ x-ray diffraction with synchrotron radiation experiments [7] provide the evolution of distributions of pressure in each phase, the concentration of high-pressure phases, grain size, as well as sample thickness profile. Their postprocessing leads to various important discoveries. Thus, it was found for  $\alpha$ - $\omega$  PT in severely predeformed Zr [7] that the minimum pressure for strain-induced PT is independent of the plastic strain tensor and its entire path. This means that, in contrast to the existing view, strain-induced PTs can be studied under compression in traditional DAC. However, in DAC, pressure grows during compression. In contrast, in RDAC, one can produce strain-induced PT at almost constant pressure close to the minimum pressure for PT. It was proven earlier [9] for more than 60 materials (simple metals and alloys, minerals, oxides, etc.) that, for monotonous and quasi-monotonous loadings and plastic strain exceeding a certain critical value, the initially-isotropic polycrystals deform as the perfectly plastic (i.e., without strain hardening or softening) and isotropic material with a strain tensor- and strain tensor path-independent limiting surface of the perfect plasticity.

To explain the above phenomena, a four-scale theory was developed, and

corresponding simulations were performed (see the first analytical three-scale theory [1] and review [3]). Molecular dynamic [10,11] and first-principle [12] simulations were used to determine lattice instability conditions under all six components of the stress tensor. At the nanoscale and microscale, nucleation at various evolving dislocation configurations was studied utilizing developed nanoscale [13,14] and scale-free [15,16] phase-field approaches. The possibility of reducing PT pressure by more than an order of magnitude due to stress concentration at the shear-generated dislocation pileup is proven. At the microscale, a strain-controlled kinetic equation was derived [1] and utilized in the large-strain macroscopic theory for coupled PTs and plasticity [17,18]. At the macroscale, the behavior of the sample in DAC/RDAC is studied using the finite element approach [17,18]. Various experimental effects are reproduced. The first experimental calibration and confirmation of the strain-controlled kinetics [1] were obtained for  $\alpha$ - $\omega$  PT in Zr [7]. The obtained results offer a new fundamental understanding of strain-induced PTs under high pressure in DAC/RDAC and methods of controlling PTs and searching for new high-pressure phases. They can be applied to various other pressure-shear processes, e.g., in geophysics, during friction, high-pressure torsion, cutting, polishing, armor penetration, and ball milling, among many others. In particular, the suggested theory resolves the main puzzles of the PT-based mechanism of the deep-focus earthquake [19]. During the above studies, various new phenomena have been discovered and utilized. For example, predicting PT induced by a rotational plastic instability phenomenon allowed us to reduce the transformation pressure for obtaining superhard BN by a factor of 10 (from 55 to 5.6 GPa) [4]. Analytical prediction of singular transformation-induced plasticity (TRIP) in a shear band and self-blown-up PT-TRIP-heating phenomena have been utilized to resolve the main puzzles of the deep-focus earthquake [19].

More general aspects of our works on the interaction between plasticity, PTs, chemical reactions, and fracture are reviewed in [20,21]. They include, in particular, new thermodynamic, kinetic, and phase field approaches to PTs, dislocations, and their interaction; to fracture and its interaction with PTs; to solid-solid PTs and fracture via intermediate (or virtual) melting significantly below the melting temperature; various surface and nanoscale effects in PTs and fracture; and reaction-induced plasticity (RIP).

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## Improved Modeling of Fluid Flow in Porous Media

by Russell Johns, Member EUAS

### Short Biography

*Russell T. Johns is the George E. Trimble Chair of Energy and Mineral Sciences at the Department of Energy and Mineral Engineering at The Pennsylvania State University. He recently served as Chair of the Petroleum and Natural Gas Engineering Program from 2015 to 2018, Distinguished SPE Lecturer for 2019 – 2020, and Editor-In-Chief for all SPE technical journals from 2018 - 2020.*

*Prior to his current position, he served on the petroleum engineering faculty at The University of Texas at Austin from 1995 to 2010. He also has nine years of industrial experience as a petrophysical engineer with Shell Oil and as a hydrogeologist for Colenco Power Consulting in Baden, Switzerland. He holds a BS degree in electrical engineering from Northwestern University and MS and PhD degrees in petroleum engineering and water resources from Stanford University. He has over 250 publications in enhanced oil recovery, thermodynamics and phase behavior, unconventional gas engineering, multiphase flow in porous media, water resources, and well testing. Dr. Johns received the SPE Ferguson medal in 1993, the Society of Petroleum Engineers (SPE) Distinguished Member award in 2009, the SPE Faculty Pipeline award in 2013, the 2016 SPE international award in Reservoir Description and Dynamics, the Wilson Excellence in Research award from the College of Earth and Mineral Sciences in 2018, and the prestigious IOR Pioneer Award from SPE in 2022. He is currently director of the Enhanced Oil Recovery consortium in the EMS Energy Institute at Penn State University.*

*The research group of Dr. Johns is noted for its development of the first flash calculation algorithm for microemulsion phases where all Winsor regions (single, two, and three-phase) are modelled simultaneously. His group is also recently recognized as developing state function theory of relative permeability to fit experimental data and predict relative permeabilities away from that data set. As a part of that research, they developed an analytical function that includes connectivity (Euler number) in the relative permeability model. Finally, his group has been recognized as a leader in developing miscibility theory for gas injection applications such as injection of carbon dioxide into oil reservoirs. They developed analytical theory for solving hyperbolic equations to predict the minimum miscibility pressure (MMP) for any number of components.*

*Dr. Johns currently teaches required undergraduate courses in secondary recovery and pressure transient analysis, along with a required graduate course in thermodynamics. He is a member of numerous Penn State and professional committees. Selected abstracts from publications this year from his group are included below.*

### **Modeling of High-Pressure and High-Temperature Microemulsion Experiments using HLD-NAC-Based Equation of State**

D. Magzymov, Johns, R.T., Hashim, H., and Dindoruk, B.

SPEJ (2022)

### **Abstract**

Surfactant flooding is a promising technique that can reduce interfacial tension (IFT) between oil and water to ultralow values, mobilizing previously trapped oil. For reservoirs at moderate to high pressures, understanding and modeling how pressure affects the phase behavior of a surfactant-brine-oil system is important to the design and implementation of an efficient/cost-effective surfactant flooding project. Typically, however, phase behavior experiments and models of that phase behavior are made only at low pressures. The main objective of this paper is to show how to model experimental data in a unified way for a large range of pressure, temperature, and other parameters, using hydrophilic-lipophilic deviation (HLD) and net-average curvature (NAC)-based equation-of-state (EOS).

Pressure and temperature scans show that pressure has a significant effect on the surfactant microemulsion phase behavior, shifting it from an optimal three-phase system at low pressure to a nonoptimal two-phase system at high pressure. Further, multiple scans at different water/oil ratios (WORs) show a shift in the optimum indicating that phase behavior partitioning of the various components is changing with oil saturation. We obtained good fits of all experimental data including all two- and three-phase regions using a single tuned HLD-NAC EOS for a wide range of simultaneous variations in pressure, temperature, salinity, and overall composition. Such a simultaneous match and prediction by a single set of model parameters has never been done before. We also demonstrate the type of data needed for an accurate EOS. When input into a numerical simulator, the tuned EOS improves the predictions of the resulting phase behavior (size and shape of the two-phase lobes and three-phase regions) and IFTs with changing pressure, temperature, salinity, WORs, and surfactant/alcohol concentrations.

### **Sensitivity Analysis of Fluid–Fluid Interfacial Area, Phase Saturation and Phase Connectivity on Relative Permeability Estimation Using Machine Learning Algorithms**

S. Mukherjee and Johns, R.T.

Energies (2022)

### **Abstract**

Recent studies have shown that relative permeability can be modeled as a state function which is independent of flow direction and dependent upon phase saturation (S), phase connectivity (X), and fluid–fluid interfacial area (A). This study evaluates the impact of each of the three state parameters (S, X, and A) in the estimation of relative permeability. The relative importance of the three state parameters in four separate quadrants of S-X-A space was evaluated using a machine learning algorithm (out-of-bag predictor importance method). The results

show that relative permeability is sensitive to all the three parameters,  $S$ ,  $X$ , and  $A$ , with varying magnitudes in each of the four quadrants at a constant value of wettability. We observe that the wetting-phase relative permeability is most sensitive to saturation, while the non-wetting phase is most sensitive to phase connectivity. Although the least important, fluid–fluid interfacial area is still important to make the relative permeability a more exact state function.

### **Inclusion of variable characteristic length in microemulsion flash calculations**

D. Magzymov and Johns, R.T.

Computational Geosciences (2022)

#### **Abstract**

Recent developments in predicting microemulsion phase behavior for use in chemical flooding are based on the hydrophilic-lipophilic deviation (HLD) and net-average curvature (NAC) equation-of-state (EoS). The most advanced version of the HLD-NAC EoS assumes that the three-phase micelle characteristic length is constant as parameters like salinity and temperature vary. In this paper, we relax this assumption to improve the accuracy and thermodynamic consistency of these flash calculations. We introduce a variable characteristic length in the three-phase region based on experimental data that is monotonic with salinity or other formulation variables, such as temperature and pressure. The characteristic length at the boundary of the three-phase region is then used for flash calculations in the two-phase lobes for Winsor type I/II. The functional form of the characteristic length is made consistent with the Gibbs phase rule. The improved EoS can capture asymmetric phase behavior data around the optimum, whereas current HLD-NAC based models cannot. The variable characteristic length formulation also resolves the thermodynamic inconsistency of existing phase behavior models that give multiple solutions for the optimum. We show from experimental data and theory that the inverse of the characteristic length varies linearly with formulation variables. This important result means that it is easy to predict the characteristic length in the three-phase region, which also improves the estimation of surrounding two-phase lobes. The results show that the optimum solubilization ratio can change significantly by a factor of two when variable characteristic length is included as temperature and pressure change. This can in turn greatly impact the interfacial tension (IFT) at optimum. This improved physical understanding of microemulsion phase behavior should aid in the design of surfactant blends and improve recovery predictions in a chemical flooding simulator.

## **Modeling Contact Angle vs. Temperature for the Quartz-Water-Decane System**

T. S. Duffy, Gamwo, I. W., Johns, R.T., and Lvov S. N. D.

SPEJ (2022)

### **Abstract**

Innovative approaches are needed to improve the efficiency of oil recovery technologies to meet the growing demands of fossil-fuel based energy consumption. Enhanced oil recovery (EOR) methods such as low-salinity waterflooding and chemically tuned waterflooding aim to optimize the reservoir's wetting properties, detaching oil globules from rock surfaces and allowing easier oil flow through pore throats. This wetting behavior is commonly quantified by contact angle measurements of the rock-oil-brine interface, which have been thoroughly investigated and theorized for many systems at ambient temperatures and pressures. However, few studies exist for extending contact angle theories away from ambient conditions. In this paper, we model the contact angles of a quartz-water-decane system at elevated temperatures using the surface tension component (STC) approach. Temperature-dependent van der Waals [Lifshitz-van der Waals (LW)] interactions and hydrogen-bonding (acid-base) interactions were calculated and are incorporated into the model for the quartz-water-decane interface. The Hough and White procedure was used to create temperature-dependent dielectric functions of quartz, water, and normal decane for calculations of Hamaker coefficients. Hamaker coefficients calculated this way are highly linear with temperature and agree well with Israelachvili's approximation. The acid-base interactions likely contribute the most to system wettability changes. Resulting contact angles of the quartz-water-decane system shift from water-wet ( $16^\circ$ ) to slightly water-wet ( $57.4^\circ$ ) as temperature increases. The model was also successfully verified for the quartz-air-water system. Our results can be used in future studies to determine optimal injected water compositions for specific rock-oil-brine and other systems with consideration of reservoir temperature.

# Construction of Metaverse Center based on Advanced Intelligence

by Fuji Ren, Member EUAS



## Short Biography

*Dr. Fuji Ren is currently the Professor and Director of Affective Computing and Intelligent Robot Laboratory in Tokushima University. He is also the President of International Advanced Information Institute in Japan. He is a member of The Engineering Academy of Japan, a member of EU Academy of Sciences, a fellow of the Japan Federation of Engineering Societies, a fellow of The Institute of Electronics, Information and Communication Engineers, and a fellow of Chinese Association for Artificial Intelligence.*

*He received his B.E. degree in 1982 and M.E. degree in 1985 from the department of Computer Science, Beijing University of Posts and Telecommunications, Beijing, China. He received his Ph.D. in 1991 from Faculty of Engineering, Hokkaido University, Sapporo, Japan. From 1991 to 1994, he worked at CSK in Tokyo, Japan where he was the chief NLP researcher. He joined the Faculty of Information Sciences at Hiroshima City University as an Associate Professor in 1994. In 2001, he became a Professor in the Faculty of Engineering at Tokushima University. He has been the president of AIA International Advanced Information Institute since 2003. He serves as the Director of the Dept. of Information Science and Intelligent Systems from 2006 to 2010, the vice Dean of Information Solution Branch of Graduate School of Engineering from 2010 to 2012, and Dean of Information Solution Branch Graduate School of Engineering from 2012 to 2016 at Tokushima University.*

*He also holds professor positions at Dalian University of Technology, Harbin University of Technology and Xi'an Jiaotong University. He holds the roles of Advisory Professor at Beijing University of Posts and Telecommunications, Research Advisor at Tsinghua University, Visiting Professor at University of Science and Technology of China, Yangtze River Professor at Nanjing University, and Advisory Professor at Tongji University. He was a visiting professor at CRL (Computing Research Laboratory) at New Mexico State University, a visiting research professor in the College of Engineering, at Florida International University, and a visiting professor in Harvard University in the USA.*

## **1. Metaverse concepts and characteristics**

### **1.1 Origin of the Metaverse**

The term "Metaverse" can be traced back to American science fiction writer Neil Stephenson, who described a virtual world interconnected with the real world in his science fiction novel "SnowCrash" published in 1992. The "metaverse" appeared frequently in games or film and television works. Now sandbox gaming platform Roblox has put the "metaverse" concept in its prospectus and successfully listed on the New York Stock Exchange. Metaverse has quickly become the global focus of attention from all walks

of life, and enterprises and governments in various countries (regions) have begun to lay out the metaverse industry track.

**1.2 Connotation of the Metaverse**

At present, the industry and academia have not yet formed a unified conclusion on the concept of metaverse. The metauniverse is a new type of Internet application and social form that integrates virtual-reality and reality by integrating a variety of new technologies. It provides immersive experience based on extended reality technology, generates a mirror of the real world based on digital twin technology, and builds an economic system based on blockchain technology, which closely integrates the virtual world and the real world in economic system, social system and identity system. And allow each user to do content production and world editing.

The metaverse is not a disruptive innovation, but a comprehensive application based on multiple digital technologies "connecting the dots into a line". It integrates the achievements of information technology (5G/6G), artificial intelligence, cloud computing, big data, blockchain and digital technologies such as VR, AR, MR And modeling engine. The metaverse will lead to in-depth research and cross-interaction of basic mathematics (algorithms), informatics (programming, information entropy), life science (brain-computer access), blockchain (encrypted finance), quantum computing (computing power) and other disciplines, and is expected to promote new breakthroughs in natural science, financial economics, future-ology, philosophy, logic, ethics, science fiction and other natural and humanistic science systems.

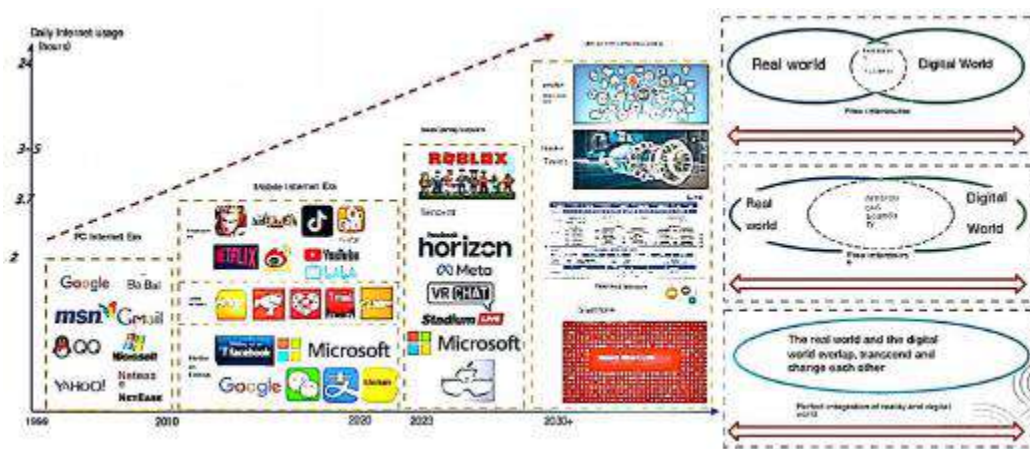


Fig. 1 The connotation of Metaverse

**1.3 Characteristics of the Metaverse**

■ **Virtual-real fusion**

Although the metaverse is the mirror image of the real world in the virtual space in the physical sense, it influences and integrates with the real world. This feature of virtual-real fusion is mainly reflected in the unity of the two identities of users in the real world and the metaverse. In the metauniverse, users complete various social activities with the help of virtual avatars. The virtual avatars uniquely correspond to their real identities and are unified and synchronized in senses and cognition. The unification of the two identities makes the boundary between virtual and reality blurred, and the virtual and real world gradually show a high degree of integration.

**■ Real-time interactivity**

Strong interaction function is a necessary condition to meet the interconnection needs between people, devices and avatars in the metaverse environment. In the metaverse environment, the highly developed Internet of things technology and network communication technology enable users to interact with the real physical world and the virtual world in real time. This real-time interaction is synchronized with the user's vision, hearing and touch in real time with a realistic interactive experience and negligible delay, so that the user can have an immersive sensory experience and a deep immersive sense of presence.

**■ High degree of civilization**

In the metaverse, users carry out various social activities through virtual avatars, and virtual avatars can communicate with each other without the restriction of time and space, which endows the metaverse with the social characteristics similar to the real society, and gradually evolves a virtual society which is born from the real society and has certain independence, thus further generating the virtual civilization in the metaverse. Therefore, the metaverse is a virtual world with a high degree of civilization. This civilization is the product of human social activities reproduced in the metaverse, including a stable economic system and a self-contained political and cultural system.

**■ Technical integration**

The realization of various ecological ideas of the metaverse cannot be completed by a single technology, and the integration and application of various digital intelligent technologies can give the possibility of the generation and operation of the metaverse. The underlying technologies of the metaverse are called "BIGANT" : blockchain, interactive technology, video games, artificial intelligence, networking and computing, and the Internet of Things. For example, interaction, technology and high-speed communication technology are the basis of immersion. Blockchain technology supports the continuous development of social civilization in the metaverse and is the core infrastructure of the metaverse.

**2. Applied Research in the Metaverse**

The technology and scene of the current metaverse are in the period of exploration and integration. It is expected that the first stage of development will take platforms such as games as the entry point for social interaction in the virtual world to form the embryonic form of immersive experiences. In the second stage, real elements such as consumption, logistics and life services will be widely connected in the virtual platform, so that the metaverse can be integrated into social life. In the third stage, the "virtual-real unification" is used to realize the inseparability of the virtual-real world. Domestic and foreign scholars have studied the application of metaverse from many aspects

In terms of cognitive interaction, the emerging virtual scene brings real interactive experience for users to meet their spiritual needs and bring social and economic value. As a new social civilization system, the metaverse separates human consciousness from matter and forms a state of high interconnection. In the exploration of Lee et al<sup>[1]</sup>, it is believed that the current brain-computer interface combined with metaverse related technologies can provide users with friendly and more intuitive communication methods through brain signals. Therefore, through the integration of information technology and brain science, the metaverse can gradually realize "intellectual reproduction", "intellectual interaction" and "intellectual immortality" in the virtual world, providing a new form for the survival of human intelligence<sup>[2]</sup>.

In terms of commercial life, the metaverse has become a new tuycere for reconstructing

commercial forms and lifestyles. It has made rapid changes in vertical commercial routes such as tourism, entertainment, art and office, rewritten industrial forms and innovating organizational forms, and promoted the upgrading of commercial development and lifestyles<sup>[3]</sup>. Jeong et al<sup>[4]</sup> proposed that the metaverse characterized by interaction also combines digital twin with real-time business, overcomes the limitations of existing online shopping, breaks the deficiencies of the existing flat online mode such as boring content, limited communication, and lack of experience, and improves information communication to realize mode innovation. Characters characterized by virtual people<sup>[5]</sup>, such as the virtual news anchor and the virtual singer Luo Tianyi of SMG Convergence Media Center, show the initial business closed loop of operating entertainment and social platforms from the perspective of individual IP.

In terms of industrial production, the metaverse will connect the dots of new technologies and create a new ecology where new information and communication technologies are deeply integrated with the real economy, thereby transforming the management mechanism, enabling technological production, and the integration of value-added industries. Digital twin is the application of the initial stage of the metaverse in industrial production, especially in manufacturing industries with high complexity such as automobiles and airplanes. Vachalek et al<sup>[6]</sup> explain the connotation of Industry 4.0 in terms of a Siemens-supported project in the automotive industry that uses digital twins to optimize production processes, proactive maintenance, and continuous improvement of process data processing. Qi et al<sup>[7]</sup> compared the application of big data and intelligent manufacturing in product design, production planning, manufacturing and predictive maintenance in manufacturing, and proposed that intelligent manufacturing is becoming the focus of global manufacturing transformation and upgrading.

In terms of culture and education, Metauniverse has operability in innovating talent training mode, empowering smart education environment, providing diversified educational resources, supporting diversified learning and life, and realizing intelligent teaching evaluation. Many understandings of the educational metaverse generally stay at the educational application level of the metaverse, such as the creation of virtual identities and immersive interactions. For example, Lu Lili et al<sup>[8]</sup>, in discussing the future teaching mode under the metaverse, proposed a kind of "virtual" and "reality" barrier to break down the concept of "online" and "offline", and formed a "chaotic" new universe that subverted and transcend the pattern and thinking of the previous generation of Internet. Context knowledge construction can solve the problem of weak connection between objective knowledge world and subjective virtual world in the metaverse<sup>[9]</sup>. Xin Haixia<sup>[10]</sup> took the metaverse as a technical concept and discussed that the metaverse drives the library to realize object twin, index twin and decision twin.

### **3. Metaverse technology system based on advanced intelligence**

#### **3.1 Six layers of metaverse architecture**

The metaverse can be divided into six levels.

##### **■ Physical layer**

The first layer is the physical layer. The bottom layer of the Internet is also the physical layer, which has optical fibers and cables to build a network. The metaverse is also based on the ICT network, and the Internet is an infrastructure of the metaverse. In addition, the hardware devices of virtual reality, augmented reality, and mixed reality, including VR, AR, MR, and XR, are the lowest layer of the metaverse, the physical layer.

##### **■ Data layer**

The second layer is the data layer. The metaverse must be an interconnected, digital

symbiosis that relies on bandwidth, storage, and computing power. IT (Information Technology), CT (communication Technology) and DT (Data Technology) platforms are the most fundamental platforms of the metaverse.

#### ■ **Algorithm layer**

The third layer is the algorithm layer. There are three elements in the algorithm layer: the first one is privacy calculation. In the metaverse, users' browsing, consumption, preferences and other data are valuable, and privacy protection and privacy computing will be a core topic. The second is AIGC. AIGC is different from PGC (expert creation of content), UGC (customer creation of content), OGC (institution creation of content), it is based on AI to create content, there must be AIGC in the metaverse, which needs AI to produce a lot of content in the digital world and virtual reality.

#### ■ **Layer of governance**

The fourth layer is the governance layer. It's about how the metaverse is organized, how it works, how it becomes an infinite game. At this level, we need to rely on blockchain. Ethereum is a blockchain, an ownerless network where many creative things are published every week. On Ethereum, there are millions of developers around the world, who don't belong to any organization, working 24/7 to figure out how to make something fun and useful.

#### ■ **Layer of excitement**

The fifth layer is the incentive mechanism. The virtual reality world must have its own currency system. The metaverse financial market is a digital financial market rather than a traditional financial market. The practice of blockchain over the past 12 years has established a very complete and well-functioning decentralized financial market system for the metaverse, on which the metaverse must be built.

#### ■ **Application layer**

The top layer is the application layer. At this level, there are various content creators and various forms of application innovation. In the application layer, we discuss the digital existence and digital production of human beings, and the production includes the production of virtual services and virtual goods.

### **3.2 Technical system**

The metaverse technology system is called BIGANT, which is composed of six supporting technologies, namely Blockchain technology, Interactivity technology, video Game technology, artificial intelligence technology, Network and computing technology, Internet of Things. We believe that we need to elevate artificial intelligence technology to the metaverse brain and become the most core technology. We proposed A BIGANT on top of BIGANT, adding Artificial Emotion into the technology system. In the ABIGANT technology framework, AI will become the core technology as the core brain of ANT. Artificial emotion, blockchain, interactive technology, game technology, network and computing technology, and Internet of Things technology will be important limbs. As the meta-universe is a new type of Internet application and social form that integrates virtual-reality with human subjects and provides people with immersive experience, it is impossible to bring huge virtual content and immersive experience to users without AI technology as the brain command. Similarly, the absence of artificial emotions (including emotion perception and emotion creation) is incomplete. For example, users who are immersed in the game world, especially teenagers, are at risk for health and social problems if their emotional state is not perceived. Similarly, immersive experiences are lacking without emotional interaction. So in A BIGANT technology system, we add artificial emotion, and put AI technology at the very core.

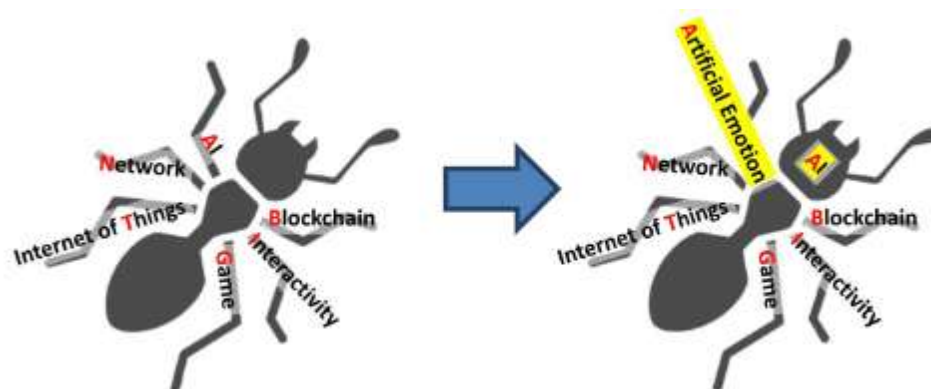


Fig. 2 BIGANT vs A BIGANT

### ■ Artificial Intelligence Technology

Through blockchain and AI technology, the threshold of content creation is reduced and the extensibility of the game is improved. Artificial intelligence technology is ubiquitous at all levels of the metaverse, in various applications, and in various scenarios. These include smart contracts in blockchain, AI recognition in interaction, automatic generation of code characters, items and even plots in games, AI capabilities in intelligent networks, data AI in the Internet of things, etc., as well as speech semantic recognition and communication of virtual characters in the metauniverse, AI recommendation of social relationships, and AI of various DAOs Operation, AI construction of various virtual scenes, various analysis and prediction reasoning, etc.

### ■ Blockchain Technology

Blockchain is the most important foundation to support the metaverse economic system! Metaverse a fixed decentralized, the user's virtual assets must be able to cross each sub-metaverse for circulation and transaction, in order to form a huge economic system.

Through blockchain technologies and applications such as NFT (non-homogeneous Token), DAO, smart contract, DeFi, and so on, it will stimulate the era of creator economy and spawn massive content innovation. Based on blockchain technology, a decentralized metaverse clearing and settlement platform and value transfer mechanism will be effectively built to ensure the attribution and circulation of value, and realize the stability, efficiency, transparency and certainty of the metaverse economic system operation.

### ■ Interaction technology

Through AR, VR and other interactive technologies to improve the immersion of the game. Human interaction technology is the biggest bottleneck restricting the immersion of the current metaverse. Composite interaction technology also includes all kinds of brain-computer interfaces, which is also the ultimate development direction of interaction technology. In the future, with the development of human-computer interaction technology represented by VR and AR, the immersion of virtual open world games carried by more realistic and high-frequency human-computer interaction is also expected to be greatly improved, so as to narrow the gap with the mature form of the metaverse.

### ■ Game Technology

It includes not only 3D modeling and real-time rendering related to game engine, but also 3D engine and simulation technology related to digital animation. The former is the key technology of the virtual world development to liberate the public productivity, and the latter is the key tool of the physical world virtualization and digitization. Both of them need to greatly reduce the production threshold, so as to greatly accelerate the process of

the real world digitization. The biggest technical threshold lies in the simulation technology, that is, the things after the digital twin must obey the laws of physics, gravity, electromagnetic laws, and electromagnetic wave laws, such as light, radio waves, pressure and sound laws.

#### ■ **Network and Computing Technology**

Metaverse requires high synchronization and low latency, so that users can get a real-time, smooth and perfect experience. In the metaverse, a large amount of data needs to be transmitted rapidly and relies on strong communication infrastructure. Edge computing is often considered to be the key infrastructure of the metaverse. By using an open platform near the source of data, the nearest service is directly provided, so as to help end users complement local computing power, improve processing efficiency, and reduce network delay and network congestion risk as much as possible.

#### ■ **Internet of Things Technology**

The Internet of Things technology not only undertakes the front-end collection and processing function of the digitalization of the physical world, but also undertakes the function of infiltrating and even managing the physical world of the virtual world of the symbiosis of the meta-universe. Only when the interconnection of everything is truly realized, can the metauniverse realize the symbiosis between virtual and real be truly possible! The development of physical network technology provides the virtual world after the digital twin with real-time, accurate and continuous fresh data supply, so that people in the virtual world of the meta-universe can explore the details of the physical world without going out of the Internet.

#### ■ **Artificial Emotion Technology**

In the context of the metaverse, sociability and emotion are essential attributes for future virtual humans. People express their emotions through facial expressions, body movements and voice intonation, and perceive other people's emotions through vision, hearing, touch and other senses and the corresponding brain functional areas. Affective computing aims to give computers the ability to observe, interpret and generate various emotional features like human beings, and finally enable computers to interact with humans naturally and harmoniously.

### **3.3 Advanced intelligent Technology**

Metaverse is a new type of Internet application and social form that integrates virtuality and reality with human as the main body. It provides people with immersive experience and allows users to produce content and edit the world. At present, and for a long time to come, games may be the most dazzling scene world of the metaverse. But even this metaverse game would not be complete without artificial emotions, including emotion perception and emotion generation. For example, users who are immersed in the game world, especially teenagers, can have serious problems if their emotional state is not perceived, including health problems and social problems. Similarly, without emotional interaction, immersive experiences fall short. In order to promote the establishment of BIGANT core technology system, it needs to be supplemented and expanded by advanced intelligence.

The so-called advanced intelligence is the research paradigm of artificial intelligence and natural intelligence fused with affective computing. The fusion of natural intelligence and artificial intelligence has achieved good results in many industries, including speech recognition, image processing, machine translation, etc. Affective computing will also be an important element of the metaverse.

#### 4. Metaverse construction plan

China sees the metaverse as the next generation of digital economy and has promulgated many policies to promote technological development. For example, at the 2022 Global Investment Promotion Conference, Shanghai released investment promotion plans for the four "new tracks" of metauniverse, green and low-carbon, smart terminal and digital economy. It is expected that by 2025, the city's green and low-carbon industry scale will strive to exceed 500 billion yuan, the metaverse industry scale will exceed 350 billion yuan, and the intelligent terminal industry scale will exceed 700 billion yuan.

Based on advanced intelligent technology, we have planned and laid out five research areas. They are real-time cloud rendering, NFT, XR, human-computer interaction, and AIGC.

##### ■ Real-time cloud rendering

In the metaverse world, all social relationships such as cities, companies, and people can be reconstructed. Everything from character depictions to simple gestures, accessories, and scenes need to be rendered. In the movie "Transformers 3", the production of a scene "Drillers destroy skyscrapers" involved more than 200,000 parts, and each frame took 288 hours to render, which required more than 200,000 hours of rendering for tens of seconds of footage. If you want to realize the scene of players wearing XR devices in the movie "Ready Player One" roaming in the virtual network world, then the high real-time performance, high interactivity and high immersion of this metauniverse are very demanding on the computing power of the terminal device. In order to break through the computing power limit, the adoption of cloud rendering technology will be essential. Computation and rendering become critical infrastructure for the metaverse. Therefore, real-time cloud rendering technology is an important infrastructure of the metaverse, which is also known as the "engine" of the metaverse.



Fig. 3 Real-time cloud rendering

##### ■ NFT

NFT refers to non-homogeneous token, which is essentially a trusted digital equity certificate with unique characteristics in the blockchain network. It is a kind of data object that can record and process multi-dimensional and complex attributes on the blockchain. NFT and metaverse are interdependent and co-flourishing.

First, NFT defines the metaverse as an operational collection of shared online worlds, so that users can use tokens to transact in the metaverse through digital identities. VR and AR avatars represent digital images created by users, which can be used in multiple games or social applications. And virtual property purchased on one platform retains value on the

other. Secondly, NFT is equal to anchor value, each NFT is uniquely corresponding to a certain real thing, users can truly enjoy the unique digital ownership of web3.0, and based on this unique and scarce value anchor can be traded, and the transaction will produce an economy, and the metaverse can be operated normally.

#### ■ XR

XR includes AR (augmented reality), VR (virtual reality), MR (mixed reality), is through the corresponding hardware equipment, combined with a variety of software technology means, the virtual content and the real scene fusion, in the XR virtual studio to build a dreamlike virtual world. XR hardware is the hardware entrance of the metaverse era and will become the next generation of computing platform. XR is also the most feasible path to combine virtual and reality.

#### ■ Human-computer interaction

Human-computer interaction is one of the key technologies of the metaverse. In the metaverse, humans in the real world can interact with agents (virtual humans, digital property, digital objects, etc.) in the virtual world. In the early days of the metaverse, humans still interacted with the virtual world through their fingers and eyes, as if playing an "immersive video game." The diversity of its interactive devices will be greatly expanded. For example, cameras and inertial sensors will capture human body movements, voice and other commands in video games, and game plot feedback will also be displayed to humans through smart glasses and smart helmets.

#### ■ AIGC

AI Generated Content (AIGC) is the content generated by AI, which is characterized by automated production and high efficiency. With the maturity of natural language generation technology NLG and AI models, AIGC has gradually attracted people's attention. Now it can automatically generate text, pictures, audio, video, and even 3D models and codes. AIGC will greatly promote the development of the metaverse, where a large number of digital native content needs to be created by AI. In terms of AI-generated text, AI can already write poems, emails, advertisements, scripts and novels. In terms of AI-generated images, the level of AI painting has made great progress this year, and the algorithm model behind it has also been iterated. It has been able to generate works comparable to that of professional painters, and the efficiency of generating images has also changed from hours at the beginning of the year to minutes or even tens of seconds now. In terms of AI-generated audio, the AI Podcast.ai generated a 20-minute interview podcast between Jobs and Joe Rogan, a well-known US host, which sounded like the real thing.

### 5. Recent Progress

The team has built a metaverse center based on XR technology in the University of Electronic Science and Technology of China. The center focuses on practical applications such as virtual scenes and virtual characters, and relies on the metaverse technology base to build a technology ecology. It covers content production, authentication mechanism, data processing, virtual-real interface, network environment and other ecology, and constructs cloud digital content collaborative creation platform, blockchains based digital asset authentication technology, multi-modal fusion interaction technology, virtual human, virtual live broadcast, low-delay HD video dissemination and other applications.

The center uses virtual scene production technology to migrate the beautiful scenery of Jiuzhaigou Valley into digital assets and move the scenery into the metauniverse. At the same time, it generates high-quality metauniverse content based on digital human technology, motion capture technology, affective computing technology and AIGC technology, which can achieve the following effects:

■ **Virtual-real Fusion**

Through LED virtual shooting technology, the real object is perfectly integrated into the virtual scene, and it is difficult to distinguish the real from the fake. LED screen for the virtual scene, LED screen in front of the real existence of people or things. Through ray tracing and color adjustment, the audience can not see the difference between the screen in front of the screen during the shooting. Break the sense of space, so that the physical and virtual scene into one.



**Fig. 2a** Virtual-real Fusion

■ **Virtual-real Interaction**

LED virtual shooting + virtual human technology to achieve virtual and real character interaction. A real person or physical object is arranged in front of the LED screen, and a virtual character is placed in the virtual scene in the LED screen, which is controlled by a model wearing a motion capture device. Real person and real object achieve the effect of virtual and real dialogue.

**Fig. 3** Virtual-real Interaction

■ **Multi-person Collaboration in the Metaverse**



Based on real-time cloud rendering technology, anyone can enter the virtual scene at any time and anywhere. In addition to watching the virtual scene displayed in this project, the audience can also enter the virtual scene through the mobile phone, and operate the role in the virtual scene to freely explore the virtual scene.

#### ■ Full Motion Capture

The real person wears motion capture equipment (including body motion capture, facial expression capture, and finger motion capture) to operate the virtual character for effect display.



Fig. 4 Full Motion Capture

#### ■ Display of Simulation Robot

In this project, a simulation robot is placed in front of the LED screen, and the simulation robot has a dialogue with the virtual person in the LED screen. Show the effect of simulated robot interaction.



Fig. 5 Display of Simulation Robot

#### ■ Artificial Intelligence

Artificial intelligence (AI) emotional question (4) answering function is realized by simulation robot combined with NLP emotional question answering technology. In the exhibition hall, the camera was simulated to capture the facial emotion of the audience to

show the emotion capture effect in the dark light environment.



**Fig. 6** Artificial Intelligence

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# Atomic Layer Deposition of GdF<sub>3</sub> Thin Films

by Markku Leskelä, Member EUAS

## Short Biography

**Markku Leskelä** (born 1950) received both M.Sc. (1974) and PhD (1980) degrees from Helsinki University of Technology. During 1979-1986 he worked at University of Oulu and Helsinki University of Technology as associate professor or acting professor, in 1986-1990 at University of Turku as professor and in 1990-2018 at University of Helsinki as professor of inorganic chemistry. He made sabbatical visits in 1983 (University of Utrecht), 1987-1988 (University of Florida) and in 1999 (University of Paris VI). During 2004-2009 he served as Academy professor. Since 2019 he has worked as emeritus professor at University of Helsinki.

His research interests cover luminescent materials, catalytic activation of small molecules with metal compounds, and development of chemistry for Atomic Layer Deposition of thin films – the latter topic being dominating during last five years. He has worked as vice-director (2002-2007) and director (2012-2017) in two centers of excellence funded by Academy of Finland. He has published about 730 original and 60 review papers which have been cited more than 34 000 times (h-index 88; Web of Science). He holds more than 40 patents. He was nominated in 2004 as ISI Highly Cited Author in materials science. He has received several honors and awards: Magnus Ehrnrooth Foundation Award in Chemistry (2002), SVR I (2005), A.I. Virtanen award (2011), American Vacuum Society ALD award (2012), Honorary award of Finnish Academy of Sciences and Letters (2014), Honorary member (2014) and honorary chairman (2019) of Finnish Chemical Society, Honorary doctor (University of Tartu 2016). He is a member of four academies of sciences. He has and has had several positions of trust in universities (for example board of trustees of University of Helsinki 2010-2017), scientific societies, academies and foundations. He has been the president of the Finnish Academy of Technical Sciences 2019-2022 and the chairman of The Council of Finnish Academies (CoFA) 2021-2022.

**E. Atosuo, K. Mizohata, M. Mattinen, M. Mäntymäki, M. Vehkamäki, M. Leskelä & M. Ritala: Atomic Layer Deposition of GdF<sub>3</sub> Thin Films. J. Vac. Sci. Technol. A 40 (2022) 022404 (7 pp.)**

Gadolinium fluoride is an attractive optical material with applications in, e.g., deep-UV lithography, solar cells, and medical imaging. Despite the interest toward this material, no atomic layer deposition (ALD) process has been published. In this article, an ALD process for GdF<sub>3</sub> using Gd(thd)<sub>3</sub> and NH<sub>4</sub>F as precursors is presented. The deposition was studied at temperatures 275–375 °C, but 285–375 °C produce the purest films. The saturation of the growth per cycle (GPC) with respect to precursor pulses and purges was proved at 300 °C. The GPC value at this temperature is ~0.26 Å, and the deposition temperature has very little effect on the GPC. According to x-ray diffraction, all the films consist of orthorhombic GdF<sub>3</sub>. The impurity contents, evaluated by time-of-flight elastic recoil detection analysis, is low, and the films are close to stoichiometric. The nitrogen content is

less than <0.04 at. %. The antireflection properties were qualitatively evaluated by UV-vis spectrometry in a transmission mode at a 190–1100 nm range: on sapphire substrates, GdF<sub>3</sub> serves as an antireflective coating. Dielectric properties of the films were studied, and for example, a permittivity value of 9.3 was measured for a ~64 nm film deposited at 300 °C.

**S. Ghafourisaleh, M. Leskelä, M. Putkonen & M. Ritala: Molecular Layer Deposition (MLD) of Thermally Stable Polybenzimidazole (PBI) Thin Films for Protective Coating Applications. *Adv. Mater. Inter.* 9 (2022) 2200370 (12 pp).**

The deposition of polybenzimidazole (PBI)-like thin films by molecular layer deposition is reported here for the first time using isophthalic acid (IPA) and 3,3'-diaminobenzidine (DAB) as monomers and trimethylaluminum (TMA) as a linker precursor. Two precursor pulsing sequences are tested, the ABCB (TMA + IPA + DAB + IPA) and ABC (TMA + IPA + DAB) type MLD processes result in different types of PBI-like films. With the ABCB sequence thin film growth per cycle (GPC) of 6.0 Å is obtained at 225–280 °C, whereas GPC of 7.0 Å is obtained with the ABC sequence. Films are characterized in detail by Fourier transform infrared spectroscopy, scanning electron microscopy, thermogravimetric analysis, time-of-flight elastic recoil detection analysis, and atomic force microscopy. The films have good thermal stability and withstand annealing at 400 °C in both air and nitrogen. PBI nanostructures are prepared by depositing PBI-like film on electro-blown polyvinylpyrrolidone fibers and removing the template fibers by annealing or dissolution into ethanol.

**A. Weiß, G. Popov, P. Jalkanen, E. Atosuo, M. Vehkamäki, A. Vihervaara, M. Leskelä, M. Ritala & M. Kemell: Atomic Layer Deposition of CsI and CsPbI<sub>3</sub>. *Chem. Mater.* 34 (2022) 6087-6097.**

Cesium iodide (CsI) is a well-established scintillator material that also serves as a precursor for all-inorganic halide perovskite solar absorbers, such as CsPbI<sub>3</sub>. However, the lack of conformal and scalable methods to deposit halide perovskite thin films remains a major challenge on their way to commercialization. In this work, we employ atomic layer deposition (ALD) as the key method due to its inherent scalability to large areas and complex-shaped surfaces. We demonstrate two new ALD processes for the deposition of CsI and CsPbI<sub>3</sub> thin films. The CsI process relies on cesium bis(trimethylsilyl) amide (Cs(btsa)) and tin(IV) iodide (SnI<sub>4</sub>) as precursors and yields high-purity, uniform, and phase-pure thin films. This process works in a wide temperature range (140–350 °C) and exhibits a large growth per cycle value (GPC) of 3.3 Å (85% of a CsI monolayer). Furthermore, we convert CsI into CsPbI<sub>3</sub> perovskite by exposing a CsI film to our earlier PbI<sub>2</sub> ALD process. We demonstrate the deposition of phase-pure  $\gamma$ - or  $\delta$ -CsPbI<sub>3</sub> perovskite thin films, depending on the applied deposition temperature and number of PbI<sub>2</sub> cycles. We believe that the ALD-based approach described in this work will offer a viable alternative for depositing perovskite thin films in applications that involve complex high aspect ratio structures or large substrate areas.

**V.A. Lovikka, K. Airola, E. McGuinness, C. Zhang, M. Vehkamäki, M. Kemell, M. Losego, M. Ritala & M. Leskelä: Toposelective Vapor Deposition of Hybrid and Inorganic Materials Inside Nanocavities by Polymeric Templating and Vapor Phase Infiltration. *Nanoscale Adv.* 4 (2022) 4102-4113.**

Selective deposition of hybrid and inorganic materials inside nanostructures could enable major nanotechnological advances. However, inserting ready-made composites inside nanocavities may be difficult, and therefore, stepwise approaches are needed. In this paper, a poly(ethyl acrylate) template is grown selectively inside cavities via condensation-controlled toposelective vapor deposition, and the polymer is then hybridized by alumina, titania, or zinc oxide. The hybridization is carried out by infiltrating the polymer with a vapor-phase metalorganic precursor and water vapor either via a short-pulse (atomic layer deposition, ALD) or a long-pulse (vapor phase infiltration, VPI) sequence. When the polymer-MOx hybrid material is calcined at 450 °C in air, an inorganic phase is left as the residue. Various suspected confinement effects are discussed. The infiltration of inorganic materials is reduced in deeper layers of the cavity-grown polymer and is dependent on the cavity geometry. The structure of the inorganic deposition after calcination varies from scattered particles and their aggregates to cavity-capping films or cavity-filling low-density porous deposition, and the inorganic deposition is often anisotropically cracked. A large part of the infiltration is achieved already during the short-pulse experiments with a commercial ALD reactor. Furthermore, the infiltrated polymer is more resistant to dissolution in acetone whereas the inorganic component can still be heavily affected by phosphoric acid.

**C. Zhang, E. Tois, M. Leskelä & M. Ritala: Substrate-Dependent Area-Selective Atomic Layer Deposition of Noble Metals from Metal Beta-diketonate Precursors. *Chem. Mater.* 34 (2022) 8379-8388.**

Area-selective ALD of Ir, Ru, and Rh with excellent substrate selectivity was achieved by using metal  $\beta$ -diketonates, i.e., Ir(acac)<sub>3</sub>, Ru(thd)<sub>3</sub>, and Rh(acac)<sub>3</sub>, as precursors with either O<sub>2</sub> or air as a coreactant. Native SiO<sub>2</sub> and Ru were identified as growth surfaces while low-k SiOC, native oxide terminated Cu and Co, Al<sub>2</sub>O<sub>3</sub>, ZrO<sub>2</sub>, and HfO<sub>2</sub> were identified as the nongrowth surfaces. UV (254 nm) irradiation in air was proven efficient to activate the low-k SiOC surface for the noble metal growth. UV exposure of 1 min was sufficient for the growth activation yet without causing any damage to the low-k material. Selective growth of the noble metals was successfully demonstrated on a UV-irradiated test chip that has micro- and nanometer-scale low-k SiOC/Cu patterns. At the optimal selective deposition temperatures, that is 225 °C for the Ir, 300 °C for the Ru, and 250 °C for the Rh, films with a thickness of at least 10 nm for Ir and ~30 nm for Ru and Rh can be selectively deposited on the UV-activated low-k SiOC regions, while no growth occurs on Cu regions, as characterized by SEM, TEM, and EDS.

**G. Popov, G. Bačić, C. Van Dijck, L. Junkers, A. Weiss, M. Mattinen, A. Vihervaara, P. Jalkanen, K. Mizohata, M. Leskelä, J. Masuda, S. Barry, M. Ritala & M. Kemell: Atomic Layer Deposition of PbCl<sub>2</sub>, PbBr<sub>2</sub> and Mixed Lead Halide (Cl, Br, I) PbX<sub>n</sub>Y<sub>2-n</sub> Thin Films. *Dalton Trans.* 51 (2022) 15142-15157.**

Atomic layer deposition offers outstanding film uniformity and conformality on substrates with high aspect ratio features. These qualities are essential for mixed-halide perovskite films applied in tandem solar cells, transistors and light-emitting diodes. The optical and electronic properties of mixed-halide perovskites can be adjusted by adjusting the ratios of different halides. So far ALD is only capable of depositing iodine-based halide perovskites whereas other halide processes are lacking. We describe six new low temperature ( $\leq 100$  °C) ALD processes for  $\text{PbCl}_2$  and  $\text{PbBr}_2$  that are crucial steps for the deposition of mixed-halide perovskites with ALD. Lead bis[bis(trimethylsilyl)amide]- $\text{GaCl}_3$  and  $-\text{TiBr}_4$  processes yield the purest, crystalline, uniform and conformal films of  $\text{PbCl}_2$  and  $\text{PbBr}_2$  respectively. We show that these two processes in combination with a  $\text{PbI}_2$  process from the literature deposit mixed lead halide films. The four less optimal processes revealed that reaction by-products in lead halide deposition processes may cause film etching or incorporate themselves into the film.

**A. Weiß, J. Goldmann, S. Kettunen, G. Popov, T. Iivonen, M. Mattinen, P. Jalkanen, T. Hatanpää, M. Leskelä, M. Ritala & M. Kemell: Conversion of ALD CuO Thin Films into Transparent Conductive p-type CuI Thin Films. Adv. Mater. Interface 9 (2022)**

Copper iodide (CuI) is a high-performance p-type transparent semiconductor that can be used in numerous applications, such as transistors, diodes, and solar cells. However, the lack of conformal and scalable methods to deposit CuI thin films limits its establishment in applications that involve complex-shaped and/or large substrate areas. In this work, atomic layer deposition (ALD) is employed to enable scalable and conformal thin film deposition. A two-step approach relying on ALD of CuO and its subsequent conversion to CuI via exposure to HI vapor at room temperature is demonstrated. The resulting CuI films are phase-pure, uniform, and of high purity. Furthermore, CuI films on several substrates such as Si, amorphous  $\text{Al}_2\text{O}_3$ , n-type  $\text{TiO}_2$ , and  $\gamma\text{-CsPbI}_3$  perovskite are prepared. With the resulting n- $\text{TiO}_2$ /p-CuI structure, the easy and straightforward fabrication of a diode structure as a proof-of-concept device is demonstrated. Moreover, the successful deposition of CuI on  $\gamma\text{-CsPbI}_3$  proves the compatibility of the process for using CuI as the hole transport layer in perovskite solar cell applications in the nip-configuration. It is believed that the ALD-based approach described in this work will offer a viable alternative for depositing transparent conductive p-type CuI thin films in applications that involve complex high aspect ratio structures and large substrate areas.

## Interactive Granular Computing (IGrC) and Related Works

by Andrzej Skowron, Member EUAS



### Short Biography

*Andrzej Skowron, an EurAI (ECCAI), AAIA Fellow and IRSS Fellow, and the Member of EU Academy of Sciences, received the Ph. D. and D. Sci. (habilitation) from the University of Warsaw in Poland. In 1991 he received the Scientific Title of Professor. He is a Full Professor in the Systems Research Institute, Polish Academy of Sciences. He is Emeritus Professor in Faculty of Mathematics, Computer Science and Mechanics at the University of Warsaw. Andrzej Skowron is the (co)author of more than 500 scientific publications including edited and (co-)authored books and volumes of conference proceedings. His areas of expertise include reasoning with incomplete information, approximate reasoning, soft computing methods and applications, rough sets, rough mereology, granular computing, intelligent systems, knowledge discovery and data mining, decision support systems, adaptive and autonomous systems, perception based computing, and interactive computational systems. He was the supervisor of more than 20 PhD Theses. In the period of 1995-2009 he was the Editor-in-Chief of Fundamenta Informaticae, an international journal. He is in the Editorial Boards of many others international journals. Andrzej Skowron was the President of the International Rough Set Society from 1996 to 2000. He has delivered numerous invited talks at international conferences including a plenary talk at the 16th IFIP World Computer Congress (Beijing, 2000), a keynote talk at the 8<sup>th</sup> Joint Conference on Information Sciences (JCIS 2005) (encompassing 12 individual conferences and workshops) (USA, 2005), an invited talk at the 2006 IEEE/WIC/ACM International Conference on Intelligent Agent Technology (IAT 2006) and on Web Intelligence (WI 2006) (Hong Kong, 2006), and a plenary talk at the 2nd World Congress on Biologically Inspired Computing (Japan, 2010). He has served as (co-)program chair or PC member of more than 200 international conferences. He was involved in numerous research and commercial projects including dialog based search engine (Nutech), fraud detection for Bank of America (Nutech), logistic project for General Motors (Nutech), algorithmic trading (Adgam), control of UAV (Linköping University), and medical decision support (e.g., in Polish-American Pediatric Clinic in Cracow). In 2012, 2016, 2017 Andrzej Skowron was in the ICI Thomson Reuters/ Clarivate Analytics lists of the most cited researchers in Computer Science (globally).*

## Abstract

This article is a continuation of Andrzej Skowron's articles published, in particular in EU ACADEMY ANNUAL REPORTS 2019-2021 and focuses on works related to Interactive Granular Computing (IGrC). More details about IGrC can be found on this site <https://dblp.org/pid/s/AndrzejSkowron.html>, in papers related to IGrC and in the recent invited lectures (see, e.g., keynote talk at Information Processing and Management of Uncertainty in Knowledge-Based Systems (IPMU 2022): Perceptual Rough Set Approach in Interactive Granular Computing; keynote talk at 18th Conference on Computer Science and Intelligence Systems (FedCSIS 2022): Rough Sets Turn 40: From Information Systems to Intelligent Systems; invited plenary talk at the special session of IEEE Intelligent Systems 2022 Conference (IEEE IS 2022): (with Dominik Ślęzak) Rough sets turn 40: What next?; Plenary talk at Optimization, Learning and Analytics in Business (OLAB 2022): Decision Support in Problem Solving by Intelligent Systems Based on Interactive Granular Computing). Here we discuss in more detail related works developed in different areas which stimulated the development of IGrC.

## IGrC and Related Works

We discuss motivations for developing IGrC which are nowadays spread over many different areas such as multi-agent systems, robotics, cognitive science, machine learning, computational intelligence, swarm intelligence, complex (adaptive) systems, to name a few of them. In these domains different aspects important for IGrC are pointed out. In developing of IGrC, we use the above mentioned evidences gathered in different areas to develop a model on which analysis and synthesis of Intelligent Systems dealing with complex phenomena can be based.

Let us consider more details about these related works.

For example, in *cognitive science*, it was emphasized in [1] that the traditional mechanistic computing model is not satisfactory for dealing with perception. Hence, such a model is not relevant for Intelligent Systems dealing with complex phenomena because separating the desired systems from the physical reality does not result satisfactory solutions. It was observed [2] that the *Turing test*, used so far, should be modified to a new one making it possible to put in sync not only language and reasoning but also issues related to perception and action.

In *multi-agent systems* [3-4] an intuitive idea of interaction of abstract and physical world is used without building more solid foundations for such computing model which can't be fully embedded in mathematical manifold [5]. Attempts to restrict such modeling only in the abstract world was criticized by Edmund Husserl, the founder of *phenomenology*, because following this leads to separating the designed systems from *human experience* [5].

It should be noted that contrary to the traditional mathematical modeling, that has been successful for a few centuries, in the context of experience concerning to *complex phenomena*, only pure mathematical approaches do not work [6]. In particular, the methods currently used in *data driven learning* [7] are not satisfactory because they do not provide the necessary tools for modeling perception (understanding) of the perceived complex situations in the physical world. In particular, methods related to control of *attention* [8] of Intelligent Systems should be developed. Such methods should be based on new approaches of reasoning that can make it possible to decide *when, where, how, or what* the system composed out of complex granules (c-granules, for short) should perceive in the

physical world. It is visible that modeling of *interactions between abstract and physical worlds* can't be realized by pure mathematical objects only.

In developing of a new computing model, one should also take into account that Intelligent Systems dealing with complex phenomena are perceiving complex situations in the real physical world under uncertainty due to complexity of these situations, unexpected interaction with the environment as well as bounded perceiving abilities of Intelligent Systems. Here the questions posed by Gurevich, in his lecture (see <https://www.youtube.com/watch?v=FX2J24u92GI>), is very relevant. His questions regarding 'What is a state?' and 'What is the transition relation?' become fundamental in developing the new computing model. Linking Intelligent Systems with the situations in the physical reality by providing continuous interaction with this reality should lead to gathering perceived data on the basis of which relevant but only temporary models can be induced. Moreover, strategies for adapting their *behaviour* to perceived changes in the environment are necessary. Intelligent Systems should be equipped with the relevant mechanisms aiming to control their behaviour to satisfy their needs expressed by the constraints related to, e.g., preserving some invariants or properties of trajectories of computations.

Making progress in developing *new reasoning methods* is crucial for design of Intelligent Systems dealing with complex phenomena. Important issues of IGrC are closely related to reasoning. Among them there are several challenges. Some of them, as we mentioned above, are related to the control of attention. Let us discuss shortly a little more about this.

Intelligent Systems dealing with complex phenomena can't be separated from *dialogues with human experts* because we do not have still satisfactory formal modeling tools that can do reasoning based on analogy; *analogy reasoning* is still in the infancy age [9] and *practical judgment* is out of jurisdiction of reasoning [8]. Hence, in developing Intelligent Systems dealing with complex phenomena, one can't separate them from the interactions with domain experts and other physical objects (e.g., patients in the medical applications or domain data bases). Here, developing methods providing tools for dialogue and interaction with humans are necessary. It should be noted that from this point of view one should take into account the challenge mentioned by Pearl [10] about the necessity of building the proper *interfaces between humans and systems*. Along this line different directions of research, called *Human-Centered AI* or *Human-in-the-Loop Machine Learning* [11-12] are emerging. In relation to the above discussion about experience based reasoning and necessity to have domain experts-in-the loop of machine learning, one can be referred to the article namely, *Where did IBM go wrong with Watson Health?* (see: <https://qz.com/2129025/where-did-ibm-go-wrong-with-watson-health>).

It should be also stressed that developing strategies of reasoning for adaptation of the c-granule or system behaviour, according to the perceived differences between expected and results in reality, is one of the great challenges.

Long time ago the *brittleness* drawback of expert systems, such as MYCIN [13] was recognised. Perceptual brittleness is related to the fact that the existing machine learning algorithm do not actually learn to perceive the world in a way that can generalize properly under uncertainty (see: [https://www.womencorporatedirectors.org/WCD/News/JAN-Feb2020/Reality Light .pdf](https://www.womencorporatedirectors.org/WCD/News/JAN-Feb2020/Reality%20Light.pdf)).

To deal with this challenge it is necessary first to develop the relevant computing model for modeling perception of situations in the physical world. One should note that such a model can't be purely abstract because perception concerns the physical objects which are not abstract (mathematical). IGrC model aims to deal with such challenges. Let us also

recall, that understanding of interactions is one of the basic issues in complex systems [14]. Moreover, interactions are embedded in the physical world and they can be only perceived partially using some tools, e.g., based on IGrC.

Other challenges are related to reasoning about data, gathered through some processes of perception. For example, some properties of physical objects 'close enough to the system' may be perceived directly (e.g., by direct measurements); some other by reasoning with the use of knowledge bases and/or physical laws related to dynamical properties of perceived configuration of physical objects. Hence, the *computing model can't be embedded only in the abstract space* because computations are dependent on physical laws as it was also observed by researchers working on quantum computing [15].

In mathematical logic, we consider that such entities like formal languages for expressing formulas, relational structures (models) and satisfiability relations, are *given*. Contrary to this traditional situation, in the considered case of Intelligent Systems dealing with complex phenomena, *these entities should be discovered (induced) from gathered data*. Moreover, this process often should be realised through hierarchical learning [16-19]. In IGrC one should consider complex reasoning strategies making it possible to construct complex entities, called c-granules. These strategies should support (i) construction of configurations of c-granules and initiate interactions of objects in them, (ii) perceiving properties of objects and interactions between them as well as (iii) performing reasoning over information gathered in informational layers of generated c-granules to control computations toward achieving by c-granule(s) needs or goals, e.g., estimation of satisfiability degree of given specification. It is worthwhile mentioning that the main idea of c-granules is consistent with the idea of computational building blocks which according to Valiant (see: <http://people.seas.harvard.edu/~valiant/researchinterests.htm>) is necessary for cognition. In the Intelligent Systems based on IGrC, such reasoning, called *judgment*, should be performed on information embedded in informational layers of c-granules. This information is gathered during interactions with other c-granules and the environment over interactive granular computations. Control of c-granules is responsible for generating computations which makes it possible to efficiently perform the judgment process.

Let us note that the task specifications for Intelligent Systems are often expressed using complex vague concepts expressed in natural language. Such concepts may be not directly understandable by the system and it is necessary to provide the reasoning with *decomposition strategies* leading, after multilevel decomposition, to concepts for which is possible to induce models by the system and next in a bottom up approach approximate the whole hierarchy. In this decomposition experience based reasoning by experts is used. This is emphasised by Zadeh [20-21] in discussion on *information granulation* and *divide-and-conquer strategy realised by humans*.

Crucial objects constructed in IGrC are *complex games*. Any complex game consists of a family of complex vague concepts labeled by decisions represented by specifications of actions/ plans triggered by these concepts (when they are satisfied to satisfactory degree). Reasoning strategies leading to inducing approximate models of such concepts as well as conclusions about satisfiability of such guards in the currently perceived situation should be provided. Many examples of such strategies are used in Machine Learning [22], e.g., in reinforcement learning [23]. However, scalability of these methods for Intelligent Systems dealing with complex phenomena in the real physical world is still a great challenge.

In general, new methods of reasoning should be developed for generating *of intelligent behaviours of interacting societies of c-granules* (whether they are living organisms or physical objects that are not living organisms) aiming to satisfy the input requirements formulated for them in Intelligent Systems [24].

It is also worthwhile to mention that based on above mentioned reasoning strategies one can define *generalised approximation spaces for adaptive approximation of vague concepts*. This is a new approach in rough sets [25-28] where membership degrees of the perceived situations are derived using reasoning, called judgment.

We would like to also emphasize the role of reasoning, called judgment, for the control of a c-granule. The further development of judgment methods will play the principal role in further development of Intelligent Systems. These reasoning methods are far beyond the existing deductive methods, well already developed in mathematical logic, or even inductive reasoning (e.g., in Machine Learning). They should take into account, e.g., experience as well as explanation of behaviour. These reasoning methods should be grounded on a new computing model making it possible to perform reasoning from sensory measurement to perception (i.e., understanding the perceived situation). We propose to base such a model on interactive c-granules having their informational parts grounded in the physical world.

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# Remote Sensing from High up in Space to Deep Down in Earth

by Manfred F. Buchroithner EUAS

## Short Biography

*Manfred Ferdinand Buchroithner (\*17-12-1950) studied Geology & Palaeontology at the University of Graz/Austria and both Remote Sensing and Cartography at ITC/Netherlands. He obtained his PhD in 1977 in Graz. In 1982 he went as Fulbright Scholar to the USA (Fort Worth/Texas, Boulder/Colorado and Stanford University/California). During the following years at the Institute for Cartography of the Austrian Academy of Sciences in Vienna and as Director of the Joanneum Research Institute of Digital Image Processing and Computer Graphics in Graz he spent several months of postdoctoral research at the Finnish National Research Center/VTT in Espoo near Helsinki and at the Jet Propulsion Laboratory/JPL of NASA in Pasadena. In 1985 he obtained his habilitation (venia legendi) for both General Geology and Remote Sensing. From 1992 to 2016 he was Full Professor, holding the Chair of Cartography at TU Dresden, Germany. Subsequently he held the position of a Senior Professor until the end of 2019. M. F. Buchroithner led many expeditions to high mountain regions in the Andes, Alps, Balkan mountain ranges, Kilimanjaro Massif, Altai mountains, most of the regions of High Asia (Tian Shan, Pamir, Hindu Kush, Karakorum, Himalaya, Tibet incl. Nyenchen Tanglha Mountains and Kailash) and to Borneo/Malaysia. He spent semesters as Invited Professor at the Universities of Munich/Germany, Salzburg/Austria (twice), Bergamo/Italy, COMSATS/Islamabad, and the École Nationale Supérieure des Mines des Paris in Sophia Antipolis/France and also gave invited guest lectures at various Chinese universities. He supervised and successfully graduated more than 50 doctoral students. Buchroithner both authored and edited several books on cartographic, GIT and remote sensing issues and has more than 500 publications incl. maps and several educational films to his credit. He holds international patents in 3D cartography, is member of several learned societies and obtained a series of national and international scientific awards, i.a. the Friedrich Hopfner Medal (A) and the Denny Medal (UK).*

## Advances in Mars Research and Exploration

*A 2022 Book Editorial from:*

**Bhardwaj, A., Sam, L., Buchroithner, M.F. & Galofre, A.G. (Ed.s, 2022): Advances in Mars Research and Exploration. Frontiers in Astronomy and Space Science, 9: 971104. August 2022. 2 pp. Taylor & Francis. DOI:10.3389/fspas.2022.971104.**

The pursuit of finding habitable conditions or life outside our planet has always been fascinating. In terms of habitability, Mars is the most Earth-like planet within our solar system as it displays comparable physical determinants such as radius, mass, and temperature, and physicochemical markers such as available energy, substrate stability, suitable chemistry, and past liquid stability. In addition, the Martian regolith and

subsurface contain water in frozen and possibly in liquid or transient liquid states; Mars has moderate surface gravity to enable future colonization; and the Martian climate, although harsh, can still theoretically support life forms analogous to terrestrial extremophiles. Thus, Mars research and exploration holds a significant place in planetary sciences, advancing our knowledge beyond the Earth.

The interest towards Mars research and exploration has gained significant momentum in the past three decades owing to the advances in computing, hardware, remote sensors, public data availability, and outreach. The next stages of this exploration demand more multidisciplinary efforts to effectively use the vast planetary data being gathered using various missions, platforms, and techniques. With this overview, our Research Topic aimed to bring together research and reviews from the Mars community covering topics on geomorphology, atmosphere, geochemistry, and future exploration. The editorial team consisted of academics from early, mid, and advanced career stages, offering valuable perspectives and feedbacks throughout the editorial process. After thorough review, all the accepted papers in the present Research Topic were novel, comprehensive, and informative with emphasis on the systematic and recent advances in our knowledge, tools, techniques, and methods for Mars research and exploration.

Within Martian geomorphology and geochemistry disciplines, two papers were accepted for publication. The first such paper by Howari et al. investigates certain aspects of recurring slope lineae (RSL), the dark albedo features which are often interpreted as possible transiently flowing water on Martian surface. Using multisensory datasets from High Resolution Imaging Science Experiment (HiRISE), Compact Reconnaissance Imaging Spectrometer for Mars (CRISM), Context Camera (CTX), and Mars Orbiter Laser Altimeter (MOLA), Howari et al. start with providing an updated global distribution map of RSL sites, and they further go on to perform a geomorphological and compositional analysis of Asimov and Hale craters, two confirmed RSL sites. Howari et al. also investigate the possibility of RSL activity due to deliquescence mediated by favourable temperature and humidity conditions, concluding that the local temperatures in Asimov Crater are high enough to allow deliquescence during the months of RSL activity with a water vapor column nearly five times higher than those measured before RSL appearance. The second paper addressing Martian geomorphology, authored by Chao and Zhibao, investigates the distribution characteristics and patterns of dune landforms. This study also took a multisensory approach, taking key inputs from CTX, Thermal Radiation Imaging System (THEMIS), HiRISE, and MOLA. The results from Chao and Zhibao indicate that the Martian dunefields are spatially distinct, scattered, and mainly concentrated in high-latitude and polar regions. Similar to their terrestrial counterparts, Martian dunes are mainly located in low-lying geomorphic units which favour sand accumulation. Based on these results, Chao and Zhibao conclude the limited sand supply as an important feature of the Martian dune development conditions, and their spatially scattered nature can provide important clues to understanding the Martian aeolian environment and evolutionary history.

The other published papers explored various aspects of the Martian electromagnetic and radiation environment. For example, Gonçalves et al. validate a model which is used to predict the radiation environment expected at different locations on the Martian orbit, atmosphere and surface, as a function of epoch, latitude and longitude. The model is called the detailed Martian Energetic Radiation Environment Model (dMEREM), developed for

the European Space Agency, and it takes into account the specific atmospheric and soil composition, based on different particle propagation codes for primary Galactic Cosmic Rays or Solar Particle Events. Gonçalves et al. validate dMEREM with differential proton fluxes measured with the NASA Curiosity rover Radiation Assessment Detector (RAD) at the Gale Crater, at the surface of Mars. The authors report a good agreement between the proton fluxes measured at the surface with RAD and the corresponding dMEREM predictions, thus proving the usefulness of dMEREM in the assessment of the expected ionising radiation field on the surface of Mars. The only review article in this Research Topic, authored by Mittelholz and Johnson discusses the Martian crustal magnetic field, discussing its presence, magnitude, and significance from the Martian subsurface to its upper atmosphere. Research on Mars' crustal magnetic field can offer vital clues about the planet's interior evolution and surface crustal modification. While available datasets have provided useful information on the acquisition and modification of magnetization in the crust, the authors highlight several research gaps regarding the nature and origin of crustal magnetization, and the past of Martian magnetism. Mittelholz and Johnson also discuss the ways in which all these research questions can be addressed through laboratory analysis, modelling and new datasets.

Finally, two of the published papers aimed at future Mars exploration. The paper by *Poian et al.* argues in favour of the concept of science autonomy to reduce data redundancy. As a pioneering work in this domain, the authors develop a proof-of-concept for Mars Organic Molecule Analyzer (MOMA) instrument onboard the planned ExoMars rover, where MOMA will be able to perform selected onboard science data analyses and then act upon those analyses through self-adjustment and tuning of instrument parameters. *Poian et al.* also discuss the challenges and limitations of this implementation for future missions. Another paper by *Abel et al.* covers all the more important topic of *in-situ* resource utilisation (ISRU) for future Mars missions. The authors integrated climate data into a radiative transfer model to show the usefulness of photovoltaics-based power systems as an adequate and practical solution to sustain a crewed mission for an extended period and that too over a large fraction of the Martian surface. Thus, all the published studies in this Research Topic demonstrate the importance of different research and exploration activities aimed at improving our understanding of the Red Planet. Many progresses are expected in relation with the forthcoming exciting Mars missions which are supposed to target the current four goals, prioritised by the Mars Exploration Program Analysis Group (MEPAG), pertaining to Martian habitability, climate, geology, and preparation for human exploration.

#### **Quantitative assessment of ground deformation risks, controlling factors and movement trends for onshore petroleum and gas industry using satellite Radar remote sensing and spatial statistics**

**Bayramov, E., Buchroithner, M-F., Kada, M. & Bayramov, R. (2022): Quantitative assessment of ground deformation risks, controlling factors and movement trends for onshore petroleum and gas industry using satellite Radar remote sensing and spatial statistics. In: Georisk: Assessment and Management of Risk for Engineered Systems and Geohazards. Vol.12 (2022), 2: 283 – 300**

A number of productive oil and gas fields are located in the Absheron Peninsula of Azerbaijan. The primary goal of the presented study was to quantitatively assess the ground deformation (subsidence and uplift) rates of oil and gas fields, determine natural and man-made influencing factors and predict deformation trends. Persistent Scatterer Interferometric Synthetic Aperture Radar technique was used for the present studies to detect ground deformation rates and velocities in the Absheron oil and gas fields. The existence of ground deformation processes was observed for the period of 2015–2017 with three hotspots of highest subsidence rates and three hotspots of highest uplift rates in oil and gas fields. The determined maximum displacement rates of subsidence and uplift processes were  $-26$  mm/y and  $+23$  mm/y, respectively. However spatial density analysis of deformation velocity presented the natural patterns of uplift and subsidence tectonic processes. This allowed to determine that two oil and gas fields hold a higher probability of being affected by man-made oil and gas exploration activities, whereas the one oil field is affected by both natural and man-made processes. Geographically Weighted Regression analysis revealed that well concentration and elevation factors provided 32% of explanation to subsidence processes.

# Combining an Intensive Green Roof with Seismic Retrofitting of Typical Reinforced Concrete Buildings in Israel

**by Yuri Ribakov, Member EUAS**

## Short Biography

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*Ph.D. 1998 – 2001 Department of Civil Engineering, Technion - Israel Institute of Technology, Haifa, Israel.*

*M.Sc. 1995-1998 Department of Civil Engineering, Technion - Israel Institute of Technology, Haifa, Israel.*

*B.Sc. 1984-1991 Faculty of Civil Engineering, Ukrainian Institute of Water Management Engineering, Rivne, Ukraine (with first class honors).*

## Professional Experience

*I have a total more than 20 years of industrial, teaching and research experience in structural engineering.*

*2018 – present Head, Division of Structural Engineering, Department of Civil Engineering, Faculty of Engineering, Ariel University, Ariel, Israel.*

*2015 – present Full Professor, Department of Civil Engineering, Faculty of Engineering, Ariel University, Ariel, Israel.*

*2011 – 2014 Head, Department of Civil Engng, Faculty of Engineering, Ariel University,*

*2010 – 2015 Associate Professor, Department of Civil Engineering, Faculty of Engineering, Ariel University, Ariel, Israel.*

*2005 – 2010 Senior Lecturer, Department of Civil Engineering, Faculty of Engineering, Ariel University, Ariel, Israel.*

*2005 – 2008 Adjunct Senior Lecturer, Department of Civil Engineering, Faculty of Engineering, Ben Gurion University of Negev, Beer Sheva, Israel.*

*2000 – 2005 Lecturer, Department of Civil Engineering, Faculty of Engineering, Ariel University, Ariel, Israel.*

*1995 - 2000 Instructor, Structural Engineering Division, Faculty of Civil Engineering, Technion - Israel Institute of Technology, Haifa, Israel.*

*1992 - 1994 Deputy Chairman, Building Department, United Municipal Structures, Rivne, Ukraine.*

*1991 - 1992 Engineer - Researcher, Building Materials Division, Faculty of Civil Engineering, Ukrainian Institute of Water Management Engineering, Rivne, Ukraine.*

*1990–1991 Senior laboratory assistant, Division of Geomechanics and Foundations, Faculty of Civil Engineering, Ukrainian Institute of Water Management Engineering, Rivne, Ukraine.*

## Research Experience & Interests

*Structural Engineering in general, Earthquake Engineering, Structural Dynamics, Seismic Design and Reinforced Concrete Structures and Elements in particular.*

## Honors & Awards

*1999 Tuvia Netzer award – given for the research entitled “Influence of dampers on response of tall buildings to earthquakes”.*

*2000 Abraham and Miriam Gutwirth Research Award.*

*2004 Award for excellence in research and teaching, Ariel University.*

*2005 Award for excellence in research and teaching, Ariel University.*

2006 Award for excellence in research and teaching, Ariel University.  
 2007 Award for excellence in research and teaching, Ariel University.  
 2008 Award for excellence in research and teaching, Ariel University.  
 2010 Award for excellence in research and teaching, Ariel University.  
 2011 Award for excellence in research and teaching, Ariel University.  
 2012 Award for excellence in research and teaching, Ariel University.  
 2013 Award for excellence in research and teaching, Ariel University.  
 2013 Reviewing Excellence Award, Engineering Structures, Elsevier.  
 2014 Outstanding Reviewer Award, Engineering Structures, Elsevier.  
 2019 Award for excellence in research, Ariel University.

#### **Research Grants**

2008 – 2011 Y. Ribakov (PI 1) and G. Agranovich (PI 2). *Improving Seismic Response of Structures Using Optimal Dampers. Ministry of National Infrastructures, Israel.*

2012 Y. Ribakov (PI 1) and G. Agranovich (PI 2). *Optimization of Hybrid Energy Dissipation Systems for Improving Structural Seismic Response. The Ministry of Energy and Water Resources of Israel.*

2013 – 2015 Y. Ribakov (PI 1) and S. Pushkar (PI 2). *Seismic resistant of green buildings. The Ministry of Environmental Protection of Israel.*

2014 – 2015 M. Ben Chaim (PI 1) and Y. Ribakov (PI 2). *Investigation of the Possible Impact on the Environment of Converting the Existing Vehicle Engines in Israel to Natural Gas. The Ministry of Environmental Protection of Israel.*

### **Combining an Intensive Green Roof with Seismic Retrofitting of Typical Reinforced Concrete Buildings in Israel**

Svetlana Pushkar, Ido Halperin , Yuri Ribakov  
 Materials, 2022 Jan 24;15(3):889. doi: 10.3390/ma15030889

#### **Abstract**

This study suggests an intensive green roof as part of a sustainable and hazard-resistant conceptual design for the retrofitting of old buildings in Israel. The roof is suggested to be built with waste-based materials. A five-story reinforced concrete residential building was retrofitted with: Case 1: concrete wall strengthening (CWS)-conventional concrete + conventional green roof; Case 2: CWS-waste-included concrete + waste-based green roof; Case 3: seismic isolation columns (SIC)-conventional concrete + conventional green roof; and Case 4: SIC-waste-included concrete + waste-based green roof. Palekastro, Nuweiba, Tabas, and Erzincan ground motions were used for a structural dynamic time-history analysis of the retrofitted buildings. Life cycle assessments of cases 1-4 were performed using ReCiPe 2016 midpoint and endpoint evaluations. A two-stage analysis of variance (ANOVA) was used to analyze the ReCiPe endpoint results. According to the seismic results, Case 3 and Case 4 were much more preferable to Case 1 and Case 2, whereas according to the environmental evaluations, Case 4 was the most preferable to the other cases.

**Using Experimental Statistical Models for Predicting Strength and Deformability of Self-Compacting Concrete with Ground Blast-Furnace Slag**

Vadim Zhitkovsky, Leonid Dvorkin, Dmyrto Kochkarev, Yuri Ribakov  
Materials, 2022 Jun 9; 15(12):4110, doi: 10.3390/ma15124110.

**Abstract**

Ground blast-furnace slag is one of the waste products available in Ukraine and other countries. It is obtained at metallurgical enterprises in huge quantities and can be efficiently used for concrete production. The article is devoted to obtaining experimental-statistical models of the influence of technological factors that determine the composition of self-compacting concrete (SCC) based on ground blast-furnace slag and polycarboxylate superplasticizer on compressive strength, tensile strength, prismatic strength, elastic modulus and crack resistance. Analysis of the investigated factors' influence on the specified SCC properties is carried out and positive influence of blast-furnace slag and superplasticizer simultaneous action on durability and deformation characteristics is studied. A design method of SCC composition design using the obtained mathematical models is developed. It allows for the consideration of a set of necessary parameters simultaneously. A numerical example is given.

**Experimental Verification of Theoretical Stress-Strain Model for Compressed Concrete Considering Post-Peak Stage**

Iakov Iskhakov, Ilya Frolov and Yuri Ribakov  
*MDPI Materials Journal*, 2022, 15, 6064.

**Abstract**

The theoretical stress-strain model for compressed composite cement materials' behavior without empirical coefficients includes the following main parameters describing concrete behavior: stresses and strains corresponding to the border between the elastic and non-elastic behavior stages of a concrete specimen, ultimate elastic strains, and stresses and strains at the end of the post-peak region. Particular attention is focused on the descending branch of the stress-strain diagram, as well as on the analysis of concrete elastic and plastic potentials. These potentials are important for assessing the dynamic response of the concrete element section, as well as for concrete creep analysis. The present research is aimed at experimental verification of the above-mentioned theoretical model. The obtained experimental results are in good agreement with the theoretical ones, which confirms the model's accuracy and enables a significant reduction in the empirical coefficients number in compressed reinforced concrete elements design. This, in turn, represents the scientific novelty of this study.

**Life-Cycle Assessment of Contemporary and Classical Seismic Retrofitting Approaches Applied to a Reinforced Concrete Building in Israel**

S. Pushkar, I. Halperin and Y. Ribakov

**Abstract**

This study aims to select an eco-friendly earthquake-resistant design using life-cycle assessments (LCAs). The study compares LCAs of three retrofitting cases: concrete shear-wall strengthening (Case 1); reinforced concrete column jacketing with shear-wall strengthening (Case 2); and high-damping rubber bearing base isolation with viscous fluid damping devices (Case 3). These cases were applied to a five-story reinforced concrete building built according to the design principles widely used in Israel in the 1970s. The seismic-bearing capacity of the retrofitted building was improved in all three cases, where Case 3 was observed as being the most effective retrofitting measure. The environmental performance of the retrofitting measures was assessed using the ReCiPe 2016 midpoint, which indicated that Case 3 was the best with the least environmental impact, Case 1 was intermediate with moderate environmental impact, and Case 2 was the worst with the most environmental impact. However, the ReCiPe 2016 endpoint single-score results showed that Case 3 caused significantly less damage than Cases 1 and 2, which caused similar significant environmental damage. These results indicate that LCA should be used to select an eco-friendly earthquake-resistant design.

# Large Seasonal Fluctuations of Groundwater Radioiodine Speciation and Concentrations in a Riparian Wetland in South Carolina

by Peter H. Santschi, Member EUAS



## Short Biography

*Dr. Peter H. Santschi is a Regents Professor of Oceanography and Marine Sciences at the Texas A&M University, Galveston, TX, USA. He received his training in Geochemistry and Oceanography during his post-graduate work at L-DEO at Columbia University, N.Y., after graduating from the University of Bern, Switzerland, with a Ph.D. in Chemistry. Dr Santschi's research interests include Marine Chemistry, Environmental Chemistry and Environmental Radiochemistry; trace element interactions with natural organic matter; Tracer applications in natural water systems using stable and radioactive isotopes. Since 2000, he is associate editor of the journal Marine Chemistry. He is an author of well over 300 journal articles and 45 book chapters on these subjects, which, over the years, have received more than 15,000 citations. More on his research can be found at <https://www.tamug.edu/mars/faculty-bios/PeterHSantschi.html> and <https://scholar.google.com/citations?user=ZKGyOTsAAAAJ&hl=en&oi=ao>.*

*His total of 400+ peer-reviewed publications, according to the ISI Web of Science (all databases as of August 3, 2020), attest to his productivity, while his citation record is a testimony of his impact. Santschi's record is thus not only of quantity alone but predominantly of quality. Metrics establishing scientific impact are difficult to come by, but if the citation count and other indexes (e.g., h-index from ISI, all databases) may serve as a measure of scientific impact, then his 400+ publications have been cited over 17,000 times, with an average citation per publication of over 42. Other indexes for his publications (ISI h-index = 71 and productivity m-index =  $h/\Delta t = 1.51$  with  $\Delta t = 47$  years since the 1st publication in 1974; g-index = 137; and Google Scholar h-index = 87 and i-10 index = 293, with well over 25,000 citations) are exceptional.*

*Peter H. Santschi received **numerous national and international awards**, e.g., he was elected Member of the European Union Academy of Sciences (EUAS) (2020), Geochemical Fellow of the Geochemical Society and the European Association of Geochemistry (2017); Fellow of the American Geophysical Union (2014), which are given annually to only 0.1% of the 60,000 members; received the Distinguished Achievement Awards in Graduate Student Mentoring (2013) from Texas A&M's Association of Former Students; Regents Professor of Texas A&M University (2009), and received the Association of Former Student Distinguished Achievement Award for Research from Texas A&M University (2004). These awards were not possible without many collaborative and/or supportive scientists.*

***His international pre-eminence** is not only demonstrated by the prestigious awards that he received, but also by the fact that he was invited as a member of Academic Advisory or Review Panels, as well as a Visiting Professor at national and international Universities, e.g., at Lamont-Doherty Earth Observatory of Columbia University (1982-1988), University of Rhode Island, School of Oceanography (1986), Dept. of Geology and Dept. of Chemistry, University of Geneva, Geneva, Switzerland (1996), Dept. of Chemistry and Biochemistry, University of Bern, Bern, Switzerland (2002), Dept. of Chemistry, University of Geneva, Geneva, Switzerland (2003), Swiss Institute of Technology, ETH, Zurich, Switzerland (2003), National Taiwan University, Taipei, Taiwan (2003), and Hong Kong University of Science and Technology (2004), National Center for Oceanographic Research, NCOR (2008).*

***Summary of Accomplishments in Environmental Science.** During his 45-plus year career in environmental science, Santschi has gained and communicated novel insights into some of the blueprints of the aquatic environment, spanning from rain water, rivers and lakes to groundwater, from surface to deep ocean. During*

his long research career, he, together with 40+ graduate students, post-doctoral fellows and scientists all over the world, was able to pioneer new concepts and approaches that were truly **transformational**. The unifying theme of his research has been the **study of the self-cleansing capacity of natural aquatic systems**: in particular, the importance of natural organic matter compounds for particle, radionuclide, and trace element cycling in aquatic systems. The importance of natural organic matter was not obvious in aquatic chemistry, as for many decades, the dogma was that metal behavior is mostly controlled by inorganic ligand interactions. His research involves the main agents that can ameliorate impact (e.g., toxicity, mobility) of potential pollutants to aquatic biota, i.e., microbially produced macromolecular substances that occur in the colloidal phase. This phase is mostly composed of nano-sized exopolymeric substances, as well as terrestrially derived humic substances, both of which can, at times, greatly help to control the efficiency of the self-cleansing capacity of aquatic systems. Natural colloids in aquatic systems are thus, to a large extent, derived from biological production and degradation of natural particles. Therefore, Peter's main contributions and impacts in environmental geochemistry are on the role of macromolecular natural organic matter, trace metal, and radionuclide speciation, transport, and cycling.

Dr. Santschi's **seminal contributions** to science, more specifically to the field of environmental biogeochemistry and radiochemistry, have thus included major **transformational** breakthroughs, e.g., the Colloidal (or Brownian) Pumping Concept that led to paradigm shifts in aquatic science (see below), and sustained impact, with his most cited papers providing unifying chemical and physico-chemical concepts explain pollutant behavior in aquatic environments, including articles published from the 1980s, 1990s, and 2000s. This transformational "Colloidal or Brownian Pumping Model" was able to simulate observations of apparent particle concentration effects on both the widely observed particle-water distribution coefficients and the model kinetic constants of trace element and radionuclide uptake onto natural particles, given the observed colloidal fractions of trace metals and radionuclides. His work then stimulated many other researchers to build on these novel concepts. Over the years following this transformational work, he tackled the challenging question of macromolecular organic compounds that occur in the colloidal phase and act as carrier molecules for specific trace elements and radionuclides. Due to the numerous difficulties in finding such compounds at relevant but trace levels in the midst of thousands of other compounds, selective separation and purification chemistry had to be thoroughly tested, before state-of-the-art instrumentation can be applied.

### Abstracts of Recent Publications

1. **Kaplan, D.I., Nichols, R., Xu, C., Lin, P., Yeager, C.M., Santschi, P.H. 2022. Large seasonal fluctuations of groundwater radioiodine speciation and concentrations in a riparian wetland in South Carolina. STOTEN.**

**Abstract:** Recent studies evaluating multiple years of groundwater radioiodine (<sup>129</sup>I) concentration in a riparian wetland located in South Carolina, USA identified strong seasonal concentration fluctuations, such that summer concentrations were much greater than winter concentrations. These fluctuations were observed only in the wetlands but not in the upland portion of the plume and only with <sup>129</sup>I, and not with other contaminants of anthropogenic origin: nitrate/nitrite, strontium-90, technetium-99, tritium, or uranium. This unexplained observation was hypothesized to be the result of strongly coupled processes involving hydrology, water temperature, microbiology, and chemistry. To test this hypothesis, an extensive historical groundwater database was evaluated, and additional measurements of total iodine and iodine speciation were made from recently collected samples. During the summer, the water table decreased by as much as 0.7 m, surface water temperature increased by as much as 15 °C, and total iodine concentrations were consistently greater (up to 680%) than the following winter months. Most of the additional iodine observed in the summer could be attributed to proportional gains inorganic-iodine, and not iodide or iodate. Furthermore, <sup>129</sup>I concentrations were

observed to be two-orders-of-magnitude greater at the bottom of the upland aquifer than at the top. A coupled hydrological and biogeochemical conceptual model is proposed to tie these observations together. First, as the surface water temperature increased during the summer, microbial activity was enhanced, which in turn stimulated the formation of mobile organo-I. Hydrological processes were also likely involved in the observed iodine seasonal changes: (1) as the water table decreased in summer, the remaining upland water entering the wetland was comprised of a greater proportion of water containing elevated iodine concentrations from the low depths, and (2) waterflow paths in summer changed such that the wells intercepted more of the contaminant plume and less of the diluting rainwater (due to evapotranspiration) and stream water (as the lower levels promote a predominantly recharging system). These results underscore the importance of coupled processes influencing contaminant concentrations, and the need to assess seasonal contaminant variations to optimize long-term monitoring programs of wetlands.

- 2. Xu, C., Lin, P., Garimella, R., Li, D., Xing, W., Patterson, N., Kaplan, D.I., Yeager, C.M., Hatcher, P.G., Santschi, P.H. 2022. <sup>1</sup>H-<sup>13</sup>C heteronuclear single quantum coherence NMR evidence for iodination of natural organic matter influencing organo-iodine mobility in the environment. STOTEN.**

**Abstract:** The complex biogeochemical behavior of iodine (I) isotopes and their interaction with natural organic matter (NOM) pose a challenge for transport models. Here, we present results from iodination experiments with humic acid (HA) and fulvic acid (FA) using <sup>1</sup>H-<sup>13</sup>C heteronuclear single quantum coherence (HSQC) nuclear magnetic resonance (NMR) spectroscopy. Even though not a quantitative approach, <sup>1</sup>H-<sup>13</sup>C HSQC NMR corroborated that iodination of NOM occurs primarily through aromatic electrophilic substitution of proton by I, and also revealed how iodination chemically alters HA and FA in a manner that potentially affects the mobility of iodinated NOM in the environment. Three types of iodination experiments were conducted with HA and FA: a) non-enzymatic iodination by IO<sub>3</sub><sup>-</sup> (pH 3) and I<sup>-</sup> (pH 4 and 7), b) addition of lactoperoxidase to promote I<sup>-</sup>-iodination in the presence of the cosubstrate, H<sub>2</sub>O<sub>2</sub> (pH 7), and c) addition of laccase for facilitating I<sup>-</sup>-iodination in the presence of O<sub>2</sub>, with or without a mediator (pH 4). When mediators or H<sub>2</sub>O<sub>2</sub> were present, extracellular oxidases and peroxidases enhanced I<sup>-</sup> incorporation into NOM by between 54% and 3400%. Iodination of HA, which was less than that of FA, enhanced HA's stability (inferred from increases in aliphatic compounds, decreases in carbohydrate moieties, and thus increased molecular hydrophobicity) yet reduced HA's tendency to incorporate more iodine. As such, HA is expected to act more as a sink for iodine in the environment. In contrast, iodination of FA appeared to generate additional iodine binding sites, which resulted in greater iodine uptake capability and enhanced mobility (inferred from decreases in aliphatic compounds, increases in carbohydrates, and thus decreases in molecular hydrophobicity). These results indicate that certain NOM moieties may enhance while others may inhibit

radioiodine mobility in the aqueous environment.

- 3. Weerakkody, W.S., Ling, K., Hsieh, H.-H., Abedneko, V.G., Shyu, J.-F., Lee, T.-M., Shih, Y.-Y., Ranatunga, K., Santschi, P.H., Hung, C.-C. 2023. Carbon capture by the macroalgae, *Sarcodia suae*, using aquaculture wastewater and green energy in subtropical regions. STOTEN, 855 (2023) 158850.**

**Abstract:** Rapid growth in the aquaculture industry and corresponding increases in nutrient and organic carbon levels in coastal regions can lead to eutrophication and increased greenhouse gas emissions. Macroalgae are the organisms primarily responsible for the capture of CO<sub>2</sub> and removal of nutrients from coastal waters. In the current study, we developed a novel wastewater treatment system in which the red macroalga, *Sarcodia suae*, is used to capture CO<sub>2</sub> under thermo- static conditions in subtropical regions. In 2020 (without temperature control), the carbon capture rate (CCR) of *Sarcodia suae* varied considerably with the season: winter/spring (2.1–3.9 g-C m<sup>-2</sup> d<sup>-1</sup>) and summer (0.09 g-C m<sup>-2</sup> d<sup>-1</sup>). In 2021, solar powered cooling reduced summer seawater temperatures from 31 to 33 °C to 23–25 °C with a corresponding increase in the mean CCR: winter/spring (2–7 g-C m<sup>-2</sup> d<sup>-1</sup>) and summer (1.33 g-C m<sup>-2</sup> d<sup>-1</sup>). The proposed aquaculture wastewater system proved highly efficient in removing nitrogen (20.7 mg-N g<sup>-1</sup> DW d<sup>-1</sup>, DW = dry weight) and phosphorus (4.4 mg-P g<sup>-1</sup> DW d<sup>-1</sup>). Furthermore, the high density of *Sarcodia* (1.10 ± 0.03 g cm<sup>-3</sup>) would permit the harvesting and subsequent dumping of *Sarcodia* in deep off-shore waters. This study demonstrated a low-cost land-based seaweed cultivation system for capturing CO<sub>2</sub> and excess nutrients from aquaculture wastewater year-round under temperature-controlled environments in subtropical regions.

- 4. Lin, T.-Y., Chen, C.-L., Shih, Y.-T., Hsieh, H.-H., Huang, W.-J., Santschi, P.H. Hung' C.-C. 2023. A smallholders' mariculture device for rearing seafood: environmentally friendly, and providing improved quality. Sustainability, 15, 110.3390/su15010862.**

**Abstract:** The aquaculture industry in Taiwan grosses more than USD 1.1 billion annually; however, it also generates considerable waste discharge (causing eutrophication in estuarine and coastal waters) and heavy groundwater withdrawals (causing land subsidence in coastal areas). Many aquaculture facilities using earth ponds are affected by benthic algae, resulting in an earthy odor, and fixed-cage farms are difficult to relocate during cold weather events. In this study, we tested small-scale (~15 ton) mobile cage tanks for the nearshore rearing of white shrimp and grouper in the Yung-An district of Kaohsiung, Taiwan. At the conclusion of the mariculture ex-periment, the content of free amino acids in shrimp and groupers reared in our mobile tanks sur-passed that in animals reared locally in traditional earthy ponds. In a blind taste test involving 42 volunteers, groupers reared in mobile cage tanks were deemed more palatable than those raised in ponds. Our results

demonstrate that small-scale mobile cage tanks are a feasible approach to the sustainable rearing of high-quality shrimp or fish. Note that wastewater from the mobile tanks is easily diluted by seawater, thereby reducing the likelihood of eutrophication in coastal regions. The proposed system could also be used for recreational fishing activities to increase income for smallholders of fishermen and/or aquaculture farmers.

## Development of Novel Nanomaterials for Energy and Environmental Applications

by Yoshio Bando, Member EUAS



### Short Biography

*Prof. Yoshio Bando has been leading the communities of nanomaterials and electron microscopy for many years. Holding a PhD degree from Osaka University, he joined the National Institute for Research in Inorganic Materials (NIRIM) in 1975. In 2001, NIRIM was merged with the National Research Institute for Metals to form the National Institute for Materials Science (NIMS), and he was appointed as Director of the Advanced Beam Analysis Group, followed by being appointed Director-General of International Center for Young Scientist. He became a NIMS Fellow in 2004. From 2008 to March 2017, he was responsible for the operation of MANA with the appointed position of Chief Operating Officer (COO). In addition, he was adjunct professor at the University of Tokyo (2009-2012) and guest professor of Waseda University (2008-2016). After retirement of NIMS in 2017, he has been appointed as Distinguished Professor at the University of Wollongong (UOW) from 2017 to 2021, Australia. He was also Professor at Institute for Molecular Plus, Tianjin University China from 2018 to 2021. He is now an Emeritus Fellow of NIMS and Honorary Professors at UOW and University of Queensland (UQ), Australia. He is also Distinguished Scientist at King Saud University (KSU), Saudi Arabia. He has received many prestigious awards and fellowships, including the "Sacred Treasure" given from the Japanese Emperor in 2017, The 3rd Thomson Reuters Research Front Award in 2012, The Tsukuba Prize in 2005, Academician, The Commendation Award by the Minister of State for Science and Technology in 1998, The Academic Award of the Ceramic Society of Japan in 1997, The Seto Award of Electron Microscopy Society of Japan in 1994 and others. He was appointed as adjunct member of the Science Council of Japan in 2006. He is also a Fellow of the American Ceramic Society and the Royal Society of Chemistry. He served as Editor-in-Chief of Journal of Electron Microscopy and Editorial Board Members of "Nano Energy", "Small", "Nanotechnology", "Materials Horizon", "Nanomaterials" and others. He has been selected as ISI Highly Cited Researcher in Materials Science in 2012, 2014, 2015, 2016 2017, 2018, 2019, 2020, 2021 and 2022. To date, he has authored about 940 original/review research papers that have been cited more than 67,400 times with h-index of 136 (Web of Science in 2022). He has registered 43 foreign patents and 70 Japanese patents.*

## Research Activities

### **1. MOF-on-MOF nanoarchitectures for selectively functionalized nitrogen-doped carbon-graphitic carbon/carbon nanotubes heterostructure with high capacitive deionization performance<sup>1)</sup>**

Carbon-carbon heterostructures are an emerging material paradigm to promote the development of capacitive deionization (CDI). The synthesis of this heterostructure with designed functionalities derived from metal-organic frameworks (MOFs) is interesting, but it has always been challenging. We develop MOF-on-MOF nanoarchitectures to obtain a selectively functionalized nitrogen-doped carbon@graphitic carbon/carbon nanotubes heterostructure (NC@GC/CNTs) via the direct pyrolysis of elaborately designed ZIF-L@ZIF-67 core-shell precursors. In this core-shell nanoarchitecture, the inner Zn-based ZIF-L provides a well-defined 2D interface for the oriented growth of the Co-based ZIF-67 outer layer, which will then convert to NC nanosheets with a high nitrogen doping content and large specific surface area for the accommodation of more ions. Meanwhile, the outer ZIF-67 layer creates highly graphitized GC/CNTs architecture offering fast electron transfer and good chemical stability, and it addresses the possible aggregation or collapse of the inner ZIF-L precursors during pyrolysis. As expected, the newly developed NC@GC/CNTs material with well-designed functionalities exhibits high salt adsorption capacity, rapid salt adsorption rate, and excellent CDI cycling stability, which highlight the significance of the carbon-carbon heterostructure to potential CDI applications and the importance of MOF-on-MOF nanoarchitectures on nanomaterials synthetic chemistry.

### **2. Ion transport channels in redox flow deionization enable ultra-high desalination performance<sup>2)</sup>**

Redox flow deionization (RFD) is an emerging derivative of redox flow cell technology that desalinizes salt water while simultaneously storing energy. However, conventional RFDs are limited by high specific energy consumption and low salt removal rates caused by low ionic conductivity in low-salinity ranges (especially  $< 3000 \text{ mg L}^{-1}$ ). This study investigates the potential of ion transport channels composed of ion exchangers to enhance ionic conductivity in low-salinity ranges. The RFD cell with ion exchangers (IE-RFD) exhibited significantly lower resistance and specific energy consumption than conventional RFD cells when processing low salinity feeds.

A finite element analysis demonstrated that the current density in the ion exchangers, especially where the ion exchangers were in contact, was much higher than that of the surrounding solution, indicating effective ion transport in low-salinity ranges. The IE-RFD cell showed excellent desalination performance (99.4% at 10 000 mg L<sup>-1</sup>) and low energy consumption (0.99 Wh L<sup>-1</sup>). We did not observe any deterioration in performance over 10 d of continuous desalination. Compared with other electrochemical desalination technologies, e.g., membrane capacitive deionization, flow capacitive deionization, and traditional RFD, the IE-RFD is superior in terms of energy consumption, salt removal ability, and stability. This study described an efficient strategy to enhance the desalination performance of RFDs through ion transport channels. With further optimization, this technology could help to alleviate the critical global demand for fresh water using minimal energy.

## **References**

1. Y. Zhang, J. Wu, S. Zhang, N. Shang, X. Zhao, S. M. Alshehri, T. Ahamad, Y. Yamauchi, X. Xu and Y. Bando, "MOF-on-MOF nanoarchitectures for selectively functionalized nitrogen-doped carbon-graphitic carbon/ carbon nanotubes heterostructure with high capacitive deionization performance", *Nano Energy*, 97, 107146 (2022).
2. P. Lin, T. Yang, Z. Li, W. Xia, X. Xuan, X. Sun, Smashers, T. Ahamad, Y. Yamauchi, X. Xu and Y. Bando, "Ion transport channels in redox flow deionization enable ultra-high desalination performance", *Nano Energy*, 102, 1076522022 (2022).

# Energy Storage through Innovative Synthesis and Processing of Nanomaterials

by Leon L. Shaw, Member EUAS

## Short Biography

### **Current Positions**

- *Rowe Family Endowed Chair Professor in Sustainable Energy, Department of Mechanical, Materials & Aerospace Engineering, Illinois Institute of Technology (IIT), Chicago, Illinois, USA*
- *Professor of Materials Science and Engineering, Department of Mechanical, Materials & Aerospace Engineering, Illinois Institute of Technology (IIT), Chicago, Illinois, USA*
- *Director of the Thermal Processing Technology Center, Illinois Institute of Technology (IIT), Chicago, Illinois, USA*

### **Education**

- Ph. D. Materials Science and Engineering, University of Florida, Gainesville, Florida, USA, 1992*  
*Minor Mechanics and Engineering Science, Univers. of Florida, Gainesville, Florida, USA, 1992*  
*M. S. Materials Science and Engineering, University of Florida, USA, 1992*  
*M. Eng. Mechanical Engineering, Fuzhou University, Fuzhou, Fujian, China, 1987*  
*B. S. Materials Engineering, Fuzhou University, Fuzhou, Fujian, China, 1980*

### **Professional Activities**

- Member Editorial Board for “Scientific Reports”*  
*Member Editorial Board for “Batteries”*  
*Member Editorial Board for “Journal of Sol-Gel Science and Technology”*  
*Member International Advisory Committee of THERMEC’ 2011, 2013, 2016, and 2018*  
*Member ASM International*  
*Member TMS*  
*Member American Ceramic Society*  
*Member Electrochemical Society*

*Guest Editor Metallurgical and Materials Transactions (1998), Materials Science and Engineering (1998,2001, 2007), Journal of Materials Engineering and Performance (2005), Journal of Materials Science (2011)*

### **Awards and Honors**

- *Fellow, ASM International (since 2004)*
- *Fellow, World Academy of Materials and Manufacturing Engineering, Poland (since 2005)*
- *Member, Connecticut Academy of Science and Engineering (since 2006)*
- *Member, EU Academy of Sciences (since 2019)*
- *Fellow, International Association of Advanced Materials (since 2020)*
- *“Researchers to Know in 2020” recognized by Illinois Science & Technology Coalition.*
- *“Excellence in Research Award for 2020”, Department of Mechanical, Materials and Aerospace Engineering, Illinois Institute of Technology.*
- *“IAAM Fellow Lecture” at the Advanced Materials Lecture Series, published at the Open Access Video Proceedings of Advanced Materials: VPOAM-2020- RG-E-12, 2020.*
- *“Energy Award” in 2018 presented by International Association of Advanced Materials.*
- *“Energy Award Lecture” in the Plenary Session of the 20<sup>th</sup> Assembly of the European Advanced Materials Congress 2018.*
- *Outstanding Poster Award, MS&T’ 2011, October 16 – 20, 2011, Columbus, OH (2011).*
- *The John & Virginia Towers Distinguished Lecture, Michigan Technological University, April 2010*
- *2006 Outstanding Faculty Member Award of the Materials Science and Engineering Program, UConn.*
- *Listed in Marquis Who’s Who in the World (since 2005), Marquis Who’s Who in American Education (since 2005), Marquis Who’s Who in Finance and Business (since 2005), Marquis Who’s Who in Science and Engineering (since 2004), and Marquis Who’s Who in America (since 2001)*

- *The Best Poster Award in the 14<sup>th</sup> Solid Freeform Fabrication (SFF) Annual Meeting, Austin, TX, August 2003.*
- *UConn Metallurgy and Materials Engineering 2001 Outstanding Department Member Award.*
- *UConn School of Engineering Outstanding Junior Faculty Award, 2000.*
- *UConn Metallurgy and Materials Engineering 1999 Outstanding Department Member Award.*
- *Honorary Advisory Professorship of Harbin Institute of Technology, Harbin, China (since 1999).*
- *Honorary Guest Professorship of Fuzhou University, Fuzhou, China (since 1999).*
- *Olin Junior Faculty Development Award, Olin Corporation (1995)*
- *Los Alamos National Laboratory J. Robert Oppenheimer Postdoctoral Fellowship Award, 1994 (awarded, but accepted UConn's faculty position).*
- *First place of the ASM International Graduate Student Paper Contest, ASM International (1992).*
- *Oak Ridge National Laboratory Eugene P. Wigner Fellowship Award, 1992 (awarded, but accepted Systran's Research Scientist position).*
- *Lifetime Member of Alpha Sigma Mu (International Metallurgical Honorary Society) since 1990.*

#### **Publications, Patents and Presentations**

- *Over 320 publications including 3 edited books, 10 book chapters, 228 archival refereed journal articles, 4 editorial materials, and 77 conference proceedings*
- *Citation: 12,809; h-index: 59; i10-index: 194 (Google Scholar)*
- *Top 1.4% citations for career-long impact among all scientific fields and top 0.2% citations for career-long impact in the subfield of "materials" (based on the composite score c compiled by Elsevier).*
- *More than 320 presentations including 80+ keynote presentations, plenary lectures and invited talks at various national and international conferences as well as a wide range of universities and companies in and outside the United States.*
- *Leon Shaw's research is focusing on materials synthesis and processing for energy storage recently.*

#### **Recent Publications from Shaw's Group**

1. **B. Liu, M. Luo, Z. Wang, C. Passolano and L. Shaw, "On the Specific Capacity and Cycle Stability of Si@void@C Anodes: Effects of Particle Size and Charge/Discharge Protocol," *Batteries*, 8, 154 (2022).**

**Abstract:** Silicon has potential to be a high-performance anode material, but its practical application is impeded by huge volume expansion during lithiation. Many studies have revealed that the huge volume expansion problem can be mitigated by introducing engineered voids into Si/C core-shell structures. In this study, a Si/C core/shell structure with engineered voids, termed as Si@void@C, is investigated for its specific capacity and cycle stability as a function of particle size and charge/discharge protocol. The study shows that finer Si@void@C particles result in higher specific capacities, but with little impact on the cycle stability. Further, lower and upper cutoff voltages in charge/discharge have profound impact on the specific capacity and cycle stability. Importantly, cutoff voltages in formation cycles have long-lasting effects on the cycle stability, indicating the critical role of forming a robust solid electrolyte interphase (SEI) layer during formation cycles. Using constant current charge followed by potentiostatic hold charge can further improve the cycle stability and minimize the sharp capacity decay in the first 20 – 40 cycles. With proper choices of charge/discharge protocols, the specific capacities of Si@void@C anodes at the electrode level are 66.8%, 38.2% and 22.7% higher than those of graphite anodes at the 1<sup>st</sup>, 300<sup>th</sup> and 500<sup>th</sup> cycles, respectively, proving

that Si@void@C has promising potential to replace graphite anodes for practical applications in the future.

2. C. Chen, V. R. Tatagari, H. Lin and L. Shaw, “Investigating TEP as a Greener Alternative to NMP in Ni-rich Cathode Fabrication,” *Journal of Energy Chemistry*, in press.

**Abstract:** In the past decade, the surging demand for portable electronics, electric vehicles, and stationary energy storage grids has triggered a noticeable rise in the production of Li-ion batteries (LIBs). However, this swift rise is now hindered by relying on the use of N-methyl-2-pyrrolidone (NMP), a repro-toxic solvent, in the current cathode processing of LIBs. To overcome this challenge, here we have investigated triethyl phosphate (TEP) as a greener alternative to NMP. The compatibility with polyvinylidene fluoride (PVDF) binder, the slurry rheology, the electrode morphology and cell performance with Ni-rich cathodes are characterized. The results show that TEP-based samples possess indistinguishable characteristics in all aspects studied when compared with NMP, revealing that TEP is a promising substitute for NMP in processing Ni-rich cathodes. It is anticipated that this green solvent, TEP, will draw attention from industry in the real-world LIB application in the future.

3. J. Wei, L. Shaw and W. Chen, “Mechanism of Cr Migration in Hybrid Layered NaCrO<sub>2</sub> Cathode,” *Physical Review Materials*, **6**, 095403 (2022).

**Abstract:** The Cr migration and O3→P3 phase transformation in layered NaCrO<sub>2</sub> restrict its application as a promising cathode material with high reversible capacity and good cycle retention. The hybrid phased NaCrO<sub>2</sub> with alternating octahedral and prismatic Na layers is often more stable than the O3 stacking in highly charged states. To suppress the undesirable Cr migration, a systematic first-principles study on the Cr migration in layered O3 and biphasic O2P NaCrO<sub>2</sub> is performed to understand the migration process and discover potential strategies to suppress it. Firstly, three factors are found to affect the Cr migration energy ( $E_{\text{mig}}$ ): the Na concentration, local 3D configuration, and 2D in-plane geometry. A low Na concentration and two special 3D configurations facilitate the Cr migration. Then, the Cr migration barriers in both O3 and biphasic NaCrO<sub>2</sub> are found positively correlated with the Cr  $E_{\text{mig}}$ . The Cr migration is triggered by the Na diffusion while the overall migration barrier remains similar as the sole Cr migration. Lastly, the Cr migration of 17 doped O3 and O2P NaCrO<sub>2</sub> is studied. Optimal dopants for Cr migration suppression are identified by considering both Cr and dopant  $E_{\text{mig}}$ . The comparative study of the Cr migration between O3 and O2P NaCrO<sub>2</sub> points out the significant role of hybrid phases in the application of layered cathode materials.

4. Q. He, M. Ashuri, Y. Liu, B. Liu and L. Shaw, “Silicon Micro-Reactor as a Fast Charge, Long Cycle Life Anode with High Initial Coulombic

**Efficiency for Li-ion Batteries,”** *ACS Appl. Energy Mater.*, 4 [5] 4744 – 4757 (2021).

**Abstract:** Applications of silicon as a high-performance anode material has been impeded by its low intrinsic conductivity and huge volume expansion (> 300%) during lithiation. To address these problems, nano-Si particles along with conductive coatings and engineered voids are often employed, but this results in high cost anodes. Here, we report a scalable synthesis method that can realize high specific capacity (~800 mAh g<sup>-1</sup>), ultrafast charge/discharge (at 8 A g<sup>-1</sup> Si) and high initial Coulombic efficiency (~90%) with long cycle life (1000 cycles) at the same time. To achieve 1000 cycle stability, micron-sized Si particles are subjected to high-energy ball milling to create nanostructured Si building blocks with nano-channel shaped voids encapsulated inside a nitrogen (N)-doped carbon shell (termed as Si micro-reactor). The nano-channel voids inside a Si micro-reactor not only offer the space to accommodate the volume expansion of Si, but also provide fast pathways for Li ion diffusion into the center of the nanostructured Si core and thus ultrafast charge/discharge capability. The porous N-doped carbon shell helps to improve the conductivity while allowing fast Li ion transport and confining the volume expansion within the Si micro-reactor. Submicron-sized Si micro-reactors with limited specific surface area (35 m<sup>2</sup> g<sup>-1</sup>) afford sufficient electrode/electrolyte interfacial area for fast lithiation/delithiation, leading to the specific capacity ranging from ~800 to 420 mAh g<sup>-1</sup> under ultrafast charging conditions (8 A g<sup>-1</sup>), but not too much interfacial area for surface side reactions and thus high initial coulombic efficiency (~90%). Since Si micro-reactors with superior electrochemical properties are synthesized via an industrially scalable and eco-friendly method, they have the potential for practical applications in the future.

**5. M. Luo, M.-T. F. Rodrigues, L. Shaw and D. P. Abraham, “Examining Effects of Negative to Positive Capacity Ratio in 3-Electrode Lithium-ion Cells with Layered Oxide Cathode and Si Anode,”** *ACS Appl. Energy Mater.*, 5 [5] 5513-5518 (2022).

**Abstract:** In practical applications, the areal specific capacity ratios of the negative to positive electrode (N:P ratio) is crucial for full cell design in order to achieve both high energy density and long lifetime battery. In this study, the effect of N:P ratio (1.22 and 1.45) on electrochemical performance has been investigated in NMC/Si cells. With individual electrode potentials monitored in three-electrode cells, different depths of lithiation/delithiation at the anode and cathode were found to play an important role on cell performance. With less lithiation at the anode, the higher N:P ratio cell displays superior performance, including greater reversibility, better capacity retention and lower impedance rise, due to less volume change of silicon during cycling. Our data demonstrate that deterioration of the Si anode during cycling is the predominant factor determining the degradation in full cell performance.

# Two-dimensional Turbulence : A Physicist Approach

by Patrick Tabeling, Member EUAS

## Short Biography

*Patrick Tabeling is leader of the group MMN, a prominent team in the field of microfluidics. Visiting researcher in Chicago University (1984-1985), Directeur de Recherches CNRS at ENS (1985-2001), visiting professor to UCLA, Directeur de Recherches, Professor at ESPCI. He is cofounder of the Institut Pierre-Gilles de Gennes, and has been its director for the period July 2011-July 2018. He is the author of 200 papers, 30 patents, 100 invited talks in international conferences. He is member of Academia Europae. He is the cofounder of MicroFactory and Minos Biosciences. He published the book entitled "An introduction to microfluidics" (Oxford University Press (2005)), the second edition appearing in 2023.*

## Abstracts of some papers

### **Two-dimensional turbulence : a physicist approach(2002)**

**P Tabeling**

**Physics reports 362 (1), 1-62 (2002)**

Much progress has been made on two-dimensional turbulence, these last two decades, but still, a number of fundamental questions remain unanswered. The objective of the present review is to collect and organize the available information on the subject, emphasizing on aspects accessible to experiment, and outlining contributions made on simple flow configurations. Whenever possible, open questions are made explicit. Various subjects are presented: coherent structures, statistical theories, inverse cascade of energy, condensed states, Richardson law, direct cascade of enstrophy, and the inter-play between cascades and coherent structures. The review offers a physicist's view on two-dimensional turbulence in the sense that experimental facts play an important role in the presentation, technical issues are described without much detail, sometimes in an oversimplified form, and physical arguments are given

### **Local investigation of superfluid turbulence (2003)**

**J Maurer, P Tabeling**

**EPL (Europhysics Letters) 43 (1), 29 (2003)**

We investigate flows of helium IV driven by two counter-rotating disks, in a range of

temperatures varying between 1.4 and 2.3 K. The local pressure fluctuations obtained on a small total-head tube are analyzed. Above  $T_\lambda$ , the sensor allows to measure the local velocity fluctuations, and below  $T_\lambda$ , it determines the local fluctuations of a linear combination of the normal and superfluid flow components. Above and below  $T_\lambda$ , Kolmogorov spectra are clearly obtained, with similar Kolmogorov constants. Evidence for persistence of inertial range intermittency in the superfluid region is presented. At all temperatures below  $T_\lambda$ , the structure function exponents are found indistinguishable from those currently observed in normal fluid turbulence.

### **Slippage of water past superhydrophobic carbon nanotube forests in microchannels (2006).**

**P Joseph, C Cottin-Bizonne, JM Benoit, C Ybert, C Journet, P Tabeling, ...**  
**Physical review letters 97 (15), 156104**

We present in this Letter an experimental characterization of liquid flow slippage over superhydrophobic surfaces made of carbon nanotube forests, incorporated in microchannels. We make use of a particle image velocimetry technique to achieve the submicrometric resolution on the flow profile necessary for accurate measurement of the surface hydrodynamic properties. We demonstrate boundary slippage on the Cassie superhydrophobic state, associated with slip lengths of a few microns, while a vanishing slip length is found in the Wenzel state when the liquid impregnates the surface. Varying the lateral roughness scale  $L$  of our carbon nanotube forest-based superhydrophobic surfaces, we demonstrate that the slip length varies linearly with  $L$  in line with theoretical predictions for slippage on patterned surfaces.

### **Nanofluidics at the Debye layer at hydrophilic and hydrophobic surfaces (2008).**

**CI Bouzigues, P Tabeling, L Bocquet**  
**Physical Review Letters 101 (11), 114503**

By using evanescent waves, we study equilibrium and dynamical properties of liquid-solid interfaces in the Debye layer for hydrophilic and hydrophobic surfaces. We measure velocity profiles and nanotracer concentration and diffusion profiles between 20 and 300 nm from the walls in pressure-driven and electro-osmotic flows. We extract electrostatic and zeta potentials and determine hydrodynamic slip lengths with 10 nm accuracy. The spectacular amplification of the zeta potential resulting from hydrodynamic slippage allows us to clarify for the first time the dynamic origin of the zeta potential.

### **Monodisperse colloids synthesized by microfluidic technology (2010)**

**F Malloggi, N Pannacci, R Attia, F Monti, P Mary, H Willaime, P Tabeling, ...**

Langmuir 26 (4), 2369-2373

Limitations in the methods employed to generate micrometric colloidal droplets hinder the emergence of key applications in the fields of material science and drug delivery. Through the use of dedicated nanofluidic devices and by taking advantage of an original physical effect called capillary focusing, we could circumvent some of these limitations. The nanofluidic (i.e., submicrometric) devices introduced herein are made of soft materials, and their fabrication relies upon rapid technologies. The objects that we have generated are simple droplets, multiple droplets, particles, and Janus particles whose sizes lie between 900 nm and 3  $\mu\text{m}$  (i.e., within the colloidal range). Colloidal droplets have been assembled on-chip into clusters and crystals, yielding discrete diffraction patterns.

### **Droplet based microfluidics at the femtoliter scale (2015).**

M Leman, F Abouakil, AD Griffiths, P Tabeling  
Lab on a Chip 15 (3), 753-765

We have built a toolbox of modules for droplet-based microfluidic operations on femtolitre volume droplets. We have demonstrated monodisperse production, sorting, coalescence, splitting, mixing, off-chip incubation and re-injection at high frequencies (up to 3 kHz). We describe the constraints and limitations under which satisfactory performances are obtained, and discuss the physics that controls each operation. For some operations, such as internal mixing, we obtained outstanding performances: for instance, in 75 fL droplets the mixing time was 45  $\mu\text{s}$ , 35-fold faster than previously reported for a droplet microreactor. In practice, in all cases, a level of control comparable to nanolitre or picolitre droplet manipulation was obtained despite the 3 to 6 order of magnitude reduction in droplet volume.

### **Universal diagram for the kinetics of particle deposition in microchannels (2018)**

CM Cejas, F Monti, M Truchet, JP Burnouf, P Tabeling  
Physical Review E 98 (6), 062606

Why do particles, suspended in a fluid and traveling in a channel, deposit onto walls? The question has far-reaching implications in different domains (filtering, syringeability, fouling, etc.). Close to a channel wall, particles are subject to a variety of effects, which control their trajectories: hydrodynamic forces, diffusion, van der Waals adhesion forces, and electrostatic forces. The existing theories and phenomenologies, due to their inherent limitations, and the numerical and experimental studies, due to their scarcity, did not allow thus far to establish a general description of the deposition process. By coupling microfluidic experiments, theory, and numerics, we succeed in establishing a general description of the phenomenon. We discover that the problem is particularly rich. We show the existence of three regimes: van der Waals, Debye, and diffusive, each including various subregimes.

## **Microfluidic actuators based on temperature-responsive hydrogels (2018)**

L d'Eramo, B Chollet, M Leman, E Martwong, M Li, H Geisler, J Dupire, ...  
*Microsystems & Nanoengineering* 4 (1), 1-7 (2016)

The concept of using stimuli-responsive hydrogels to actuate fluids in microfluidic devices is particularly attractive, but limitations, in terms of spatial resolution, speed, reliability and integration, have hindered its development during the past two decades. By patterning and grafting poly (N-isopropylacrylamide) PNIPAM hydrogel films on plane substrates with a 2  $\mu\text{m}$  horizontal resolution and closing the system afterward, we have succeeded in unblocking bottlenecks that thermo-sensitive hydrogel technology has been challenged with until now. In this paper, we demonstrate, for the first time with this technology, devices with up to 7800 actuated micro-cages that sequester and release solutes, along with valves actuated individually with closing and opening switching times of  $0.6\pm 0.1$  and  $0.25\pm 0.15$  s, respectively.

## **Foams as self-assembling amorphous photonic band gap material (2019)**

J Ricouvier, P Tabeling, P Yazhgur  
*Proceedings of the National Academy of Sciences* 116 (19), 9202-9207 (2019)

We show that slightly polydisperse disordered 2D foams can be used as a self-assembled template for isotropic photonic band gap (PBG) materials for transverse electric (TE) polarization. Calculations based on in-house experimental and simulated foam structures demonstrate that, at sufficient refractive index contrast, a dry foam organization with threefold nodes and long slender Plateau borders is especially advantageous to open a large PBG. A transition from dry to wet foam structure rapidly closes the PBG mainly by formation of bigger fourfold nodes, filling the PBG with defect modes. By tuning the foam area fraction, we find an optimal quantity of dielectric material, which maximizes the PBG in experimental systems. The obtained results have a potential to be extended to 3D foams to produce a next generation of self-assembled disordered PBG materials

## **Performing POC molecular testing for SARS-COV-2 with RNA extraction and isothermal amplification (2021)**

P Garneret, E Coz, E Martin, JC Manuguerra, E Brient-Litzler, V Enouf, ...  
*PLoS One* 16 (1), e0243712

To respond to the urgent need for COVID-19 testing, countries perform nucleic acid amplification tests (NAAT) for the detection of SARS-CoV-2 in centralized laboratories. Real-time RT—PCR (Reverse transcription—Polymerase Chain Reaction), used to amplify and detect the viral RNA., is considered, as the current gold standard for diagnostics. It is an efficient process, but the complex engineering required for automated

RNA extraction and temperature cycling makes it incompatible for use in point of care settings [1]. In the present work, by harnessing progress made in the past two decades in isothermal amplification and paper microfluidics, we created a portable test, in which SARS-CoV-2 RNA is extracted, amplified isothermally by RT—LAMP (Loop-mediated Isothermal Amplification), and detected using intercalating dyes or fluorescent probes. Depending on the viral load in the tested samples, the detection takes between twenty minutes and one hour. Using a set of 16 pools of naso-pharyngeal swab eluates, we estimated a limit of detection comparable to real-time RT-PCR (i.e. 1 genome copies per microliter of clinical sample) and no cross-reaction with eight major respiratory viruses currently circulating in Europe. We designed and fabricated an easy-to-use portable device called “COVIDISC” to carry out the test at the point of care. The low cost of the materials along with the absence of complex equipment will expedite the widespread dissemination of this device. What is proposed here is a new efficient tool to help managing the pandemics.

## More Developments in Ion-Solid Interactions

by William J. Weber, Member EUAS



### Short Biography

**Professor, Department of Materials Science and Engineering, The University of Tennessee - Knoxville**

*Prof. William J. Weber received his PhD in Nuclear Engineering from the University of Wisconsin - Madison, USA. He joined Pacific Northwest National Laboratory (PNNL) in 1977 as a research scientist and was appointed Laboratory Fellow in 1997. During 1983, he was a visiting scientist at the Institute for Transuranium Elements in Karlsruhe, Germany. He is currently a professor in the Department of Materials Science and Engineering at the University of Tennessee and Director of the Ion Beam Materials Laboratory. From 2010 through 2020, he was the Governor's Chair Professor for Radiation Effects in Materials at the University of Tennessee, with a joint appointment at Oak Ridge National Laboratory. His research has encompassed the fundamental aspects of radiation-solid interactions, radiation effects in materials, ion beam modification and analysis of materials, and defects and defect processes in materials. Much of his current research emphasizes the coupling of electronic and atomic energy dissipation processes and their role on radiation effects, defect evolution, formation of novel nanostructures, creation of new functionalities, and the response of materials to extreme environments. He is a member of the EU Academy of Sciences (2016), Fellow of the American Ceramic Society (2000), Fellow of the American Association for the Advancement of Science (2006), Fellow of the Materials Research Society (2008), Fellow of the American Physical Society (2010) and Fellow of the Ion Beam Society of India (2016). He is the recipient of the James I. Mueller Award from the American Ceramic Society (2020); Lee Hsun Lecture Award (2015); the Outstanding Young Alumni Award (1983) and the Distinguished Alumni Award (2009) from the University of Wisconsin - Oshkosh; the PNNL Laboratory Director's Award for Individual Lifetime Achievement in Science & Technology (2009); the PNNL Laboratory Director's Award for Scientific and Engineering Excellence (1995); the PNNL Chester L. Cooper Mentor of the Year Award (2005); and the U.S. Department of Energy's Materials Science Award for Research with Significant Implication for DOE Related Technologies (1995). He has published more than 597 journal articles, 118 peer-reviewed conference papers, and 14 book chapters. Based on the Web of Science, his publications have over 26,000 citations, with an h-index of 80; based on Scopus, his publications have over 27,330 citations, with an h-index of 81; based on Google Scholar, his publications have over 34,600 citations, with an h-index of 90.*

The interaction of energetic ions with a solid is well known to result in inelastic energy loss to electrons and elastic energy loss to atomic nuclei in the solid. However, the coupled effects of these energy loss pathways and the critical role of energy dissipation processes

on defect production and the evolution of defects, nanostructures and phase transformations under far from equilibrium conditions in materials are complex and not well understood. Particularly challenging are the dynamics of energy transfer processes to electrons and the exchange of energy between electrons and the atomic nuclei via electron-phonon coupling. In general, the electrons along the ion path undergo a high degree of excitation and electron–electron scattering, and they subsequently transfer much of their energy, via electron–phonon coupling, to atoms in the same region, causing a highly-localized thermal spike. Following thermalization of the electrons and recombination of electrons and holes, a high density of localized electronic defects (trapped electrons, holes and excitons) may remain. This partitioning of energy deposition and energy dissipation on the electronic and atomic structures are important to the control of ion beam modification methods to create defects and nanoscale structures that tailor materials properties or create new functionalities, as well as the development of radiation-tolerant materials and devices. Predicting and modeling such complex processes, which are temporally and spatially coupled, are grand challenges that demand fundamental understanding of materials processes at the level of electrons and atoms over several orders of magnitude in time scale, from femtoseconds to nanoseconds.

Oxide perovskites exhibit fascinating properties that identify them as key materials for the next generation of multifunctional devices, and ion-beam modification can be used to tune their functionality. While it is well-established that atomic-level defects are created by elastic (nuclear) energy transfer,  $S_n$ , from charged particles to atomic nuclei, the effects of inelastic (electronic) energy loss,  $S_e$ , to target electrons is more complicated. High-energy ions with  $S_e$  values above a threshold interact synergistically with pre-existing disorder in  $\text{SrTiO}_3$  and  $\text{KTaO}_3$  to form amorphous nanotracks along ion trajectories at 300 K. The nanotrack cross-sections increase with  $S_e$  and the level of pre-existing disorder, and the inelastic energy loss threshold,  $S_{et}$ , decreases with increasing level of disorder. Application of the analytical thermal spike model suggests a decrease in effective melting temperature and increase in efficiency of track formation with increasing disorder. Molecular dynamics simulations combined with the inelastic thermal spike model confirm that the formation of these amorphous tracks is due to melt-quenching along the ion trajectory. While high energy ions contribute to damage production above  $S_{et}$ , the effects of inelastic energy loss on pre-existing disorder below  $S_{et}$  have not been studied in detail. To investigate this, pre-damaged surface layers of  $\text{SrTiO}_3$  have been irradiated with 200 keV electrons, 2 MeV He, 1.2 MeV C, 5 MeV C and 12 MeV O ions, and pre-damaged surface layers of  $\text{KTaO}_3$  have been irradiated with 5 MeV C and 12 MeV O ions. The results indicate two distinct regimes of ionization-induced recovery in  $\text{SrTiO}_3$  and only a single recovery regime in  $\text{KTaO}_3$ . While melt-quenching does not occur for these ions, the inelastic thermal spike for C and O ions, with  $S_e$  between 1.6 and 3 keV/nm, causes sufficient local heating via electron-phonon coupling to induce defect recovery in both  $\text{SrTiO}_3$  and  $\text{KTaO}_3$ , which has been confirmed by MD simulations for the case of  $\text{SrTiO}_3$ . At lower values of  $S_e$ , the efficiency of defect recovery decreases by several orders magnitude for 2 MeV He ions and 200 keV electrons in  $\text{SrTiO}_3$ , and this recovery is attributed to local electronic excitations that enhance defect mobility. In undamaged  $\text{KTaO}_3$ , irradiation with 200 keV electrons results in ionization-induced damage formation.

Oxygen vacancies are known to play a central role in the optoelectronic properties of oxide perovskites. A detailed description of the exact mechanisms by which oxygen vacancies govern such properties is still quite incomplete. The unambiguous identification

of oxygen vacancies has been a subject of intense discussion. Interest in oxygen vacancies is not purely academic, but also of technical interest. Precise control of oxygen vacancies has technological benefits in optoelectronic devices. Irradiation constitutes an efficient and reliable strategy to introduce, monitor, and characterize oxygen vacancies. The primary experimental results obtained for oxygen vacancy centers under high energy electron irradiation (100 keV-1 MeV) in  $\text{LiNbO}_3$  and under high-energy (1-20 MeV) heavy ion irradiation in  $\text{SrTiO}_3$  have been reviewed. In both cases, the experiments have used *real-time* and *in-situ* optical detection. Our current view is that a consistent picture is now emerging on the structure and relevant optical features (absorption and emission spectra) of these vacancy centers. One key aspect pertains to the generation of self-trapped electrons as small polarons from irradiation of the crystal lattice and the stabilization of the small polarons by oxygen vacancies. What has been learned by observing the interplay between polarons and vacancies has inspired new models for color centers in dielectric crystals.

The initial luminescence yield of amorphous silica under ion irradiation has been studied at temperatures between 30-100 K, using swift ions of different masses and energies. The intensity of the 2.1 eV emission band, ascribed to the intrinsic recombination of self-trapped excitons (STEs), has been found to vary systematically with ion mass, energy and irradiation temperature. A detailed model has been developed to quantitatively describe those variations in terms of the competition between non-radiative Auger recombination, STE formation, STE thermal dissociation, and subsequent STE hopping and capture at non-radiative sinks. The model, which uses a thermal spike approach to describe the effect of swift ion irradiation, is found to quantitatively predict the experimental data without adjustable parameters. It provides new insights into the interactions of carriers in an ion track and the behavior of the luminescence emissions during ion irradiation (ionoluminescence). The model is found to predict the correct temperature dependence of the yield if an activation energy for STE thermal migration of 0.12 eV is assumed, which is in good agreement with values previously reported.

High-entropy pyrochlore oxides have recently gained recognition for their low thermal conductivity and tunable mechanical capabilities, but little is known about their irradiation behavior. In recent work, the heavy-ion irradiation response of single-crystal, high-entropy oxides (HEO) with the pyrochlore structure have been investigated. The damage accumulation behavior at 300 K due to 4 MeV Au ion irradiation of a  $\langle 100 \rangle$ -oriented HEO single crystal has been investigated by Rutherford backscattering spectrometry in channeling mode and transmission electron microscopy. The results reveal that this high-entropy pyrochlore goes amorphous at a dose of 0.13 dpa. In another HEO single-crystal composition, the amorphization due to 23 MeV Ni ions has been characterized by Raman spectroscopy, and the results reveal that amorphization occurs at a dose of 2.5 dpa in the near-surface region, which suggests that the high electronic energy loss may be causing simultaneous damage annealing.

**Select Publications Related to This Research**

1. W. J. Weber, H. Xue, E. Zarkadoula, and Y. Zhang, Two regimes of ionization-induced recovery in SrTiO<sub>3</sub> under irradiation, *Scripta Materialia* **173**: 154-157 (2019).
2. E. Zarkadoula, Y. Zhang, and W. J. Weber, Molecular dynamics simulations of the response of pre-damaged SrTiO<sub>3</sub> and KTaO<sub>3</sub> to fast heavy ions, *AIP Advances* **10**: 015019 (2020).
3. Y. Zhang and W. J. Weber, Ion irradiation and modification: The role of coupled electronic and nuclear energy dissipation and subsequent nonequilibrium processes in materials, *Applied Physics Reviews* **7**: 041307 (2020).
4. Y. Zhang, C. Silva, T. G. Lach, M. A. Tunes, Y. Zhou, L. Nuckols, W. L. Boldman, P. D. Rack, S. E. Donnelly, L. Jiang, L. Wang, and W. J. Weber, Role of electronic energy loss on defect production and interface stability: Comparison between ceramic materials and high-entropy alloys, *Current Opinion in Solid State & Materials Science* **26**: 101001 (2022).
5. M. L. Crespillo, J. T. Graham, F. Agulló-López, Y. Zhang, and W. J. Weber, Real-Time Identification of Oxygen Vacancy Centers in LiNbO<sub>3</sub> and SrTiO<sub>3</sub> during Irradiation with High Energy Particles, *Crystals* **11**: 315 (2021).
6. J. T. Graham, M. L. Crespillo, F. Agulló-López, and W. J. Weber, Light emission of self-trapped excitons from ion tracks in silica glass: Interplay between Auger recombination, exciton formation, thermal dissociation, and hopping, *Acta Materialia* **229**: 117829 (2022).
7. G. Velisa, E. Zarkadoula, D. Iancu, M. D. Mihai, C. Grygiel, I. Monnet, B. Kombaiyah, Y. Zhang and W. J. Weber, Near-surface modification of defective KTaO<sub>3</sub> by ionizing ion irradiation, *J. Physics D: Applied Physics* **54**: 375302 (2021).
8. D. Iancu, E. Zarkadoula, M. D. Mihai, C. Burducea, I. Burducea, M. Straticiuc, Y. Zhang, W. J. Weber, and G. Velisa, Revealing two-stage phase transition process in defective KTaO<sub>3</sub> under inelastic interactions, *Scripta Materialia* **222**: 115032 (2023).
9. C. Kinsler-Fedon, L. Nuckols, C. T. Nelson, Z. Qi, Q. Huang, D. Mandrus, Y. Zhang, W. J. Weber, and V. Keppens, Effects of Au<sup>2+</sup> irradiation induced damage in a high-entropy pyrochlore single crystal, *Scripta Materialia* **220**: 114916 (2022).

# Evaporation Flow Characteristics of Airborne Sputum Droplets with Solid Fraction of COVID 19

by Shigenao Maruyama, Member EUAS



## Short Biography

*Present Affiliation: President, National Institute of Technology, Hachinohe College, Hachinohe 039-1192, Japan*

## **Academic Qualifications**

*B.Eng. 1977, Department of Mechanical Engineering II, Tohoku University, Japan*

*M.Sc. 1979, Department of Aeronautics, Imperial College, London University, UK*

*M.Eng. 1980, Department of Mechanical Engineering, Tohoku University, Japan*

*PhD 1983, Department of Mechanical Engineering, Tohoku University, Japan*

## **Professional Carriers**

*1983 Assistant Professor, Institute of High Speed Mechanics, Tohoku University*

*1988 Visiting Scholar, School of Mechanical Engineering, Purdue University, USA*

*1989 Associate Professor, Institute of Fluid Science, Tohoku University*

*1997 Professor, Institute of Fluid Science, Tohoku University.*

*2005-2006 Specially Appointed Assistant to the President, Tohoku University*

*2006-2009 Councilor, Tohoku University*

*2006-2008 Special Advisor to President, Tohoku University*

*2006-2013 Special Advisor for Centenary Events and Alumni, Tohoku University*

*2008-2011, 2015-2017 Distinguished Professor of Tohoku University*

*2016 Visiting Professor, INSA de Lyon*

*2017- President, National Institute of Technology, Hachinohe College*

## **Awards**

*Japan Society of Mechanical Engineers (JSME), Award for Young Engineers, 1989*

*Fluid Science Foundation, Award for Fluid Science, 1995*

*Heat Transfer Society of Japan (HTSJ), Award for Scientific Contribution, 1998, 2016*

*JSME Medal for Outstanding Paper, 1999, 2013*

*HTSJ, Award for Scientific Measurement, 1999*

*JSME Tohoku Division, Award for Technical Contribution, 2001*

*Japan Society of Applied Electromagnetic and Mechanics, Best Technical Contribution Award, 2001*

*JSME Thermal Engineering Division, Award for Academic Achievements, 2001*

*HTSJ, Award for Technical Contribution, 2002*

*Societe Francaise de Themique, 2002 International SFT Award, 2002*

*JSME Thermal Engineering Division, Award for Contribution, 2003*

*JSME Fellow, 2004*

*Government of Japan, Japanese Medal of Honor (Medal with Purple Ribbon), 2012*

*JSME Thermal Engineering Division, Award for Achievements (Research), 2012*  
*HTSJ Honorary Member, 2020*

## Research Activities

Professor Shigenao Maruyama specializes in thermal engineering. He has published more than 10 books and 300 academic research papers, and has acquired 60 patents. He investigated various aspects of fluid flow and energy exchange. Based on the principle that conventional heat transfer and thermal control focuses on the enhancement of heat transfer and temperature control of equipment, he has proposed a novel concept of heat-transfer control, in which the heat transfer is actively enhanced or reduced. The proposed active thermal insulation system and a heat-transfer control device utilizes Peltier effects. His work is interdisciplinary utilizing knowledge from various academic disciplines. He has co-authored and edited Thermodynamics (JSME Text series) [1], one of the bestselling books on thermodynamics for mechanical engineering students in Japan. He has also published a book to educate the public thermal science [2], and a novel describing accidents in Fukushima Daiichi nuclear plants [3].

Some aspects of his research activities are as follows:

**Radiative heat transfer:** Detailed studies on radiative heat transfer, which is energy transfer by infrared or electromagnetic waves, has been carried out. A generalized analysis method to calculate radiative heat transfer was proposed [4], and this method was applied to analyze heat transfer in semi-conductor processes [5] and industrial furnaces. This method was also applied to large-scale environmental energy transfer processes, such as heat transfer in fogs and clouds [6]. Thermal emission from nano-scale structures was also investigated [7]. These results were published in a monograph [8] which is the first textbook on radiative heat transfer in Japan.

**Natural convection:** Natural convection induced by temperature differences in fluid and the gravitational force was studied, and a generalized description was presented [9]. These results were applied to the cooling fins of electronic devices [10]. This research has been extended to understanding large-scale natural convection in oceanography. The upwelling velocity of deep seawater in the ocean which was proposed by Stommel to be a perpetual salt fountain, was successfully measured for the first time in the world [11].

**Active heat-transfer control by Peltier elements:** Peltier elements, used as cooling equipment, have been applied to a heat-transfer control device. This device has been utilized to the heat-transfer control of equipment in a microgravity environment [12], in an active catheter, and in artificial heart muscles [13]. Furthermore, this heat-transfer control has been applied to the fields of oriental medicine and cryosurgery [14]. The concept of heat-transfer control has been expanded to fusion of thermal engineering and medical engineering [15].

## **Evaporation flow characteristics of airborne sputum droplets with solid fraction: Effects of humidity field evolutions [23]**

The continuance of the COVID-19 pandemic largely depends on the spread of virus-carrying aerosols in ambient air. The mechanism of virus transmission and infection remains under intense investigation. In this study, an evaporation flow model of airborne sputum droplets is proposed which considers the evolution effects

of the humidity field under different particle distributions and solid/salt fraction interactions. The incompressible Navier–Stokes equations characterize a stream of airflow jets, and the convection-diffusion-evaporation process is used to account for the inhomogeneous humidity field caused by the respiratory tract. Momentum equations for droplet dynamics which involve the effects of drag, gravity, and Brownian motion on sputum droplets are introduced to quantify the transport of droplets in a humidity field. The Lattice Boltzmann method is used to track the evolution of the aerosol in space and time under different ambient temperature and relative humidity conditions. The results of the simulation demonstrate that airborne humidity accelerates the evaporation rate of droplet, while supersaturated humid air forms a vapor mass in front of the respiratory tract. Despite the short lifespan of this phenomenon, it significantly hinders the evaporation of the droplets. Besides, the droplet vortex dynamics in a humidity field are sensitive to the droplet size.

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# Research Activities on Shape Memory Polymers (SMPs)

by Jinlian Hu, Member EUAS

## Short Biography

*Director of the Laboratory of Wearable Materials for Healthcare.*

*Fellow, National Academy of Inventors, USA (FNAI, 2022-)*

*Fellow, International Association of Advanced Materials, Sweden, (FIAAM, (2022-)*

*Fellow, Royal Society of Chemistry (FRSC, 2016-)*

*Fellow of HK Institution of Textiles and Apparel (FHKITA, 2001-)*

*Fellow of the Textile Institute, UK (FTI, 1997-)*

*Chairman for Hong Kong Federation of Invention and Innovation.*

*Adjunct Dean of Modern Textile College of Wuhan Textile University.*

*Principal Consultant of Zhejiang Institute of Modern Textile Industry.*

*Visiting professor/chair professor to a number of universities in different parts of the world.*

*Committee member of National Laboratory and Chairman of HKFii.*

*China National Talent award winner.*

*China Textile Academic Leader award winner.*

*Distinguished Achievement Award winner in Basic or Applied Fiber Science in US.*

*First-Class Prize and Sang Ma Textile Science and Technology Award winner.*

*Included in the list of Top 2% world's most highly cited scientists by Stanford Ranking (actual 228 out of 315721 in materials science, 0.07%).*

*Overall ranking of 23663 among ~10 million scientists worldwide.*

*Google H-index of 64 with 16269 citations.*

*Over 400 refereed journal Papers, 14 books, 32 book chapters, 100 patents, ~130 plenary/keynote conference lectures.*

*The highest International Consultancy Award winner.*

*The highest International Consultancy Award winner in HKPolyU.*

*Technology Transfer Award winner in HKPolyU.*

*Project Manager for over 100 Projects from industry, NSFC, ITF, etc.*

*Plenary/keynote speaker at conferences and organizations (~200)*

*Breakthrough work interviewed by influential TV programs: Associated Press (USA), Discovery Chanel and HK TV headline news.*

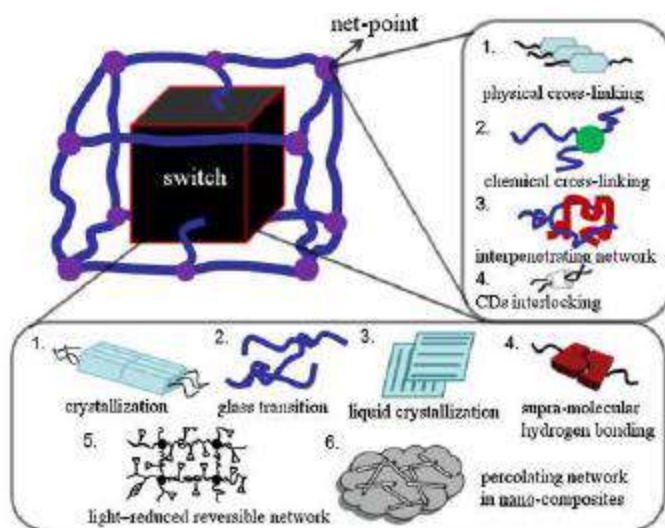
*Reviewer for >130 journals including Science and Nature.*

*Chairman or Committee member for international conferences cross different continents.*

*Major fields of research in Traditional Chinese medical therapies and their materials, energy materials and healthcare, personal protective equipment against infectious diseases, spider silks and their relatives as biomaterials, as well as two-dimensional nanomaterials for sensing element.*

Prof. Hu is a pioneer, sustained and distinguished academic leader in shape memory polymers (SMPs). Started from the pioneer usage of SMPs in innovative intelligent textiles, she has made the significant contributions to fundamental research of SMPs on theory and practice. She built the structure model and intrinsic relationship between structure, properties and performance. Moreover, she extended the SMPs application in biomaterials, animal hairs, artificial muscles, fibres, textiles, artificial spider silks, etc. The uniqueness of her research is the integration of theory and practice from molecular design, polymer processing and functional customization to manufacture commercial products.

Innovatively, she established a “*netpoint-switch-rubbery*” 3-phase structural model for SMPs and proposed a programming principle of “*stress memory*” to explain shape memory behaviours. In the 3-phase structural model, SMPs consist of both switch units and net-points (Fig. 1). The net-points determine the permanent shape and can be made of either chemical or physical cross-links, with an interpenetrated or interlocked supramolecular complex. The driving force for strain recovery in SMPs is the entropic elasticity of the polymer network. Similarly, the switch unit is responsible for controlling the shape fixity and recovery upon a specific and predetermined external stimulus. Based on the structural model, shape memory polymers and their composites have been creatively applied to biomedical fields for cardiovascular stent, bone regeneration, nerve repairing, wound healing, orthopaedics and cell manipulation.



**Fig. 1** “*netpoint-switch-rubbery*” 3-phase structural model.

Fig. 2 schematically describes the “*stress memory*” programming principle: ①heating the specimen to high temperature above its transition level, ②stretching the specimen to a certain strain level at high temperature, ③holding the specimen under the given strain level at high temperature to nullify the viscous stress, ④allowing the specimen to store the generated stress by cooling to room temperature, ⑤re-heating the specimen at the same constraint strain level to trigger memory stress. Based on stress memory SMPs, artificial muscles with extra-ordinary functions, namely, both Isotonic and Isometric, have also been achieved. In addition, SMP solutions have been applied for finishing to reach wrinkle free functions in cotton, and its blends as well as wool fabrics, even hair treatment.

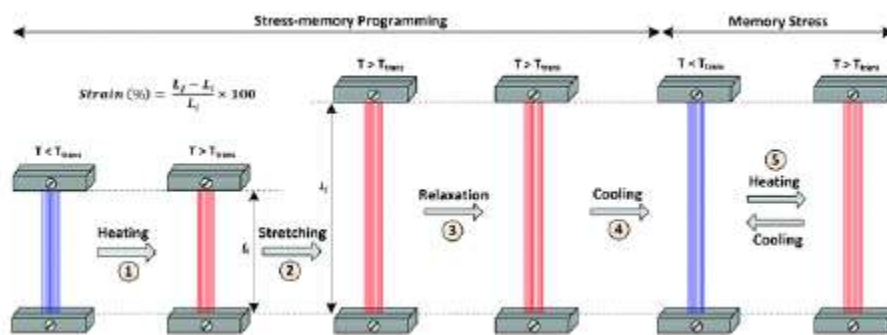


Fig. 2 “stress memory” programming principle.

Significantly, she developed the world first intrinsic shape memory fibres, which is going to be commercialized for smart textiles. Smart compression stocking derived from shape memory fibres with stress memory capability has been studied with programmability and various textile designs.

Inspired by the fact that spider silk, particularly dragline silk, has super-contraction, which is actually identical to shape memory, she established a model to explain such correspondences, which suits for other natural protein fibres. Moreover, artificial spider silks mimicking its structures have been accomplished both by biological and chemical methods in parallel. Based on the model for spider silk, she discovered stress memory properties and potential application of animal hairs. For example, smart wool fabrics have been studied and applied for personal thermal management and smart garment. This can inspire many people to make smart garments with various functions. Extraordinary properties, including super-toughness, water collection and shape memory have been reproduced, which contributes to high performance fibres and materials in artificial spider silk using scalable chemical synthesis.

Recently, she developed an electrochemical method to solve the preparation puzzle of two-dimensional nanomaterials such as MXene. Importantly, she innovatively combined two-dimensional nanomaterials with indoor textiles, which serve as mechanically flexible and flame-retardant fire alarm sensors for repeatable contact/non-contact fire monitoring. Smart textiles could be potentially used as perceptive layer of Internet of Things.

Educated in textile engineering and materials, Professor Hu obtained her PhD from the University of Manchester in 1994, then UMIST, is a world-renowned expert in shape memory polymers for fibres, textiles and biomedical applications, a top 2% world's most highly cited scientists by Stanford Ranking (actual 228 out of 315721 in materials science, 0.07%), overall ranking of 23663 among ~10 million scientists worldwide. Professor Jinlian Hu is a pioneer, sustained and distinguished academic leader who has made significant contributions to basic research of shape memory polymers from structure modelling, function design, fabrication and innovative applications. She has Google H-index of 64 with 16269 citations, published 14 books, 32 book chapters, 100 patents, ~130 plenary/keynote conference lectures and ~400 refereed journal Papers.

Basic Research achievements

1. Started from innovating textiles with smart properties through application of shape memory polymers (SMPs), Professor Hu is a successful scholar to have made significant contributions to basic and applied research of SMPs from structure

modelling, relationship between structure, properties and performance as well as applications to biomaterials, animal hairs, artificial muscles, fibres, textiles and artificial spider silks. The uniqueness of her research is the integration of theory and practice from molecular design, polymer processing and function designs to final products.

2. Specifically, she established a netpoint-switch-rubbery 3-phase structural model for SMPs, developed stress memory concept and theory to explain such behaviour.
3. Based on the above structural model, shape memory polymers and their composites have been innovatively applied to biomedical fields for cardiovascular stent, bone regeneration, nerve repairing, wound healing, orthopaedics and cell manipulation.
4. Based on stress memory and shape memory properties of a polymer, artificial muscles with extra-ordinary functions, namely, both Isotonic and Isometric, have also been realised.
5. SMP solutions have been applied for finishing to reach wrinkle free functions in cotton, and its blends as well as wool fabrics, even hair treatment.
6. She also developed the world first intrinsic shape memory fibres, which is going to be commercialized, various smart applications have been studied for smart textiles.
7. Smart compression stocking derived from shape memory fibres with stress memory capability has been studied with programmability and various textile designs.
8. Based on the fact that spider silk, particularly dragline silk, has supercontraction, which is actually identical to shape memory, a model to explain such correspondences was established and extended to other natural protein fibres.
9. Based on the above, artificial spider silks mimicking its structures have been accomplished both by biological and chemical methods in parallel.
10. Extraordinary properties, including super-toughness, water collection and shape memory have been reproduced, which contributes to high performance fibres and materials in artificial spider silk using scalable chemical synthesis.
11. Also based on the model for spider silk, animal hairs have been discovered to have SM properties and smart wool fabrics have been studied and applied for personal thermal management and smart garment. This can inspire many people to make smart garments with various functions.
12. Recently, she developed an electrochemical method to prepare two-dimensional nanomaterials such as MXene, which serve as mechanically flexible and flame-retardant fire alarm sensors for fire proofing and repeatable contact/non-contact fire monitoring.

# Tuning Ordering / Disordering and Properties in Architected Metastable Materials

by Jürgen Eckert, Member EUAS

## Short Biography

*Jürgen Eckert obtained his Ph.D. in Materials Science and Engineering at the Friedrich-Alexander-University Erlangen-Nuremberg, Germany in 1990. After his Ph.D. he worked for two and a half years as postdoc at the California Institute of Technology. After a short break in industry, he moved to the Leibniz-Institute for Solid State and Materials Research (IFW) Dresden, one of the leading Materials Research Science Centers in Germany. From 1996 until 2003 he was Head of the Department Metastable and Nanostructured Materials at IFW Dresden, before moving to TU Darmstadt as Full Professor for Physical Metallurgy. In 2006 he moved back to Dresden as Director of the Institute for Complex Materials at IFW Dresden and Chair for Synthesis and Analysis of Materials at Dresden University of Technology (TU) Dresden. He also served as Scientific Director of IFW Dresden (2013/2014). In 2015 he became Chair Professor of Materials Physics at Montanuniversität Leoben, and Director of the Erich Schmid Institute of Materials Science of the Austrian Academy of Sciences. He held an Adjunct Professor Position at Michigan Technological University, Houghton, USA (2002-2005), was a Visiting Professor at University of Vienna, Austria (2009/2010/2012) and was appointed Honorary Professor at Shenzhen University, PR China (2021).*

*He is an international expert in the field of metastable materials and has published more than 1300 papers in archival journals (h-index: 101 (WoSci), more than 48.500 citations), as well as more than 150 conference papers, 18 book chapters, 6 edited books, conference proceedings and journal issues, holds more than 20 patents, and delivered so far more than 245 plenary, keynote and invited presentations.*

*Jürgen Eckert was honored as Dr. honoris causa (Dr. h.c.) by the Slovak University of Technology in Bratislava, Slovak Republic (2012), and received the Gottfried Wilhelm Leibniz Award of the German Research Foundation (2009), the highest Science Prize and scientific honor in Germany. Other honors include the THERMEC 2021 Distinguished Award (2021), the European Advanced Materials Award of the International Association of Advanced Materials, Sweden (2021), an ERC-Proof of Concept Grant of the European Research Council (2019), the DGM-Prize 2014 of the German Materials Research Society, an ERC Advanced Grant of the European Research Council (2013), the ISMANAM Senior Scientist Award (2012), the Hsun Lee Lecture Award of the Chinese Academy of Sciences (2006), the Georg-Sachs-Prize of the German Materials Research Society and the Austrian Metal Industry (1997), and the FEMS Materials Science and Technology Prize of the Federation of European Materials Science Societies (FEMS) in 1997. He received the Young Scientist Award of the German Materials Research Society (1994), and the ISMANAM Young Scientist Award (1997). He is corresponding Member of the Section Mathematics-Natural Sciences of the Austrian Academy of Sciences (2017), Member of the European Academy of Sciences (2018), MRS Fellow of the Materials Research Society, USA (2018), Honorary Member of The Indian Institute of Metals, corresponding Member of the Section Technical Sciences of the Saxon Academy of Sciences and Humanities in Leipzig, Germany (2020), Foreign Fellow of the Indian National Academy of Engineering, India (2021), Fellow of the International Association of Advanced Materials (FIAAM), Sweden (2021) and was elected Full Member of Sigma Xi, The Scientific Research Honor Society, USA (2022).*

Jürgen Eckert's research activities focus on phase formation and structure-property correlations of metastable materials processed under non-equilibrium conditions; structural and functional materials with particular emphasis on

fundamentals of solidification and solid state reactions; additive manufacturing techniques; high strength, biocompatible and magnetic alloys, and materials for sustainable energy applications (e.g. next generation batteries, supercapacitors, carbon materials, materials for hydrogen production and storage) and thin film systems for flexible electronics; mechanical and electrochemical properties of bulk materials, coatings and surfaces; biologically inspired far-from-equilibrium materials and architected structures; mathematical modelling of advanced materials and processes.

Over the years, Jürgen Eckert and his team have provided seminal contributions in developing metastable advanced high-performance materials. Early work focused on amorphization and quasicrystal formation in metallic systems, and fundamental observations on establishing nanoscale grain sizes in metallic materials. The interest shifted later on to the development and property optimization of bulk metallic glasses and composites, high entropy alloys and structurally modulated systems with hierarchically tuned microstructure for creating plastically deformable and tough engineering materials. This work followed a synergistic approach by understanding how atomic scale structures, microstructural features and stress, along with processing-induced heterogeneities determine the mechanisms of plastic deformation on different length scales such as to overcome the otherwise unavoidable brittleness of glassy or nanoscale materials, and evolved into a comprehensive approach using disorder and heterogeneity concepts for creating new strategies to tailor the properties of advanced materials under non-equilibrium conditions. This allowed to create new high-strength lightweight alloys, hard and soft magnetic materials, porous bulk materials and hybrid structures for biomedical applications, materials for energy applications, and also touched on surface modification and development of architected gradient structures.

Jürgen Eckert's recent research activities focus on in-depth *in situ* and *in operando* investigations of phase transformations and structure-property correlations using local probes and high-resolution techniques for structure characterization and imaging of local structures, chemical compositions and interaction of nanoscale objects with external fields and stimuli (e.g. mechanical, thermal, electrical, magnetic fields) for creating tailored biologically inspired metastable materials with hierarchical structure and tuned disorder. This can be realized in a microscope or through flash annealing at extreme heating and cooling rates. An example for such materials is the *in situ* design and testing of glassy or nanostructured metallic alloys containing heterogeneities on different length-scales to overcome their intrinsic brittleness. The heterogeneities can be triggered through local chemical variations, modulation of short- or medium-range order or via creating locally tuned stress/strain states. The concept of *in situ* design and testing is applicable to bulk materials, granular or thin film systems and to a variety of materials, and thus opens new research avenues for designing materials with unique properties. Some of the key publications in this area include:

- F. Spieckermann, D. Şopu, V. Soprunyuk, M.B. Kerber, J. Bednarčík, A. Schökel, A. Rezvan, S. Ketov, B. Sarac, E. Schafner, J. Eckert, "Structure – Dynamics Relationships in Cryogenically Deformed Bulk Metallic Glass", *Nat. Commun.* **13**, 127 (2022).
- O. Renk, I. Weißensteiner, M. Cihova, E.-M. Steyskal, N.G. Sommer, M. Tkadletz, S. Pogatscher, P. Schmutz, J. Eckert, P.J. Uggowitzner, R. Pippan, A.M. Weinberg, "Mitigating the Detrimental Effects of Galvanic Corrosion by Nanoscale Architecture Design", *npj Mater. Degrad.* **6**, 47 (2022).
- H.P. Sheng, D. Şopu, S. Fellner, J. Eckert, C. Gammer, "Mapping Shear Bands Metallic Glasses: From Atomic Structure to Bulk Dynamics", *Phys. Rev. Lett.* **128**, 245501 (2022).
- E. Sharifikolouei, B. Sarac, Y.H. Zheng, P. Bala, J. Eckert, "Fabrication of Stainless-Steel Microfibers with Amorphous-Nanosized Microstructure with Enhanced Mechanical Properties", *Sci. Rep.* **12**, 10784 (2022).
- B. Sarac, M. Micusik, B. Putz, S. Wurster, E. Sharifikolouei, L.X. Xia, M. Omastova, F. Spieckermann, C. Mitterer, J. Eckert, "Magnetron Sputtered Non-Toxic and Precious Element-Free Ti-Zr-Ge Metallic Glass Nanofilms with Enhanced Biocorrosion Resistance", *Adv. Mater. Interfaces* **9**, 2201223 (2022).
- Q. Xu, D. Şopu, X. Yuan, D. Kiener, J. Eckert, "Interface-Related Deformation Phenomena in Metallic Glass / High Entropy Alloy Nanolaminates", *Acta Mater.* **237**, 118191 (2022).
- M.W. Kapp, O. Renk, J. Eckert, R. Pippan, "The Importance of Lamellar Architecture to Obtain Ductility in Heavily Cold-Worked Pearlitic Steels Revealed by Microbending Experiments", *Acta Mater.* **232**, 117935 (2022).
- E. Yüce, L. Zarazúa-Villalobos, B. Ter-Ovanesian, E. Sharifikolouei, Z. Najmi, F. Spieckermann, J. Eckert, B. Sarac, "New-Generation Biocompatible Ti-Based Metallic Glass Ribbons for Flexible Implants", *Mater. Des.* **223**, 111139 (2022).

The long-term perspective of these approaches is to further advance the understanding of structure-property correlations for hierarchically modulated structures and hybrid systems over a variety of different length-scales under highly non-equilibrium thermodynamic and kinetic conditions. The goal is to gain a descriptive and quantitative picture of phase formation, transformation, dynamics and property design under extreme conditions, such as ultra-fast heating and cooling on extremely short time scales with or without external mechanical, electrical or magnetic stimulus. Whereas some of these approaches are already followed for crystalline materials, research on disordered and interface dominated materials along these lines touches almost unknown grounds, since the structural diversity represented by disorder in a material represents a holy grail of materials science and promises to overcome the compositional and structural constraints of crystalline materials. The ability to predict and design disorder in architected materials with

unique functionality via property-directed material design provides vast opportunities for new structural and functional materials including high-strength-lightweight systems, biomedical implants or micromechanical components with unique performance characteristics. But not only the basic fundamental mechanisms of structure formation and property development are of interest, but also the question how the findings can be transferred into parts, devices and systems for MEMS/NEMS, sensor and actuator applications, flexible microelectronics, as well as into materials for energy applications and energy harvesting. Also biocompatible (biodegradable) bulk materials, porous structures, coatings and surfaces are in the focus of interest, e.g. for tailored orthopedic implants or for advanced personalized medical devices.

For this purpose state-of-the-art techniques from the fields of materials physics, structure analysis, *in situ* structure investigations under different applied fields (e.g. mechanical, electrical, magnetic), and also structure-biological mimetic and 3d printing techniques are used to generate architected materials built from disordered building blocks. Modelling and simulation supplement and strengthen the experimental efforts. Multi-scale modelling techniques based on hierarchies of overlapping scales including quantum mechanics based structure modelling, atomistic modelling and numerical methods can be involved. A variety of simulation and modelling of length and time scales is utilized, and complemented by Bayesian Interference (BI) and machine learning algorithms to better characterize the local property statistics not assessable with direct measurements. The outcome of this approach allows for both a quantitative parameterization of local properties and protocols by which they are, in general, to be measured. This is a vital input for property-directed material design of disordered systems, and promises to open new avenues for nanoscale structure formation in architected materials with unique functionality through generating an atomic structural – functional understanding of the properties, performance and correlation of hierarchical thin film structures and membranes, tailored interface structures, nano- and multiscale hybrid systems and tailored lattice materials.

# Cooling Performance & Flow Characteristics of a Combustor Liner Plate

by Phil Ligrani, Member EUAS

## Short Biography

*Eminent Scholar in Propulsion, Professor of Mechanical and Aerospace Engineering, Department of Mechanical and Aerospace Engineering, Propulsion Research Center, 5000 Technology Drive, University of Alabama at Huntsville*

## **PROFESSIONAL PREPARATION**

University of Texas at Austin	Mechanical Engineering	Bachelor of Science, 1974
Stanford University	Mechanical Engineering	Master of Science, 1975
Stanford University	Mechanical Engineering	Doctor of Philosophy, 1980

## **APPOINTMENTS**

2014 – present	<i>Eminent Scholar in Propulsion, Professor of Mechanical and Aerospace Engineering, Department of Mechanical and Aerospace Engineering, University of Alabama</i>
2010 – 2014	<i>Professor of Aerospace &amp; Mechanical Eng, Saint Louis University</i>
2010 – 2013	<i>Director of Graduate Programs, Parks College, Saint Louis University</i>
2006 – 2009	<i>Statutory Professor, Department of Engineering Science, University of Oxford</i>
2006 – 2009	<i>Director, Rolls-Royce UTC (University Technology Centre)</i>
1997 – 2006	<i>Professor, Department of Mechanical Engineering, University of Utah</i>
2002 – 2006	<i>Adjunct Professor, Department of Bioengineering, University of Utah</i>
1992 – 1997	<i>Associate Professor, Department of Mechanical Engineering, University of Utah</i>

## **ARCHIVAL JOURNAL PUBLICATIONS AND RELATED ITEMS.**

As of December 2022, Dr. Ligrani is author or co-author of more than 217 publications in archival journals, including the *International Journal of Heat and Mass Transfer*, the *ASME Transactions-Journal of Turbomachinery*, the *ASME Transactions-Journal of Engineering for Gas Turbines and Power*, the *ASME Transactions-Journal of Heat Transfer*, the *ASME Transactions-Journal of Fluids Engineering*, *Nature - Scientific Reports*, the *Journal of Fluid Mechanics*, the *AIAA Journal*, *Experiments in Fluids*, *Physics of Fluids*, the *AIAA Journal of Heat Transfer and Thermophysics*, the *International Journal of Rotating Machinery*, *Separation Science and Technology*, *Sensors and Actuators A: Physical*, and the *Journal of Microcolumn Separations*. He is also author of 10 book chapters, and about 159 conference presentations and publications. A number of these are invited conference presentations at international meetings, at locations which include Korea, France, the Ukraine, Croatia, Germany, England-United Kingdom, and Belgium. From 1994 to 2022, he has also presented approximately 195 lectures at different institutions and establishments, including many invited lectures. From 2006 to 2023, he presented or is scheduled to present 9 Invited Keynote Papers, 12 Invited Papers, and 11 Invited Plenary Keynote Papers at different international conferences. Current SCOPUS Reference Citation H-INDEX is 47. Current GOOGLE SCHOLAR Reference Citation H-INDEX is 53.

## **EDITOR ACTIVITIES.**

From 1998 to 2000, Dr. Ligrani served as Guest Editor for a Special Topical Issue for *Measurement Science and Technology*. He has also served as Associate Editor for the *ASME Transactions-Journal of Heat Transfer* from 2003 to 2006, and from 2010 to 2014, and as Associate Editor for the *ASME Transactions-Journal of Fluids Engineering* from 2005 to 2008. Present editor duties include Associate Editor, *ASME Transactions-Journal of Journal of Engineering for Gas Turbines and Power* (2018-2024).

## **SELECTED RECENT HONORS, AWARDS, ACADEMIC RECOGNITIONS**

Dr. Ligrani has a strong past and present record of performing sponsored, fundamental and applied research for a variety of funding agencies, including ones in the USA and Europe. As such, he has successfully managed a wide variety of research programs, for different industrial, foundation, and government sponsors. **As of December 2022, research funding awards have been received from the following organizations:** Alabama State Innovation Program Fund, University of Alabama in Huntsville Endowment for Eminent Scholar in Propulsion, University of Alabama in Huntsville Start-Up Funds, AEDC – Arnold Engineering Development Center of Arnold Air Force Base, National Science Foundation, Honeywell Aerospace Corp., The Boeing Company, IHI Corporation, the Henry Luce Foundation, South Carolina Institute for Energy Studies (SCIES-AGTSR) of the Department of Energy, U. S. Army Aviation

Research and Technology Activity-AVSCOM, NASA-Ames Research Center, NASA-Lewis Research Center, Hispanic Research Center-Arizona State University, Turbo and Power Machinery Research Center-Seoul National University, Solar Turbines Incorporated, UCON U.S.-Japan Center-Weber State University, General Electric Corporate Research and Development Center, Pratt & Whitney Corporation-Florida, the North Atlantic Treaty Organization (NATO), Pratt & Whitney Corporation-Canada Corp., the Gas Technology Institute, Intel Corporation, HEET-High Efficiency Engines and Turbines Program - South Carolina Energy Research and Development Center, Invesys Corp. - Foxboro Company, Ceramatec Advanced Materials and Electrochemical Technologies Corp., CISCO Systems Inc., SEEDA-South East England Development Agency, EPSRC – Engineering and Physical Sciences Research Council of Great Britain, ISIS Innovation, John Fell Fund, European Community Sixth Framework Programme, Korea Institute of Geoscience and Mineral Resources - KIGAM, Lockheed Martin UK, The Royal Academy of Engineering, Rolls Royce PLC, Science and Engineering Research Council (SERC) Engineering Board of Great Britain, Office of Naval Research, Naval Postgraduate School Research Foundation, Aero-Propulsion Laboratory-Wright-Patterson Air Force Base, and Naval Postgraduate School Direct Funding.

Dr. Ligrani has a strong past and present record of working with many different collaborators and co-workers, from many locations throughout the world. Additional information on selected, currently active research projects is provided within sections which follow. (i) **Traditional Heat Transfer and Fluid Mechanics Investigations** involving electronics cooling, heat transfer augmentation, drag reduction, turbulent boundary layers, flows in channels with dimpled surfaces, flows in curved channels, elastic turbulence, slot impingement cooling, and macro-scale pumps and pump flows. Also included are **aerodynamics investigations with high-speed, compressible flows at transonic and supersonic Mach numbers**, including SWBLI – Shock Wave Boundary Layer Interactions. Related projects involve **transonic and supersonic experimental testing**. Research interests also include experimental diagnostics in high speed flows, and air breathing propulsion. (ii) **Air Breathing Engines - Gas Turbine Heat Transfer, Cooling, and Aerodynamics Losses**, including internal cooling, film cooling, impingement cooling, cooling of extremities, aerodynamic performance including aerodynamic losses, and transonic turbine flows and heat transfer. This subject area includes the effects of uses of bio-fuels, synthetic fuels, and renewable energy sources in relation to gas turbines and gas turbine heat transfer and cooling technologies. Note that an important area of turbomachinery research interest involves heat transfer and aerodynamics investigations with *high-speed, compressible flows at transonic and supersonic Mach numbers*, including linear cascade studies. (iii) **Micro-Fluidics and Millimeter-Scale-Fluidics**, including micro-pump flows, and the effects of slip phenomena on gas and liquid flows in micro-scale passage flows with and without surface roughness, including the effects of hydrophobic surfaces and elastic turbulence. (iv) **Experimental Techniques**, including development of millimeter-scale multiple-hole pressure probes, subminiature hot-wire anemometry, and infrared thermography.

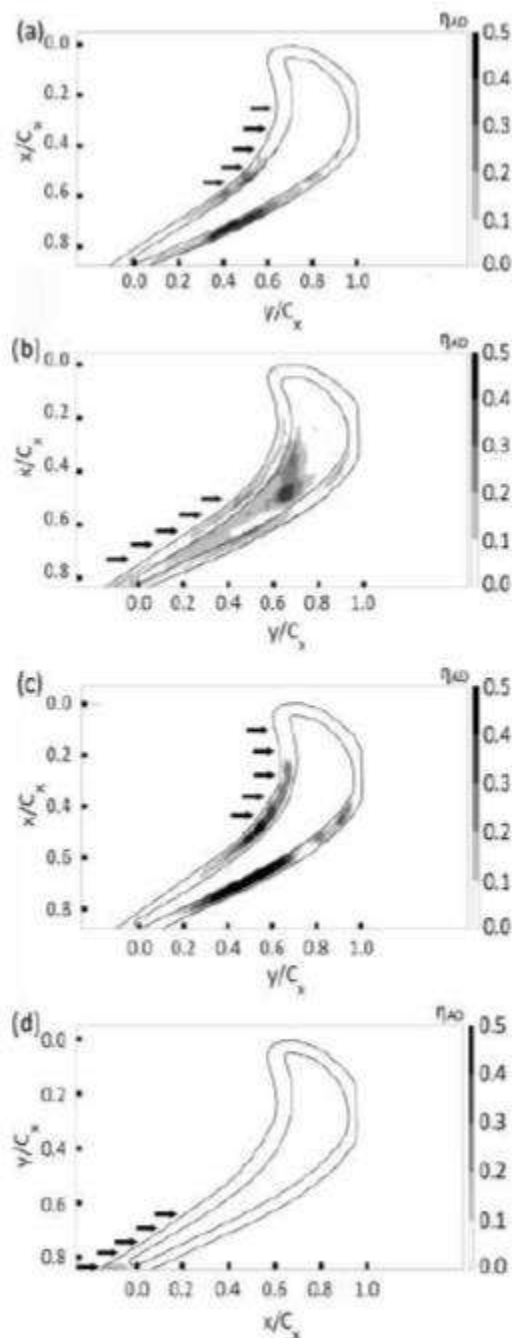
#### **COOLING PERFORMANCE AND FLOW CHARACTERISTICS OF A COMBUSTOR LINER PLATE WITH COMPOUND ANGLE AND SIMPLE ANGLE EFFUSION HOLES.**

Provided are new data for a unique compound angle arrangement, never previously considered, with  $\alpha=30^\circ$ ,  $\beta=\pm 30^\circ$ , such that the compound angle of the effusion holes changes from  $\beta=+30^\circ$  to  $\beta=-30^\circ$ , as adjacent rows of effusion holes are encountered. Also provided are data for comparison from a simple angle configuration with  $\alpha=30^\circ$ ,  $\beta=0^\circ$ . Here,  $\alpha$  denotes the film cooling hole angle of inclination and  $\beta$  denotes the film cooling hole compound angle. Coolant is supplied to both effusion hole arrays using arrays of

impingement cooling jets. The results of the numerical simulations are obtained using the ANSYS FLUENT V 21.1 numerical code, with a shear stress transport (SST)  $k-\omega$  turbulence model. Data are provided for main flow Reynolds numbers from 142,000 to 155,000, impingement flow Reynolds numbers from 7900 to 18000, effusion flow Reynolds numbers from 10,400 to 23,600, and overall blowing ratios from 3.3 to 7.4. When  $\beta$  is changed from  $0^\circ$  to  $\pm 30^\circ$ , area-averaged film cooling effectiveness values and area-averaged heat transfer coefficient magnitudes increase overall by approximately 2.89 percent and 11.7 percent, respectively. This is because the use of compound angle arrangements often inhibits the formation of the horseshoe-shaped vortex, and the resulting counter-rotating vortex legs, that often promote lift off of significant film concentrations from the test surface. The skewed and non-symmetric character of the horseshoe-shaped vortex is also increased by the use of compound angle arrangement, which also sometimes provides local improvements in surface thermal protection.

#### **EFFECTS OF PRESSURE SIDE FILM COOLING HOLE PLACEMENT AND CONDITION ON ADIABATIC FILM COOLING EFFECTIVENESS CHARACTERISTICS OF A TRANSONIC TURBINE BLADE TIP**

Investigated are the effects of film cooling hole placement location along the upper pressure side of a transonic squealer blade tip. The thermal performance of four different film cooling configurations; B1, B2, B3 and B4, are considered using the University of Alabama in Huntsville's SS/TS/WT (supersonic/transonic/wind tunnel) experimental facility and a simulated turbine blade row using a linear cascade. Contributions from the present investigation are unique because of a deficit of experimental data for film cooled squealer blades which operate with transonic flow. In addition, the present investigation is the first to consider the effects of hole placement location for upper pressure side film cooling arrangements with transonic flow conditions. Surface-varying results are provided for both the squealer blade tip surface, and for the upper pressure side of the squealer blade. These results are given for blowing ratios ranging from 0.42 to 3.20 in the form of spatially-resolved and spatially-averaged adiabatic film cooling effectiveness distributions. Because local static pressure variations and gradients vary in a significant manner at different blade locations, coolant accumulations near surfaces (and the associated surface thermal protection and film effectiveness distributions) produced by the different film cooling configurations are vastly different along the squealer blade tip surface. Examples for the B1, B2, B3, and B4 configurations are shown in parts (a), (b), (c), and (d), respectively, of the included figure for blowing ratios from 2.90 to 3.20. Such results show that the B1 and B3 film cooling configurations give substantial magnitudes of adiabatic film cooling effectiveness along the pressure side rim and the suction side rim. Also present is a considerable region of locally increased film cooling effectiveness and a wider region of surface protection within the squealer recess region for the B2 film cooling configuration.



### SLIP DUE TO RAREFACTION FOR AIR AND HELIUM INCLUDING THE INFLUENCES OF SURFACE ROUGHNESS TEXTURE.

Rarefaction slip phenomena are experimentally investigated within a Viscous Disk Pump (VDP), which produces shear-induced Couette rotating flow between a rotating disk and the bottom of a C-shaped fluid passage. The pressure gradient along the channel is characteristic of Poiseuille flow and is due to the z-gradient of viscous fluid shear, such that the local pressure gradient opposes the shear-driven fluid motion. Measured are the static pressure rise within the VDP, the volumetric flow rate, and the rotational speed of the disk. Three different levels of surface roughness are used. To characterize the surface

structure, a Wyko NT1100, white light interferometer, is used to map test surfaces at different locations for determination of magnitudes of mean roughness height  $R_a$ . Investigated are channel heights of 9.8  $\mu\text{m}$ , 19.9  $\mu\text{m}$ , 35.5  $\mu\text{m}$ , and 40.5  $\mu\text{m}$  using air and helium. Rotational speeds of the disk range from 63 1/s to 158 1/s. Experimental results show that the static pressure increase along the channel becomes smaller as the volumetric flow rate is increased, provided the rotational speed of the disk is maintained constant. The effects of the fluid medium are also considered, which show that tangential momentum accommodation coefficients for helium are generally lower than for air when compared at the same disk rotational speed and channel height. The absolute value of the slip velocity for air is smaller than for helium, provided rotational speed and flow passage height are the same. The non-dimensional slip velocity (determined as the ratio of slip velocity at the wall to the flow velocity at mid radius and mid height) is approximately independent of rotational speed, with higher non-dimensional slip velocities for helium relative to air, when compared for the same flow pass height, surface roughness texture, and disk rotational speed. Rarefaction slip effects become more pronounced as the average roughness height becomes smaller. This is illustrated by tangential momentum accommodation coefficients, which decrease as the mean roughness height  $R_a$  becomes smaller, and by absolute values of slip velocities, which increase as the mean roughness height  $R_a$  decreases.

#### **EFFECTIVE DIFFUSION FROM ELASTIC INSTABILITES WITHIN ROTATING COUETTE FLOWS.**

Considered is effective diffusion, characterized by magnitudes of effective diffusion coefficients, in order to quantify mass transport due to the onset and development of elastic instabilities. Effective diffusion coefficient magnitudes are determined using different analytic approaches, as they are applied to tracked visualizations of fluorescein dye front variations, as circumferential advection is imposed upon a flow environment produced using a rotating Couette flow arrangement. Effective diffusion coefficient results are provided for a range of flow shear rates, which are produced using different Couette flow rotation speeds and two different flow environment fluid depths. To visualize flow behavior within the rotating Couette flow environment, minute amounts of fluorescein dye are injected into the center of the flow container using a syringe pump. This dye is then redistributed within the flow by radial diffusion only when no disk rotation is used, and by radial diffusion and by circumferential advection when disk rotation is present. Associated effective diffusion coefficient values, for the latter arrangement, are compared to coefficients values with no disk rotation, which are to molecular diffusion alone, in order to quantify enhancements due to elastic instabilities. Experiments are conducted using viscoelastic fluids, which are based on a 65 percent sucrose solution, with different polymer concentrations ranging from 0 ppm to 300 ppm. Associated Reynolds numbers based on fluid depth and radially-averaged maximum flow velocity range from 0.00 to 0.5. Resulting effective diffusion coefficient values for different flow shear rates and polymer concentrations quantify the onset of elastic instabilities, as well as significant and dramatic changes to local mass transport magnitudes which are associated with further development of elastic instabilities.

#### **SPATIAL COHERENCE OF LOW-FREQUENCY UNSTEADINESS ASSOCIATED WITH DIFFERENT TYPES OF SHOCK WAVES.**

Transonic, supersonic, and hypersonic flows often involve inter-related, interacting, coupled, and three-dimensional interactions between a plethora of simultaneous physical phenomena, especially as they are present in different turbomachinery, aeronautical, and aerospace application environments. One type of phenomena, which is ubiquitously present within these environments, is shock waves, especially as they interact with adjacent turbulent flows, and as they offer fascinating possibilities for understanding and management of high-speed compressible flow environments. Using a newly-developed, transonic / supersonic wind tunnel facility (located at the University of Alabama in Huntsville), spatially- and temporally-varying flow structural characteristics are quantified for correlation and spectral analysis, using high resolution, shadowgraph flow visualization data, as well as measurements of time-varying surface static pressure and surface heat flux. Considered are different types of oblique and normal shock waves, including the source, origin, and propagation direction of shock wave unsteadiness. Interests include avenues to alter and control associated transport characteristics by control and management of associated shock wave properties and characteristics. Determined are spectral energy variations, magnitude squared coherence variations with frequency, and time lag magnitude variations with frequency, where these last two quantities are determined for different flow locations relative to shock wave locations. For an arrangement with a well-defined normal shock wave, lambda foot, and separated turbulent boundary layer, present with an inlet Mach number of 1.54, data associated with lower Strouhal numbers in vicinity of 0.0013 and 0.0039 illustrate important and pronounced interactions between the normal shock wave and the boundary layer separation zone. With Strouhal numbers in the vicinity of 0.0091, 0.0104, and 0.0260, the most pronounced and significant interactions with the normal shock wave occur with respect to the downstream boundary layer.

#### **TURBULENT HEAT TRANSFER IN CHANNELS WITH MICRO-DEPTH DIMPLES.**

Experimentally-measured heat transfer and pressure loss characteristics are considered for dimpled surfaces, placed along one surface of a channel, with different ratios of dimple depth to channel height, and for Reynolds numbers ranging from 10,000 to 70,000. With the same relative dimple spacing, relative to dimple print diameter, and the same ratio dimple depth to dimple print diameter of 0.20, results for spherical indentation dimples with micro depths of 0.03 and 0.05 (relative to channel height) are compared with thermal and flow characteristics for larger dimples with a ratio of dimple depth to channel height of 0.20. Results indicate that Nusselt number ratios and friction factor ratios are dependent upon the ratio of dimple depth to channel height. As such, the present data for dimples with ratios of dimple depth to channel height between 0.03 and 0.20 are different from previous studies with ratios of dimple depth to channel height between 0.10 and 0.78. The importance of a critical Reynolds number is also demonstrated by the results, which is determined when the ratio of viscous sublayer layer thickness to the dimple depth is equal to unity. Nusselt number enhancements for the micro dimples are generally lower at lower Reynolds numbers, but increase as the Reynolds number becomes larger and approaches the critical Reynolds number. Nusselt number enhancements are then approximately invariant with Reynolds number, when Reynolds number then exceed the critical value.

# The Fluid—Mosaic Membrane and its role in Membrane Lipid Replacement

by Garth L. Nicolson, Member EUAS

## Short Biography

### **Professor Emeritus Garth L. Nicolson, PhD, MD (H)**

*Professor Emeritus Garth L. Nicolson is the Founder, President, Chief Scientific Officer and Emeritus Research Professor of Molecular Pathology at the Institute for Molecular Medicine in Huntington Beach, California. He is also a Conjoint Emeritus Professor at the University of Newcastle (Australia). He was previously the David Bruton Jr. Chair in Cancer Research and Professor and Chairman at the University of Texas M.D. Anderson Cancer Center in Houston, and he was Professor of Internal Medicine and Professor of Pathology and Laboratory Medicine at the University of Texas Medical School, Houston. Professor Nicolson has published over 700 medical and scientific papers, including editing 20 books, and he has served on the Editorial Boards of 30 medical and scientific journals and was Senior Editor of four of these. Professor Nicolson has won many awards, such as the Burroughs Wellcome Medal of the Royal Society of Medicine (United Kingdom), Stephen Paget Award of the Metastasis Research Society, U.S. National Cancer Institute Outstanding Investigator Award, the Innovative Medicine Award of Canada and the EU Academy of Sciences. He is also a Colonel (O6, Honorary) of the U. S. Army Special Forces and a U.S. Navy SEAL (Honorary) for his work on Armed Forces and veterans' illnesses.*

### **Professional Experience:**

#### **Primary Appointment:**

*1996-Present, President and Founder, Chief Scientific Officer and Emeritus Professor of Molecular Pathology, The Institute for Molecular Medicine, PO Box 9355, S. Laguna Beach, CA 92652*

#### **Secondary Appointments:**

*2003-Present, Conjoint Emeritus Professor, Faculty of Science and Technology, University of Newcastle, Newcastle, Australia*

#### **Previous Appointments:**

*1989-00, Professor, Department of Internal Medicine, The University of Texas Medical School, Houston, TX*

*1981-99, Adjunct Professor, Department of Pathology, School of Veterinary Medicine, Texas A & M University, College Station, TX*

*1982-99, Professor, Department of Pathology and Laboratory Medicine, The University of Texas Medical School, Houston, TX*

*1980-96, David Bruton Jr. Chair in Cancer Research, Professor and Chairman, Tumor Biology, The University of Texas M. D. Anderson Cancer Center, Houston, TX*

*1980-96, Professor, The Graduate School of Biomedical Sciences, The University of Texas Health Science Center, Houston, TX*

*1980-87, Florence M. Thomas Professor of Cancer Research, The University of Texas M. D. Anderson Cancer Center, Houston, TX*

*1978-80, Professor, Department of Physiology and Biophysics, College of Medicine, University of California, Irvine, CA*

*1977-80, Associate Director, Oncology Program, University of California, Irvine, CA*

*1975-80, Professor, Department of Developmental and Cell Biology, University of California, Irvine*

*1974-76, Chairman, Department of Cancer Biology, The Salk Institute, La Jolla, CA*

*1972-74, Head, Cancer Council Laboratory, Director, Electron Microscopy Laboratory, The Salk Institute, La Jolla, CA*

*1970-71, Senior Research Associate, Cancer Council Laboratory, The Salk Institute, La Jolla, CA*

*1967-70, USPHS Predoctoral Fellow University of California, San Diego, CA*

### **Honors and Awards:**

*European Union Academy of Sciences, 2019-*

*Doctor of Medicine, M.D. (H), University of the Republic of Uruguay, 2015*

*Yanagimachi Distinguished Lectureship, University of Hawaii School of Medicine, 2012*

*John Drulle Memorial Lectureship, International Lyme and Associated Diseases Society (ILADS), 2008*

*Annual Award of the Common Cause Medical Research Foundation (Canada), 2006*

*Innovative Medicine Award (Canada), 2002*

*Stephen Paget Award, Metastasis Research Society, 1998*  
*Albert Schweitzer Award (Portugal), 1998*  
*First Norman N. Durham Lectureship, Environmental Institute, OSU, 1996*  
*Indo-American Society for Health & Laboratory Professionals Award, 1996*  
*Distinguished Presentation Award, Third International Cancer Molecular Biology Symposium, 1996*  
*COLONEL (Honorary), U. S. Army Special Forces, 1995*  
*SEAL (Honorary), U.S. Navy Special Forces, 1995*  
*Haskel Visiting Professorship, University of Pennsylvania, 1995*  
*Burroughs Wellcome Medal, Royal Society of Medicine Foundation, London, 1991*  
*Outstanding Faculty Award, The University of Texas Health Science Center at Houston, 1991*  
*U.S. National Cancer Institute U.S.S.R. Scientist Exchange Award for Collaborative Research on Molecular and Genetic Aspects of Tumor Metastasis, 1991*  
*Evan and Marion Helfaer Distinguished Lectureship, The Cancer Center of the Medical College of Wisconsin, 1990*  
*Dean's Teaching Excellence List, The University of Texas Health Science Center at Houston Graduate School of Biomedical Sciences, 1985-1994*  
*Teaching Excellence Award for Best Course, The University of Texas Medical School at Houston, 1990*  
*NCI/NIH Outstanding Investigator Award, 1987*  
*Annual Award of the Japan Histochemical Society, 1976*  
*Eli Nadel Memorial Lecture in Biochemistry, 1983*  
*Rita Ferdinand Memorial Lectureship, 1982*  
*Guy Lipscomb Memorial Lecture in Chemistry, 1980*  
*Upjohn Biology Education Award, 1976*  
*Presidential Award, Electron Microscopy Society of America, 1971*

## **1. The Fluid—Mosaic Membrane and its role in Membrane Lipid Replacement**

The Fluid–Mosaic Membrane model has been the accepted general or basic model for biomembrane structure and organization for the last 50 years (Singer, S.J.; Nicolson, G.L. The Fluid Mosaic Model of the structure of cell membranes. *Science* 1972; 175: 720-731). Previously researchers placed most membrane proteins on the exterior and interior surfaces of lipid bilayers to form trimolecular structures or as lipoprotein units arranged as modular sheets. Such membrane models were structurally and thermodynamically unsound and did not allow independent lipid and protein lateral movements. The Fluid–Mosaic Membrane Model was the only model that accounted for these and other characteristics, such as membrane asymmetry, variable lateral movements of membrane components, cis- and trans-membrane linkages and the dynamic associations of membrane components into multi-molecular complexes. Since this model was based on the available 1960s era data, it could not explain all of the properties of various membranes discovered in subsequent years. Additional data on various structures associated with membranes have now been included, resulting in the addition of membrane-associated cytoskeletal, extracellular matrix and other structures, specialized lipid-lipid and lipid-protein domains, and other configurations that can affect membrane dynamics. The presence of such specialized membrane domains has reduced significantly the extent of the fluid lipid membrane matrix as first proposed, and cellular membranes are now considered to be less fluid and more mosaic with some fluid areas, rather than a fluid matrix with predominantly mobile components. However, the fluid-lipid matrix regions remain very important in cell membranes, especially those involved in the binding and release of membrane lipid vesicles and the uptake of various nutrients. Membrane phospholipids can associate spontaneously to form lipid structures and vesicles that can fuse with various cellular

membranes to transport lipids and other nutrients into cells and organelles and expel damaged lipids and toxic hydrophobic molecules from cells and tissues. This process and the clinical use of membrane phospholipid supplements has important implications for chronic illnesses and the support of healthy mitochondria, plasma membranes and other cellular membrane structures.

Nicolson GL, Ferreira de Mattos G. A brief introduction to some aspects of the Fluid—Mosaic Model of membrane structure and its importance to Membrane Lipid Replacement. *Membranes* 2021; 11(12): article 947.

Nicolson GL, Ferreira de Mattos G. Fifty years of the Fluid—Mosaic Model of biomembrane structure and organization and its importance in biomedicine with particular emphasis of Membrane Lipid Replacement. *Biomedicines* 2022; 10: article 1711.

Nicolson GL, Ferreira de Mattos G. Fluid—Mosaic model of biological membranes. *Access Science*, 2023, in press.

## **2. Membrane Lipid Replacement and its use in enhancing bioavailability and reducing symptoms in chemically exposed patients**

Previous studies indicated that lipids and nanostructured materials may improve the uptake of nutrients with moderate bioabsorption properties. Thus we evaluated the effects of Membrane Lipid Replacement (MLR) with NTFactor<sup>®</sup> Lipids (NTFL) on bioabsorption of three poorly to moderately absorbed nutrients (quercetin, curcumin and coenzyme Q10) utilizing the Caco-2 epithelial cell permeability model. Transfer across a Caco-2 epithelial cell layer has become a reference standard in the pharmaceutical and nutraceutical industries for *in vitro* prediction of *in vivo* human intestinal absorption and bioavailability of orally administered substances. When NTFL was added to each of the three test nutrients, there was increased absorption and transfer across a Caco-2 cell layer in a dose-dependent manner for the three nutrients. Using the Caco-2 bioabsorption and bioavailability *in vitro* model we found that NTFL could enhance absorption, bioavailability and uptake of nutrients while providing its own clinically demonstrated health benefits. In another study chemically-exposed veterans of the 1991 Gulf War were recruited to study the effects of NTFL in slowly removing hydrophobic organic molecules from tissues, while enhancing mitochondrial function and decreasing the severity of certain signs and symptoms associated with this multi-symptom illnesses. These subjects took 6 g per day oral glycerolphospholipids for 6 months, and the severities of over 100 signs and symptoms were self-reported at various times using illness survey forms. There were gradual and significant reductions of symptom severities in categories related to fatigue, pain, musculoskeletal, nasopharyngeal, breathing, vision, sleep, balance, urinary, gastrointestinal and chemical sensitivities. There were no adverse incidents during the study, and the all-natural oral study supplement was extremely well tolerated. Thus MLR with oral glycerolphospholipids proved to be a simple, safe and potentially effective method of slowly reducing the severities of multiple symptoms in chemically-exposed veterans.

Nicolson GL, Ferreira de Mattos G, Ash M, Settineri R, Escribá PV. Fundamentals of Membrane Lipid Replacement, a natural medicine approach to reducing fatigue, pain, and other symptoms while restoring function in chronic illnesses and aging. *Membranes* 2021;

11(12): article 944.

Nicolson GL. Membrane Lipid Replacement—a functional approach to repairing cellular membranes, reducing symptoms, and restoring function. *Functional Food Science* 2022; 2(8): 198-204.

Settineri R, Ji J, Shields ZP, Shirvani T, McLaren CE, Nicolson GL. The effects of Membrane Lipid Replacement with NTFactor<sup>®</sup> Lipids on increasing the bioavailability of three test nutrients. *Bioactive Compounds in Health & Disease* 2022; 5(5): 106-116.

Nicolson GL, Settineri R, Breeding PC. Recent research on Membrane Lipid Replacement with NTFactor Lipids<sup>®</sup>: Enhancement of nutrient bioavailability and reductions in symptom severities in chemically exposed veterans. *Townsend Letter* 2022; 472: November 1-4.

Nicolson GL, Breeding PC. Membrane Lipid Replacement with glycerolphospholipids slowly reduces self-reported symptom severities in chemically exposed Gulf War veterans. *International Journal of Translational Medicine* 2022; 2(2): 164-173.

### **3. Microbial translocation and its role in diseases of unknown origin and infectious diseases like COVID-19 and Long COVID**

Gut microbes are immunologically tolerated in the gastrointestinal tract but trigger aggressive immune responses upon translocation across the gut barrier. Although oral tolerance, a physiological process that dampens immune responses to food proteins and commensal microbiota, remains poorly defined, significant progress was made during and after the Human Immunodeficiency Virus epidemic in 1980s and the discovery of regulatory T cells in 1995. Additional insight was gained after the discoveries of innate lymphoid cells in 2008 and the functional elucidation of mucosal mast cells. Prior to the historical discovery of human pathogens, the etiologies of most human diseases were considered unknown. The same was true about many genetic disorders prior to the Human Genome Project. We have hypothesized that many of the remaining idiopathic conditions, including autoimmune, fibroproliferative, and neuropsychiatric diseases as well as some cancers can be considered microbial translocation disorders triggered by the host immune responses to extra-intestinal gut microbes. We have proposed potential interventions for intestinal barrier rehabilitation, including the use of Membrane Lipid Replacement supplements (NTFactor Lipids). This appears to be useful in reducing symptom severities in infections of SARS-CoV2 and post-infection Long COVID.

Ferreira G, Santander A, Guirado M, Sobrevia L, Nicolson GL. SARS-CoV-2, Zika viruses and Mycoplasma: structure, pathogenesis and some treatment options in emerging viral and bacterial infectious diseases. *Biochimica et Biophysica Acta Molecular Basis of Disease* 2021; 1867: 166264.

Sfera A, Osorio C, Hazan S, Kozlakidis Z, Maldonado JC, Martin del Campo CMZ, Anton JJ, Rahman L, Andronescu CV, Nicolson GL. Long COVID and the neuroendocrinology of microbial translocation outside the GI tract: some treatment strategies. *Endocrines* 2022; 3: 703-725.

Sfera A, Hazan S, Klein C, Zapata-Martin del Campo CM, Sasannia S, Anton JJ, Rahman L, Andronescu CV, Sfera DO, Kozakidis Z, Nicolson GL. Microbial translocation disorders: assigning an etiology to idiopathic illnesses. *Applied Microbiology* 2023; 3(1): 212-240.

#### **4. Membrane Lipid Replacement with NTFactor Lipids increases sperm motility and resistance to oxidative stress**

Sperm membrane integrity is essential in maintaining sperm viability, signaling, and motility, which are essential for fertilizing female gametes. Human and animal sperm are highly sensitive to oxidative stress as they are unable to synthesize and repair essential constituents. Important targets of this process are sperm cellular membranes. Membrane Lipid Replacement (MLR) with glycerophospholipid mixtures (NTFactor Lipids) has been shown to ameliorate oxidative stress to cells and their cellular membranes and prevent loss of function. Therefore, we tested the effects of MLR on human sperm by tracking and monitoring NTFactor Lipids incorporation into their membrane systems and studying their effects on sperm motility and viability under different experimental conditions. Incubation of human sperm with mixtures of exogenous, unoxidized GPL results in their incorporation into sperm membranes, especially mitochondrial membranes (Ferreira G, Costa C, Bassaiztegy V, Santos M, Cardozo R, Montes J, Settineri R, Nicolson GL. Incubation of human sperm with micelles made from glycerolphospholipid mixtures increases sperm motility and resistance to oxidative stress. *PLoS One* 2018; 13(6): article e0197897). We have now examined horse sperm membranes. Stallion sperm contain a high proportion of polyunsaturated fatty acids, making horse spermatozoa especially vulnerable to peroxidative damage from reactive oxygen species generated as a by-product of cell metabolism. Membrane Lipid Replacement therapy with NTFactor Lipids has been shown to reduce oxidative damage *in vitro* and *in vivo*. When oxidative damage was induced by the addition of arachidonic acid to stallion spermatozoa, the subsequent addition of NTFactor Lipids significantly reduced the percentage of 4-hydroxynonenal, a key end product of lipid peroxidation, and significantly increased the concentration of this key end product within the spent medium. Lipid replacement improved several motility parameters and significantly reduced mitochondrial ROS generation. Supplementation with NTFactor Lipids during 17°C *in vitro* sperm storage over 72 h improved sperm viability and total motility. Incubation of stallion spermatozoa with sub-µm-sized glycerolphospholipid micelles resulted in the incorporation of exogenous phospholipids into sperm membranes, diminishing lipid peroxidation and improving sperm quality *in vitro*.

Medica AJ, Aitkin RJ, Nicolson GL, Sheridan AR, Swegan A, De Luliis G, Gib Z. Glycerophospholipids protect stallion spermatozoa from oxidative damage *in vitro*. *Reproduction & Fertility* 2021; 2: 199-209.

# Pharmaceutical Formulations and Excipient Functions

by Mansoor A. Khan, Member EUAS

## Short Biography

*Dr. Mansoor A. Khan has served FDA for over 11 years as the Director of Product Quality Research and a Senior Biomedical Research Scientist (SBRS) at CDER, where he helped develop regulatory policies for reviews and compliance, and led cmc review and research teams on drug delivery systems, product stability, biotech products, and biopharmaceutics. In Sept of 2015, he joined Texas A&M University as Professor and Vice Dean at the Rangel College of Pharmacy in College Station, TX. Prior to joining FDA in 2004, Dr. Khan was a Professor of Pharmaceutics and Director of Graduate Program in the School of Pharmacy at Texas Tech University Health Science Center. He earned his Ph.D. degree in Industrial Pharmacy from the St. John's University School of Pharmacy at New York in 1992. He has published over 325 peer-reviewed manuscripts, five texts including "Quality by Design for Biopharmaceutical Drug Product Development, 30 book chapters, 250 poster presentations, and more than 275 invited presentations world-wide.*

*Dr. Khan has held several leadership positions at the American Association of Pharmaceutical Scientists (AAPS) including elected chair of pharmaceutics and drug delivery (PDD) and the founding chair of formulations design and development (FDD). He serves on the editorial board of Pharmaceutical Technology, International Journal of Pharmaceutics, AAPSPharmsciTech, and Drug Delivery and Translational Research. As a formulations expert, Dr. Khan served as a FDA representative to EMA/PDCO, WHO, USP, NIH, DoD, DARPA, NASA, and Bill and Melinda Gates Foundation. He also served as the science policy advisor to CDER Center Director where he helped resolve complex issues of drug reviews and compliance with science. He has also led the chemistry review team that approved the first 3D printed tablets in August 2015. Dr. Khan has received outstanding alumni award from St. Johns University, College of Pharmacy, Excellence Award from Texas A&M University Health Science Center, over fifteen FDA/CDER Team Excellence Awards, FDA/CDER Scientific Achievement Award, and FDA/CDER Exemplary Performance Awards. Additionally he received the AAPS Research Achievement Award in Formulations Design and Development. He is also an AAPS and AAiPS Fellow.*

## **Summary of Accomplishments and Research Efforts in the Area of Pharmaceutical Formulations and Excipient Functions**

Dr. Mansoor Khan is a Regents Professor of Pharmaceutical Sciences within the Texas A&M University Irma Lerma Rangel College of Pharmacy. He joined the University in the fall of 2015. Prior to joining Texas A&M University, Dr. Khan was a director of the division of product quality research in the US Food and Drug Administration (FDA) with an oversight of clinical pharmacology and drug formulations research to support science-based public policy decisions. Additionally, he served as the highest-ranking scientist in the federal system, SBRS (Senior Biomedical Research Service). Dr. Khan is a licensed pharmacist and has earned his PhD degree in pharmaceutics/industrial pharmacy from St. John's University in New York. Dr. Khan performs research in several areas of excipients. He is one of the rare pharmaceutical formulation scientists with over 17,000 citations, with h-index of 62 and i-10 index of 247. Now to provide some granularity, Dr. Khan's distinguished research is focused on development of novel dosage forms and delivery

systems including pediatric medications and 3D printed products, eutectic-based self nanoemulsified products, quality by design with process analytical technologies, and post-market research to identify the root cause of product failures and safety issues of metformin as well many other narrow therapeutic drugs.

### **Most recent research activities in the area of excipients**

Most recently Dr. Khan identified and submitted a patent that resolved some of the nitroso impurities of metformin in the presence of several excipients. While FDA and the firms saw a recall of more than 256 lots of extended release metformin products (between February of 2020 and June of 2021), Dr. Khan identified the reason and examples of immediate release products failure for the very first time (1. Dharani S, Mohamed EM, Khuroo T, Ali HI, Reddy IK, Rahman Z, Khan MA. In-use stability assessment of FDA approved metformin immediate release and extended release products for N-Nitrosodimethylamine and dissolution quality attributes. *Int J Pharm.* 2022 Jul 25;623:121923., 2. *Stable Pharmaceutical Composition of Metformin and Similar Drugs, Docket 13260 -P266V1 (10-28-2021)*, and 3. *Compositions Of Stable Metformin And Similar Drug Products With Control On Nitroso Impurities, PCT submitted on March11, 2022*)

### **Pediatric dosage forms and excipients**

Children require different oral dosage forms than adults. Most useful products are liquid dosage forms such as syrups and suspensions. Question were raised, mostly by scientists from Europe that pediatric excipients such as propylene glycol, polyethylene glycol, glycerine and similar cosolvents and certain surfactants such as polysorbates cause neurotoxicities in children and need to be avoided. This created difficulties for developing pediatric dosage forms. With his extensive research, Dr. Khan has cited that several approved products with these excipients have not had any meaningful adverse events, and firms can continue to use these excipients, . Moreover, drugs prescribed to children have historically been those approved for adult patients. As a result, over 80% of product labeling did not provide directions for safe and effective use in pediatric patients. The lack of availability of pediatric friendly formulations is primarily due to evolving physiological and pharmacokinetic development of children where fixed doses do not work. Often, the physicians prescribe an extemporaneous preparation where the drug product is manipulated in pharmacy with a goal to adjust the dose of the drug. However, concerns are raised by physicians and FDA alike on lack of dose accuracy, stability/sterility, pharmacokinetic/pharmacodynamics studies, efficacy and safety, and consistency in preparing extemporaneous preparations. From pediatricians' perspective, an ideal pediatric product should have ability to titrate dose (dose flexibility) so that a wide age group (0-17) of children can be covered by a single product that is easy to swallow/dissolvable form, palatable, contains minimal/safe excipients, has adequate bioavailability and is stable at high heat and humidity. Dr. Khan has promoted the development of pediatric friendly dosage with traditionally used excipients through policy, regulation, and research with continuous funding throughout his career. He presented on FDA policy and regulation on pediatric excipients, and approaches to develop pediatric dosage forms to federal agencies, and at national and internal conferences e.g. AAPS, European Pediatric Formulations Initiative (EUPFI), US Drug Information Agency (DIA), FDA and NIH. His most recent grant on pediatric products development has been funded by the NIH. Dr. Khan currently

has funding from FDA, NIPTE, and the TAMU presidential clinical research grant along with Houston Methodist partners.

Three dimensional (3D) printing or additive manufacturing is the 21<sup>st</sup> century manufacturing technology, which involves assembling parts in an assembly line to make an end-user product. The 3D printing technology involves successive layering of drugs from a digital file of computer aided design under the control of computer software. It has enormous potential across industries, and one of the most transformative applications has been in the medical field including personalized medical devices and drug products. Dr. Khan has established collaborations with Medicine, Engineering, Driscoll Children's Hospital and Houston Methodist to accomplish this. The FDA has approved about eighty-five 3D printed medical devices through 510(K) process, and just one drug product, Spiritam<sup>®</sup>. At the FDA, Dr. Khan led a team of scientists and reviewers that oversaw the approval of Spiritam<sup>®</sup>. Currently, he is working on 3D printing technologies (selective laser sintering and fused deposition modeling) for the development of dosage forms for compounding of personalized medications especially pediatric and geriatric patients. He has published research papers on 3D printing of pharmaceuticals in peer reviewed journals (104,111- 113,120,123 in CV). The 3D printing requires new excipients eg. Caldurin, that need to congeal upon laser treatment to solidify. A review of Dr. Khan's CV highlights several manuscripts that describe excipient role in pediatric product and process development. His project on 3D printing with selective laser sintering required novel excipient selection that required controlled melting and sintering under the influence of laser light, is currently funding by the National Institute of Health.

### **Excipients and Quality by Design**

Research in Dr. Khan's laboratory also includes Quality by Design (QbD) and process analytical technology (PAT) in pharmaceutical development and manufacturing. FDA encourages risk-based approaches and the adoption of QbD principles in drug product development, manufacturing, and regulation. FDA's emphasis on QbD began with the recognition that increased testing does not necessarily improve product quality. Quality must be built into the product. Pharmaceutical QbD is a systematic approach to development that begins with predefined objectives and emphasizes product and process understanding and control based on sound science and quality risk management. PAT is a mechanism to design, analyze, and control pharmaceutical manufacturing processes through the measurement of critical process parameters which affect critical quality attributes. Dr. Khan has extensively used multivariate statistical process control to understand and develop process controls. His research on QbD spans coprecipitation, encapsulation, niosomes, microparticles, nanoparticles, liposomes, freeze-drying process, granulation, ointment, cream etc. Dr. Khan has used Focused beam reflectance measurement, THz spectroscopy, near infrared, particles-vision monitoring, FTIR probes as PAT tools to understand, monitor and control various pharmaceutical manufacturing processes, and track excipients along with the API. Today he is one of the most leading authorities in the world on Quality by Design. He has coedited a book on QbD of biopharmaceutical product development along with executives and scientists from Gates Foundation, Amgen and Genetech. He has also authored or co-authored several book chapters and peer-reviewed publications (1,4-6,8,13,15,23,24,28,31 in CV). Partnering with Universities such as Wisconsin, Maryland, and UT Austin, Dr. Khan received an

FDA grant to develop Quality Score Cards. Presence of excipients places a new burden on process analytical technologies due to signal interference. Therefore, a chemometrics approach is needed to separate the excipient signal from the API signals. The excipient interference and subsequent resolution of X-ray diffractograms for quantitative evaluation of the degree of crystallinity as well as the relating NIR measurements with chemometrics represent good examples of Dr. Khan's on excipient use in quality by design. Dr. Mansoor Khan's consistent message has been that excipients are not "inert" materials. They play a significant role in the delivery of drugs to the required targets, and perform a variety of important functions, e.g., processing aids, chemical stabilizers, bioavailability enhancers, etc. A key challenge is to monitor excipients during manufacturing, as it is not easy to accurately quantify their properties in the different drug delivery systems. As shown in his paper "Rahman, Z., Zidan, A. and Khan, M, Formulation and evaluation of a protein loaded solid dispersions by non-destructive methods in the AAPS Journal., (2010), 12(2), 158-170, Dr. Khan used novel methods to precisely monitor and characterize PEG 6000 by non-destructive chemical imaging and near infrared (NIR) methods. He has also shown in other publications that excipients can be easily monitored by on-line NIR methods without the need for extensive wet chemistry methods for analyzing them. For example, the manuscript "Sulub Y, Wabuye B, Gargiulo P, Pazdan J, Cheney J, Berry J, Gupta A, Shah RB, Wu H, and Khan MA. 'Real-time on-line blend uniformity monitoring using near-infrared reflectance spectrometry: A noninvasive off-line calibration approach', Journal of Pharmaceutical & Biopharmaceutical Analysis, (2009), 49 : 48-54., indicates that excipients such as croscopolvidone, lactose, and microcrystalline cellulose could be precisely monitored quantitatively in a real-time fashion along with the API. This work emanated from the well-known FDA Novartis Cooperative Research and Development Agreement where Mansoor serves as the Principal Investigator.

### **Excipients to enhance drug solubility and bioavailability**

One particularly difficult area of drug delivery has been developing an effective delivery system for poorly soluble drugs or drugs needed for specific targeting to required tissues. In fact, a majority of newly developed drugs are poorly soluble in water. Dr. Khan's research efforts have been at the cutting edge of developing innovative drug delivery systems to overcome some of these challenges.

Lipids along with proteins and carbohydrates, are the structural components of living cells. Certain lipids such as oils have been shown to be successful carriers for administering the drugs to the body. As a result, there is a growing demand in the pharmaceutical field for the use of these lipid-based formulations, due to their ability to vastly improve the administration and therapeutic efficacy of poorly water-soluble drugs.

However, a key challenge in developing lipid-based drug delivery systems is to find the appropriate combination of all the ingredients that will optimize the desired results. Dr. Khan's expertise with the chemical nature, physical properties, interactions between drug and excipients, solubility, dispersibility in water and bioavailability enhancement, led to important contributions for the advancement of lipid delivery systems. The innovative formulations developed in his laboratories significantly added to the knowledge and scientific understanding of the surfactants as a critical component in lipid-based drug delivery systems. Due to the complexities of their use, and the fact that the surfactants can be toxic, if used in too large a quantity, Mansoor was able to balance all these competing factors to develop innovative and safe delivery systems. Based upon these many contributions, it is my opinion that Dr. Khan is at the forefront of ensuring the safe and

effective use of surfactant based formulations. For example, Dr. Khan has determined that combining the proper amount of surfactant in addition to co-surfactants, with intermediate properties between oils and surfactants, significantly reduces surface tension even further, and results in an increased dissolution of the lipids.

Dr. Khan has also made significant strides in formulating drug delivery systems in which the pharmaceuticals are neither soluble in water or oil. For example, he was among the first researchers to devise and characterize a new drug delivery system to address the challenges posed by insoluble drugs. This innovative technique is known as eutectic-based self-nanoemulsified drug delivery; for which he was granted a US patent (US Patent No. 7,588,786).

He has devised a formulation where a drug is melted into a liquid which is then used as the oily-phase of the lipid-based drug delivery system. The key to effective administration of such a delivery system is determining the proper eutectic forming agent that will force a high melting drug to melt at or below body temperature. A eutectic is a low melting mixture of compounds that when combined, their melting temperatures drop. Thus, because most drugs melt at temperatures higher than body temperature, by combining them with an effective eutectic agent greatly facilitates their delivery to the body. Dr. Khan has been able to determine that certain essential oils, such as peppermint, anise, and lemon oil act as ideal eutectic agents, causing a host of drugs to liquefy in the oil mixture and enabling an ideal lipid-based delivery system. Details of this work can be seen in a series of papers that he has published with his students, Drs Nazzal and Palamakula, and post doctoral scholars, Drs Zidan and Rahman. The cytotoxicity and permeability of numerous surfactants and cosurfactants were evaluated to select the most appropriate excipients. An example illustrating this work is provided in the manuscript, S. Nazzal, I.I. Smalyukh, O.D. Lavrentovich, and M.A. Khan, Preparation and *in-vitro* Characterization of a Eutectic-based Semisolid Self-nanoemulsified Drug Delivery System (SNEDDS) of Ubiquinone: Mechanism and Progress of Emulsion Formation, *Int. J. Pharm.* (2002), 235, 247-65.

Narrow therapeutic index (NTI) drugs are comprised of products where small differences in dose or blood concentration may lead to serious therapeutic failures and/or adverse drug reactions that are life-threatening. Examples of NTI drugs for which the quality issues have been addressed are phenytoin sodium, warfarin, tacrolimus, and theophylline. Phenytoin is a first line drug for generalized tonic-clonic epileptic seizure. The generic phenytoin differs from the brand as well among themselves in terms of the composition of inactive ingredients (qualitative and quantitative), manufacturing methods, processing parameters, in-process control, specifications, and container closure etc. This may be manifested in clinical performance when a product is switched to another product. Furthermore, differences in products clinical performances are not only because of inherent properties of the drug but may also be due to quality differences among products. Dr. Khan's studies indicated significant effect of excipient, process variables and stability on the critical quality attributes of phenytoin products. These findings are published in *International Journal of Pharmaceutics*, *Journal of Pharmaceutical Sciences* and *AAPS PharmSciTech*, and also presented to FDA for market corrections. Tacrolimus product recalls have been traced to an increase in drug crystallinity resulting in decreased dissolution and bioavailability. The degree of crystallinity measurements required a separation of excipient interference in Bragg's spacing and two theta values of tacrolimus. Dr. Khans work in this area is highly cited, and became a regulatory standard for monitoring the degree of crystallinity

Similar to phenytoin, systematic studies with subsequent impact of product withdrawals and market corrections were carried out for warfarin, levothyroxine, carbamazepine, theophylline, and divalproate NTI drugs (7,11,27,39,67,80,85-87 in CV).

### **Leadership activities**

This is another major strength and area of distinction for Dr. Khan. Dr. Khan is a leader in pharmaceutical product development and has served to set the standard nationally and internationally for development and use of pharmaceutical products. As a Professor at TAMU and ex-Director of the Division of Product Quality Research for 11.5 years, he is highly visible and well- recognized both nationally and internationally in the area of industrial pharmacy and formulations. Dr. Khan is a Fellow of the American Association of Pharmaceutical Scientists (AAPS) and recipient of the 2012 AAPS Research Achievement Award in Formulations Design and Development. He was elected Chair of AAPS Pharmaceutics and Drug Delivery Section (2009) and served as Founding Chair of AAPS Formulations Design and Development Section (2010). He has organized more than 25 workshops and symposia as Chair, Co-Chair, Moderator or a Planning Committee Member. He has been a speaker world- wide for over 250 invited presentations. His national presentations included keynote or plenary presentations in almost all major pharmaceutical conferences nationally including AAPS, Controlled Release Society, Parenteral Drug Association, USP, NIH, FDA, NASA, DARPA, National Biotech Conference/NBC, many major universities, and international conferences or workshops in most major European and Asian Countries in addition to US and Canada. Dr. Khan has had direct interactions/collaborations or Memorandum of Understandings (MOUs) or Cooperative Research and Development Agreements (CRADAs) with USP, EMA, WHO, NASA, National Institute of Pharmaceutical Education and Technology (NIPTE), Center for Pharmaceutical Processing and Research (CPPR), NIH, FIP (Europe), AAPS and over a dozen US universities. He has led or co-led the FDA's CRADAs with Novartis and Pfizer and served or continues to serve on the expert review committees of NIH, DARPA, the Bill and Melinda Gates Foundation, the USP and EMA/Pediatric Development Committee (PDCO). His strong scientific leadership and visibility are exemplified by his tenure as NIH Senior Biomedical Research Scientist (SBRS) and by his service as scientific/technical advisor to the Center and Super Office Directors for very high impact regulatory decisions leading to approvals, withdrawals/recalls, policy development and FDA action on citizen petitions. During his tenure at the FDA, he has served on more than 30 committees, notably the CDER Emerging Technology Team on which he served as lead reviewer, the Nanotechnology Working Group and Council of Scientific Enhancement (CASE).

# Global COVID-19 Wastewater Monitoring Efforts, Equity, and Gaps

by Joan Rose, Member EUAS

## Short Biography

*Dr. Joan Rose serves as the Homer Nowlin Chair in Water Research at Michigan State University, the Co-Director of the Center for Advancing Microbial Risk Assessment (CAMRA) a 10 million dollar grant funded by the EPA and US Department of Homeland Security. She is also the Director of the Center for Water Sciences (CWS). Dr. Rose received her B.S., in 1976 from University of Arizona, her MS from University of Wyoming in 1980 and Ph.D. in Microbiology from the University of Arizona in 1985. She served as a Professor in the College of Marine Science, University of South Florida (USF) from 1998-2002 and Associate Professor, Department of Marine Science, USF from 1994-1997. In 1995, she was an Assistant Professor, Department of Environmental and Occupational Health, USF, and from 1986-1989, she served as Research Associate/Lecturer, Department of Microbiology and Immunology, UAZ.*

*Dr. Rose is an international expert in water microbiology, water quality and public health safety publishing more than 300 manuscripts. She has been involved in the investigation of numerous waterborne outbreaks world-wide. Her work has examined new molecular methods for waterborne pathogens and zoonotic agents such as Cryptosporidium and enteric viruses and source tracking techniques. She has been involved in the study of water supplies, water used for food production, and coastal environments as well as water treatment wastewater treatment, reclaimed water and water reuse and quantitative microbial risk assessment. She specifically interested in microbial pathogen transport in coastal systems and has studied the impact of wastewater discharges and climate on water quality. She was named as one of the 21 most influential people in Water in the 21st Century by Water Technology Magazine in 2000 and won the Clarke Water Prize (\$50,000. prize) (one of 5 international awards for contributions to water science and technology).*

*She current serves on a number of advisory committees include 1) Chair of the Drinking Water Committee for the Science Advisory Board for the U.S. Environmental Protection Agency 2) Vice-Chair of USA National Committee for the International Water Association, 2002-05, 4) Member of the Strategic Council for IWA 2005-08, 3) Chair of the Specialist Group Health-Related Water Microbiology (IWA). 4) She is currently advisory to the Governments of Singapore and Queensland, Australia, serving as chair of the audit committee for the Public Utilities Board in Singapore for the last 4 years.*

*She was appointed to Water Science and Technology Board of National Academy of Science, National Research Council, 1998-2004 and served as Vice Chair of the Board from 2002-04. Professional society memberships include American Academy of Microbiologists, American Public Health Association, American Society of Microbiology,, American Water Works Association (AWWA), Society for Risk Analysis, International Water Assoc. and Water Environment Federation.*

*Sources of recent grant and/or contract support include NOAA, EPA, Water Environ. Research Foundation, and NSF,*

## **Positions and Honors**

### **Positions and Employment**

*1986-1989: Research Associate/Lecturer, Department of Microbiology and Immunology, and Nutrition and Food Science, University of Arizona*

*1989-1994: Assistant Professor, Department of Environmental and Occupational Health, University of South Florida*

*1994-1997: Associate Professor, Department of Marine Science, University of South Florida*

*1995: Courtesy Appointment, Associate Professor, Department of Civil and*

*Environmental Engineering, University of South Florida*

1998-2002: *Professor, College of Marine Science, University of South Florida*

2005-2014: *Co-Director, Center for Advancing Microbial Risk Assessment (CAMRA), Michigan State University (Center of Excellence DHS/EPA)*

2003-present: *Homer Nowlin Endowed Chair for Water Research, Michigan State University Honors (Most Recent)*

*Member of the National Academy of Engineering, inducted 2011*

*Awarded the KWR Water Fellow, Netherlands, October, 2016*

**Stockholm Water Prize 2016**

*Recipient of The Michigan Environmental Council's Helen & William Milliken Distinguished Service Award, 2018*

**Naughton, C.C., Roman Jr., F.A., A. F Alvarado, A.G. F.; Tariqi, A.Q.; Deeming, M.A.; Kadonsky, K.F.; Bibby, K.; Bivins, A.; Medema, G.; Ahmed, W.; Katsivelis, P. Allan, V.; Sinclair, R. and Rose J. B. 2023 Show us the Data: Global COVID-19 Wastewater Monitoring Efforts, Equity, and Gaps. FEMS Microbes.**

### **Abstract**

A year since the declaration of the global coronavirus disease 2019 (COVID-19) pandemic there were over 110 million cases and 2.5 million deaths. Learning from methods to track community spread of other viruses such as poliovirus, environmental virologists and those in the wastewater based epidemiology (WBE) field quickly adapted their existing methods to detect SARS-CoV-2 RNA in wastewater. Unlike COVID-19 case and mortality data, there was not a global dashboard to track wastewater monitoring of SARS-CoV-2 RNA worldwide. This study provides a one year review of the “COVIDPoops19” global dashboard of universities, sites, and countries monitoring SARS-CoV-2 RNA in wastewater. Methods to assemble the dashboard combined standard literature review, Google Form submissions, and daily, social media keyword searches. Over 200 universities, 1,400 sites, and 55 countries with 59 dashboards monitored wastewater for SARS-CoV-2 RNA. However, monitoring was primarily in high income countries (65%) with less access to this valuable tool in low and middle income countries (35%). Data are not widely shared publicly or accessible to researchers to further inform public health actions, perform meta-analysis, better coordinate, and determine equitable distribution of monitoring sites. For WBE to be used to its full potential during COVID-19 and beyond, show us the data.

**Key words:** Geographic Information Systems (GIS), Wastewater Based Epidemiology (WBE), SARS-CoV-2, Open Data, Public Health, COVIDPoops19 Dashboard.

**Flood, MT; Hernandez-Suarez, JS;; Nejadhashemi, AP; Martin, SL; Hyndman, D.; Rose, JB 2022. Connecting microbial,**

**nutrient, physiochemical, and land use variables for the evaluation of water quality within mixed use watersheds Jul 1 2022 Water Research 219: Article Number118526.**

**Abstract**

As non-point sources of pollution begin to overtake point sources in watersheds, source identification and complicating variables such as rainfall are growing in importance. Microbial source tracking (MST) allows for identification of fecal contamination sources in watersheds; when combined with data on land use and cooccurring variables (e.g., nutrients, sediment runoff) MST can provide a basis for understanding how to effectively remediate water quality. To determine spatial and temporal trends in microbial contamination and correlations between MST and nutrients, water samples (n = 136) were collected between April 2017 and May of 2018 during eight sampling events from 17 sites in 5 mixed-use watersheds. These samples were analyzed for three MST markers (human – B. theta; bovine – CowM2; porcine – Pig2Bac) along with E. coli, nutrients (nitrogen and phosphorus species), and physiochemical parameters. These water quality variables were then paired with data on land use, streamflow, precipitation and management practices (e.g., tile drainage, septic tank density, tillage practices) to determine if any significant relationships existed between the observed microbial contamination and these variables. The porcine marker was the only marker that was highly correlated (p value <0.05) with nitrogen and phosphorus species in multiple clustering schemes. Significant relationships were also identified between MST markers and variables that demonstrated temporal trends driven by precipitation and spatial trends driven by septic tanks and management practices (tillage and drainage) when spatial clustering was employed.

**Graydon, R.C.; Mezzacapo, M.; Boehme, J. Foldy, S.; Edge, T.A.; Brubacher, J. Chan, H.M.; Dellinger, M.; Faustman, E.M.; Rose, J.B. and Takaro, T.K. 2022. Associations between extreme precipitation, drinking water and protozoan acute gastrointestinal illnesses in four North American Great Lakes cities (2009-2014) *Journal of Water and Health* 20 (5), 849-862.**

**Abstract**

Climate change is already impacting the North American Great Lakes ecosystem, and understanding the relationship between climate events and public health, such as waterborne acute gastrointestinal illnesses (AGI), can help inform needed adaptive capacity for drinking water systems (DWSs). In this study, we assessed the effects of extreme precipitation events ( $\geq 90$ th percentile) and preceding dry periods, source water turbidity and total coliforms, and protozoan AGI - cryptosporidiosis and giardiasis - in the populations served by four DWSs that source surface water from Lake Ontario (Hamilton and Toronto, Ontario, Canada) and Lake Michigan

(Green Bay and Milwaukee, Wisconsin, USA) from January 2009 through August 2014. We used distributed lag non-linear Poisson regression models adjusted for seasonality and found extreme precipitation weeks preceded by dry periods increased the relative risk of protozoan AGI after 1 and 3-5 weeks in three of the four cities, although only statistically significant in two. Our results suggest that the risk of protozoan AGI increases with extreme precipitation preceded by a dry period. As extreme precipitation patterns (both dry and wet) become more frequent with climate change, the ability to detect changes in water quality and effectively treat source water of varying quality is increasingly important for adaptive capacity and protection of public health.

**Keywords:** climate change, cryptosporidiosis, giardiasis, Great Lakes, rain, water quality

## Activities in Materials Science, Engineering and Engineering Education

by Derek O. Northwood, Member EUAS

### Short Biography

*Professor Derek O. Northwood is a Distinguished University Professor Emeritus and Professor of Engineering Materials in the Department of Mechanical, Automotive and Materials Engineering at the University of Windsor, Windsor, Ontario, Canada. Professor Northwood has an earned doctorate in Chemical Physics (Crystallography) from the University of Surrey (UK) and a BSc (Eng) in Engineering Metallurgy from the Imperial College, University of London (UK). He is a licensed Professional Engineer in Ontario, Canada (PEng) and is a Chartered Professional Engineer (CPEng; NER), APEC Engineer, and International Professional Engineer (IntPE(AUS), in Australia. In the 40+ years as an academic, Professor Northwood has held various administrative positions including Department Head, Dean, Associate Dean of Research, Director of the Office of Research Services, President of the Industrial Research Institute, and, Research Leadership Chair, both at the University of Windsor and Ryerson University, Toronto, Canada. Professor Northwood has taught, researched and facilitated joint research and educational programs at 14 universities worldwide, including the UK, the USA, Australia, Taiwan, China, Singapore and Canada. He has published 703 papers in refereed international journals and conference proceedings, 9 chapters in books and has edited 10 books, on a wide range of topics including materials and their applications, and engineering and technology education. He has been elected Fellow of six international professional societies in Australia, Canada, the UK and the USA; namely, Fellow of the Royal Society of Canada (FRSC); Fellow of the Institution of Engineers Australia (FIEAust); Fellow of the World Institute for Engineering and Technology Education (FWIETE); Fellow of the Institute of Materials, Minerals and Mining (FIMMM); and Fellow of ASM International (FASM); and Fellow of Alpha Sigma Mu (FAΣM), The International Professional Honor Society for Materials Science and Engineering. In 2022, Professor Northwood was again recognized as being among the world's top 100,000 - or top 2% of scientists - according to the database published by Stanford University. The database recognizes the long-term career performance of scientists around the world, living or deceased, who are the most cited authors in their disciplines. It reflects six citation metrics, including total citations and number of citations to papers as single or first author between 1965 and 2019. The data was collected from the Scopus database of nearly 7 million authors out of which the top 100,000/2% were analysed. In 2022, Professor Northwood was appointed as Associate Editor of two journals: Global Journal of Engineering Education and World Transactions on Engineering and Technology Education. Professor Northwood has continued in his role as a member of the International Editorial Board for the International Journal of Computational Methods and Experimental Measurements.*

**RESEARCH ACTIVITIES AND PUBLICATIONS 2022**

As was the case for 2020 and 2021, Covid-19 restrictions have had a significant negative impact on our ability to conduct research both in my home university and with my partners across the globe.

Work had been conducted in two principal areas:

1. Developing the potential properties of traditional materials.
2. Innovation in Engineering Education

The cooperative work on "Developing the potential properties of traditional materials" with Yangzhou University has been halted and no publications have resulted in 2022.

Work has continued in the "Innovation in Engineering Education" area.

**Innovation in Engineering Education**

Since early 2020, in response to the pandemic, faculty, administrators, and staff have been challenged as how best to serve learners. *University Affairs*, the voice of the Canadian university community, posed the following question to their readers. "What is the one change you've made as a result of the pandemic that you will carry with you into the upcoming academic year and why? ["What we have learned from the Pandemic", Hannah Liddle, *University Affairs*, 63(6), 28-32, November -December 2022}.

The responses were varied and addressed societal problems as well as the learning process.

Examples included:

- Reducing carbon emissions by limiting air travel and connecting virtually;
- Making the best use of pre-recorded audio lectures for teaching transferable skills, expanding on basic curricula, hosting review sessions, and doing labs;
- Leveraging technology. Many approaches have been taken including virtual educating learners at all levels. A virtual approach has also been taken for student wellness programs in order to reach students off campus;
- "Focusing on relationships and advocating for empathy, compassion, and kindness in all the policies, procedures, grading and interactions with others." [Judy Bornais, University of Windsor]

With respect to "Leveraging Technology", Associate Professor Daniela Pusca and I have outlined a number of approaches in our paper, "Teaching and learning engineering design: creative methods for remote education."

Pusca, D., Northwood, D.O.

**Teaching and learning engineering design: creative methods for remote education**  
(2021) *World Transactions on Engineering and Technology Education*, 19 (3), pp. 306-312.

**Abstract**

The traditional engineering design class was created for integrated lecture-laboratory sessions in a face-to-face environment. With the move towards remote teaching and learning at the University of Windsor, Windsor, Canada, there was a need to make changes related to both, teaching and learning. In this article, the authors discuss issues on How much change is needed; Does tech solve education problems?; What is the impact on students' learning?; and present innovative course design strategies for remote education, based on identified problems and challenges associated with using an e-learning platform. It is the authors' opinion that both teaching and learning should be done creatively, regardless of the environment - face-to-face or remotely. In times of rapid technological changes, instructors and students should be able to use different tools associated with the learning management system (LMS) and also course-related digital tools to achieve the desired student-centred results. The purpose of this article is to present digital tools and new technology that have the potential to transform the teaching and learning experience, regardless of the learning spaces.

The importance of "Empathy" has long been recognized. As emphasized by Helen Riess [The Science of Empathy, Journal of Patient Experience, 4(2), 74-77, 2017]:

*Empathy plays a critical interpersonal and societal role, enabling sharing of experiences, needs, and desires between individuals and providing an emotional bridge that promotes pro-social behavior."*

Also, as detailed by Associate Professor Daniela Pusca and myself, empathy is at the core of a "design thinking" approach to problem solving.

Pusca, D., Northwood, D.O.

**Design thinking and its application to problem solving**

(2018) *Global Journal of Engineering Education*, 20 (1), pp. 48-53.

**Abstract**

In this article, the authors implement the design thinking paradigm as a method to find solutions for specific problems and challenges within higher education. This approach was triggered by the continuous changes in technology and the requirements of the outcome-based curriculum in regard to graduate attributes. The authors also address the question as to whether researchers should be problem focused or solution focused in the process. Problem-oriented thinking is closely linked to critical thinking, and questions like what? and why?, whereas solution-focused thinking is linked to creativity and the question how. In this context, design thinking should be thought as a form of solution-based thinking, which is implemented to produce creative future results and/or creative resolutions to wicked problems. This article identifies how design thinking was implemented to provide innovations in outcome-based teaching and learning considering aspects, such as curricula, pedagogy, assessment methods and teaching spaces. The main goal was to improve graduate attributes and, as a consequence, the academy to industry transition. Using case studies to accommodate the new generation of learners, the authors argue in the article that user-oriented and outcome-based oriented design thinking is the suitable paradigm to

ensure that these initiatives are successful.

The English poet Samuel Taylor Coleridge (1772-1834) in his poem *Love, Hope, and Patience in Education* made the case that love, hope and patience "upbear" (*support; sustain*) education. Love, hope and patience are all important components of empathy.

There are those who consider that empathy cannot be taught, but methods have been, and continue to be, developed whereby these skills can be facilitated. Significant advances in this respect have been made in nursing education. The application of these methods to engineering and technology education is an area warranting investigation in our future studies.

# Modifications to ACI 318 Shear Design Method for Prestressed Concrete Members

by Thomas Kang, Member EUAS

## Short Biography

*Dr. Thomas Kang is a full professor in the Department of Architecture & Architectural Engineering at Seoul National University (SNU), Korea. Before that, he was a professor in the School of Civil Engineering and Environmental Science at the University of Oklahoma. He also has held various affiliated positions in the U.S., Japan and South Africa, including the University of Illinois at Urbana-Champaign, University of Hawaii at Manoa, University of Tokyo and University of Cape Town. Prof. Kang received his PhD from University of California Los Angeles (UCLA) in 2004, his MS from Michigan State University in 2000, and his BS from SNU in 1998. He is a Fellow and Technical Advisory Board (TAB) member of Post-Tensioning Institute (PTI), a Fellow of American Concrete Institute (ACI), and a member of National Academy of Engineering of Korea and EU Academy of Sciences. He received the Kenneth B. Bondy Award for Most Meritorious Technical Paper as Lead Author from PTI in 2012, and the Wason Medal for Most Meritorious Paper as Lead Author from ACI in 2009. He currently serves as an Editor-in-Chief for Wind and Structures and as the Associate Editor for PTI Journal. Prof. Kang published over 150 international journal papers, including over 50 in ACI Structural Journal and over 10 in PTI Journal. His research interests include the design and behavior of reinforced, prestressed and post-tensioned concrete structures, as well as dynamic effects (wind, seismic, fire, impact & blast) on structures.*

*Dr. Kang has chaired numerous sessions/symposiums of structural engineering; delivered many plenary/keynote/invited speeches; and organized several international conferences/workshops as Chair or Co Chair. He is also one of the founding and voting members of PTI DC-20 Committee, Building Design; and has been a voting member for a variety of technical committees, including: ACI Subcommittee 318-T, Structural Concrete Building Code – Post-Tensioned Concrete; ACI Committee 369, Seismic Repair and Rehabilitation; Joint ACI-PTI Committee 320, Post-Tensioned Concrete Building Code; Joint ACI-ASCE Committees 335, Composite and Hybrid Structures; 352 Joints and Connections in Monolithic Concrete Structures; and 423, Prestressed Concrete; and Joint ACI-ASME Committee 359, Concrete Containments for Nuclear Reactors.*

## **Abstracts of Selected Recent Papers and Patent**

**Modifications to ACI 318 Shear Design Method for Prestressed Concrete Members: Detailed Method (by H. Ju, M. Yerzhanov, D. Lee, H. Shin, and T. H.-K. Kang; PCI Journal, V. 68, No. 1, Jan.-Feb. 2023)**

This paper proposes modifications to the methods for shear design of prestressed concrete one-way members specified in American Concrete Institute's Building Code Requirements for Structural Concrete (ACI 318-19) and Commentary (ACI 318R-19) to increase applicability. The current ACI 318 shear design methods have

been widely used and have a history of demonstrated safety and reliability. However, there are long-standing concerns regarding the cumbersome computational procedures specified in ACI 318, as well as the inability of the ACI 318 shear design methods to capture key influential factors. This paper provides a brief history of changes made over several decades within ACI 318 for prestressed concrete shear design and critical issues raised in previous studies. While maintaining the philosophy and safety priorities of the original pioneers in the development of shear design for prestressed concrete members, the proposed changes simplify the calculation process and provide analytical accuracies comparable to the current ACI 318 methods. These changes are affirmed by comparing the results of the modified methods with data from an extensive shear database of prestressed concrete component designs that vary in dimensional detail and material properties and shear strengths estimated using current ACI 318 methods.

**Post-Tensioned Self-Centering System Efficiency against Extreme Wind Loads (by H. Alinejad, T. H.-K. Kang, and S. Y. Jeong; ACI Structural Journal, V. 119, No. 5, Sept. 2022)**

For tall buildings, wind demand under extreme wind loads is so large that design based on conventional elastic behavior can be difficult. A practical solution is to permit inelastic behavior to introduce hysteretic damping and reduce design wind force. Therefore, the inelastic behavior of structures subject to wind load should be thoroughly investigated. Presumption is that applications currently applied in inelastic seismic design can be employed in inelastic wind design of concrete buildings. In this research, behaviors of elastic, bilinear, and self-centering single degree of freedom systems under along-wind load were studied for various design wind speeds using nonlinear time history analysis. Self-centering systems, in particular unbonded post-tensioned concrete systems given their wide use and high potential and flexibility for self-centering behavior, were found to have smaller maximum displacement than bilinear systems with differences being considerable at higher wind speeds. Results found highlight the role of post-yield stiffness in reduction of maximum displacement. Self-centering systems were also found to be highly influenced by reverse yielding values. Systems with reverse yield strength equal to standard deviation of the elastic force (about 20% of [mean + background + resonant components]) demonstrated minimum displacement. In addition, design parameters, such as ductility, overstrength, and displacement factor, are reported for inelastic design based on the concept of a response modification factor.

**Validation of Numerical Modeling Techniques for Unbonded Post-Tensioned Beams under Low Velocity Impact (by A. Nghiem, and T. H.-K. Kang; Journal of Structural Engineering, V. 148, No. 8, Aug. 2022)**

This study validates the use of available tools for nonlinear finite element dynamic analysis (NLFEDA) modeling of unbonded post-tensioned reinforced concrete (PT-RC) members under drop weight impact and is the first attempt at low-velocity impact to the authors' knowledge. The study was performed in two parts. The first portion of the study determined the appropriate mesh and material properties of the testing setup and specimens that were generated by the authors. The second portion of the study then established the level of convergence of the model based on a wide range of design and loading parameters. The NLEFDA was validated using experimental data obtained from laboratory investigations on the behavior of shear-critical and flexural PT-RC members. The interaction between the prestress, as applied from the PT tendon, and the surrounding concrete was well modeled in the presence of large shear failures of the concrete. The modeling techniques, coupled with experimental studies, can be helpful in expanding the range of understanding of the behavior of unbonded PT-RC members.

**Parametric Study on the Dynamic Behavior of Post-Tensioned Beams Using Nonlinear Finite Element Modeling (by A. Nghiem, and T. H.-K. Kang; ACI Structural Journal, V. 119, No. 4, July 2022)**

A parametric study was performed to understand the behavior of unbonded post-tensioned concrete beams under low-velocity drop-weight impact. Nonlinear finite element dynamic analysis was used for the simulation of both shear- and flexural-critical members. The modeled design parameters incorporated various concrete strengths, spacing of transverse reinforcement, and increasing levels of post-tensioning force. All beams were simulated under impact at four levels of impacting velocity of the drop hammer. Results of the parametric study were used to identify critical design and loading conditions on the dynamic behavior of unbonded post-tensioned members. Post-tensioning was shown to be beneficial for both shear and flexural resistance against low-velocity impact, and a static shear-to-flexural capacity ratio of at least 5 was found to prevent large shear failure. Additionally, the study was useful at correlating prior experimental results on the behavior of unbonded post-tensioned members, as well as developing the relationship between the peak deformation and the impacting energy and static design capacity with conservativeness.

## A review of Organic Matter in Fogs and Clouds : Origin, Processing and Fate

by Kalliat Valsaraj, Member EUAS

### Short Biography

*Professor Kalliat T Valsaraj presently holds the dual titles of the Charles and Hilda Roddey Distinguished Professor in Chemical Engineering and Ike East Professorship in Chemical Engineering at Louisiana State University in Baton Rouge, Louisiana. He is a Fellow of the American Association for the Advancement of Science (AAAS), the American Institute of Chemical Engineers (AIChE), the Royal Society of Chemistry (RSC) and the National Academy of Inventors (NAI). He received the M.Sc. in Chemistry from the Indian Institute of Technology, Madras in 1980 and a Ph.D. in Chemistry (with Chemical Engineering as Minor) from Vanderbilt University in 1983. He served as the Department Chair of the Cain Department of Chemical Engineering at LSU from 2005 to 2011, as Associate Vice Chancellor for Research and Economic Development at LSU between 2011 and 2013 and, as the Vice President for Research and Economic Development at LSU from 2013 till 2019.*

*His research area is in environmental chemical engineering. He has broad research experience in wastewater treatment, atmospheric chemistry and, modeling the fate and transport of contaminants in all three environmental media (air, water and soil/sediment). He has mentored 15 Ph.D, 23 MS students at LSU and several postdoctoral students in addition to hosting a number of visiting professors in his laboratory.*

*His present research is concerned with the transformations of pollutants on atmospheric aerosols (fog, rain, ice and snow)<sup>1</sup>, mercury sequestration in sediments, carbon sequestration<sup>2</sup> and, studies on chemical dispersant design for sub-sea oil/gas spill. His most recent research has been on the transformations and transport of microplastics in the environment<sup>3</sup>. He is currently in the process of advancing the revisions to the chemical engineering discipline as taught to undergraduate students<sup>4</sup>. Recent publications refer to this important aspect of the work.*

*He is the author of 1 textbook (with three editions), 225 peer-reviewed journal articles, 29 book chapters and 3 U.S. patents. He has made over 280 national and international presentations, invited seminars and plenary lectures on his research. His research has been supported by the NSF, EPA, DOE, DOD, USGS and several private industries.*

**P Herckes, K T Valsaraj, J L Collett, “A review of organic matter in fogs and clouds : Origin, processing and fate”, *Atmospheric Research* 132/133: 434-449 (2013).**

While fog and cloud composition has been studied for decades, most of the research was limited to inorganic species and fog acidity. Recently the focus has shifted towards organic matter in the atmospheric aqueous phase of fogs and clouds: its origin, reactivity and fate. An impressive number of fog and cloud chemistry observational studies have been performed over the last decade throughout the world. In the present work we will review the state of knowledge of atmospheric

organic matter processing by fogs, with a focus on field observations. We start by reviewing observational studies in general and then discuss our knowledge on the occurrence of organic matter in fogs, its solubility, characterization and molecular speciation. Organic carbon concentrations can vary widely from approximately 1 mg C/L in remote marine environments to more than 100 mg C/L in polluted radiation fogs, accounting for a substantial part of fogwater solutes. The carbonaceous material can enter the droplets from the gas and particle phase and the scavenging behavior of fogs will be detailed. Observational studies showed evidence of aqueous phase transformation of organic material, in particular secondary organic aerosol (SOA) generation, in fog. Recent observations of biological material in fog suggest also an impact of biological processing within the droplets on fog organic matter. The review will end with a discussion of the impact of fog on the deposition fluxes of organic material and hence its atmospheric lifetime.

**Carlos J Jimenez Haertel, Marcia McNutt, Mihrimah Ozkan, Edda Sif Pind Aradottir, Kalliat T Valsaraj, Paul R Sanberg, Shuchi Talati, Jennifer Wilcox, “The Promise of scalable direct air capture”, *Chem* (2021),**

Direct air capture (DAC) is one promising technology to remove CO<sub>2</sub> from the atmosphere. To meet the emissions goals of the Paris Agreement, there has been a noticeable rush to scale up DAC among key players in industry. This Voices asks thought leaders in academia and industry: what do you think about the potential, and feasibility, of scalable DAC? Is DAC a sustainable technology?

**A Al Harraq, PJ Brahana, O Arcemont, D Zhang, KT Valsaraj, B Bharti, “ Effects of weathering on microplastic dispersibility and pollutant uptake capacity”, *ACA Environmental Au*, 2022**

Microplastics are ubiquitous in the environment, leading to a new form of plastic pollution crisis, which has reached an alarming level worldwide. Micron and nanoscale plastics may get integrated into ecological cycles with detrimental effects on various ecosystems. Commodity plastics are widely considered to be chemically inert, and alterations in their surface properties due to environmental weathering are often overlooked. This lack of knowledge on the dynamic changes in the surface chemistry and properties of (micro)plastics has impeded their life-cycle analysis and prediction of their fate in the environment. Through simulated weathering experiments, we delineate the role of sunlight in modifying the physicochemical properties of microplastics. Within 10 days of accelerated weathering, microplastics become dramatically more dispersible in the water column and can more than double the surface uptake of common chemical pollutants, such as malachite green and lead ions. The study provides the basis for identifying the elusive link between the surface properties of microplastics and their fate in the environment.

**K Nandakumar, M Tyagi, Ye Xu, Kalliat Valsaraj, “Chemical engineering at crossroads”, *The Canadian Journal of Chemical Engineering* 100: 2011-2027 (2022).**

Through periodic introspection and assessment, the chemical engineering field has developed a mature undergraduate curriculum built on a strong science background in mathematics, physics, and chemistry. This brings a unique set of skills in transport, reaction engineering, and thermodynamics, coupled with suitable process systems engineering and process design courses, to supply well-trained engineers to a vast array of process manufacturing facilities. These facilities produce basic chemicals, pharmaceuticals, oil and gas, petrochemicals, food and agricultural products, minerals, and materials. While this maturity has served existing industries well, we argue that the chemical engineering field is at crossroads between managing the curriculum of undergraduate and graduate education to supply the needs of established industries while creating innovators for emerging industries. While this is a great opportunity for yet another introspection, we caution that the inadvertent cannibalization of the field must be avoided. We do argue in favour of adding a biology sequence and a computational science sequence to the core at the undergraduate level in a related perspective article.

## Infrared Physics & Technology in Biomedical Sciences

by Eddie Ng Yin-Kwee, Member EUAS



### Short Biography

*Dr. Eddie obtained Ph.D. at Cambridge Univ. with a Cambridge Commonwealth Scholarship.*

*He is elected as:*

*Fellow (inaugural) for National Academy of Technology (USA);*

*Academician for European Academy of Sciences and Arts (EU-Austria);*

*Fellow (Life) of the American Society of Mechanical Engineers (USA);*

*Fellow of Institute of Engineering and Technology (United Kingdom);*

*Fellow of International Engineering and Technology Institute (Hong Kong),*

*Distinguished Fellow for Institute of Data Science and Artificial Intelligence, (China), and,*

*Academician for Academy of Pedagogy and Learning, (USA).*

*Eddie received 2022 Alumni Highly Commended Award from the VC of Newcastle upon Tyne University, UK for his contributions to the society and achievements as academia.*

*He published more than 542 papers in SCI-IF int. journal (430); int. conf. proceedings (150), textbook chapters (>105) and others (32) over the 28 years. Co-edited 14 books on “Cardiac Pumping and Perfusion Engineering” by WSP (2007); “Imaging and Modelling of Human Eye” by Artech (2008); “Distributed Diagnosis and Home Healthcare, v.1” by ASP (2009); “Performance Evaluation in Breast Imaging, Tumor Detection & Analysis” by ASP (2010); “Distributed Diagnosis and Home Healthcare, v.3” by ASP (2011); “Computational Analysis of Human eye with Applications” by WSP (2011); “Human Eye Imaging and Modeling” by CRC (2011); “Multimodality Breast Imaging” by SPIE (2013); “Image Analysis and Modeling in Ophthalmology”; “Ophthalmology Imaging and Applications” by CRC (2013, 2014); “Bio-inspired Surfaces and Applications” by WSP (2016); “Application of Infrared to Biomedical Sciences” by Springer (2017) and “Computation and Mathematical Methods in Cardiovascular Physiology” by WSP (2019). Also, co-authored a textbook: “Compressor Instability with Integral Methods” by Springer (2007).*

*Since 1992, he works as Faculty in the School of Mechanical & Aerospace Engineering in Nanyang Technological University, Singapore.*

*He is included in the Stanford list of the World’s top 2% Scientists since 2019 (ranked 83 out of 64,425 as 0.001% in the field of Biomedical Engineering). The ranking method is calculated by removing the self-citation of the literature.*

*His Score in researchgate.net is one of the highest in our school (> 44.82 or higher than 97.5% of all ResearchGate members’ scores).*

*He is also ranked # 5 (Worldwide) in Google Scholar (h-index: 68) under Biomedical category [see <http://scholar.google.com.sg/citations?user=9QW1LYAAAAAJ>].*

### RESEARCH INTERESTS

- Numerical modeling in biomedical engineering (including AI in healthcare and thermal-fluids engineering such as Computational Fluid Dynamics (CFD) & Heat Transfer-CHT).
- Infrared physics & technology with its application to clinical diagnosis of health abnormalities.

**Clinical diagnosis of health abnormalities with affordable, non-invasive, and contactless active dynamic thermography technique.**

Eddie is pioneering in the early detection of human health abnormality via non-contact and non-invasive methods which leverages on AI and machine learning approaches. He derived an innovative thermograms analysis (novel tissue activities ratio, [1]) in infrared physics & technology (IRPT) and developed unique software algorithms to identify health conditions such as hot or cold spots to confirm health abnormalities inside the body. He formulated numerical algorithms (coupled CFD/CHT) [2] and designed experiments to gain physical insight into the underlying complex thermal-fluids mechanisms. He tested and refined theoretical predictions made from the detailed analysis of model systems to improve healthcare and diagnosis such as the burn injury model and bioheat physics that are adopted widely in the biomedical engineering (BME) and industry design domains [2,3,4,5,6]. His well-cited work on non-contact screening for cancer tumours, artery-stenosis, aneurysms, kidney blockage, and superficial vein finder with IRPT, have resulted in distinguished achievements and patents. These include 4 technical disclosures filing and copyrights, 3 U.S. patents on software classifiers that identifies the stages of breast cancer, and another patent on “IoT enabled EPCG-device-unit for nursing heart-health-distantly” with AusPat. Office.

With his notable citations in the field of BME-IRPT, he is well consulted for his deep technical expertise in medical scientific research by reputable global healthcare institutions (Dubai-London Clinic & Hospital), universities (Nazarbayev University of Kazakhstan; Medical University of Gdansk, Gdańsk University of Technology, Poland) and start-ups in USA, Singapore, India such as Cyrcadia Health, Sirius d’ Innovation, Niramai Health Analytix respectively. Working closely with international peers, he determined that the Infrared Diagnostic System can be used as a better objective assessment tool for complementary health screening such as computer-aided breast cancer detection methods.

He received the SPRING-Singapore Merit-Award together with a testimonial for innovation work in infrared thermal imagers to screen fever and for his significant contributions to the Singapore Standardization Program and the National Biomedical and Health Standards Executive Committee. His article "Is thermal Scanner losing its bite in mass screening of fever due to SARS?" was published in Medical Physics [7] and it is still highly relevant today in screening pandemic infectious virus that exhibits fever-like symptoms. He was approached by researchers, journalists, and scientists from countries such as France, UK, India,

USA, Denmark, Indonesia, Malta, Brazil to share his expertise on the viability of thermal scanners for mass virus screening.

Twenty-one of his research papers have been referenced in the Singapore Standard (SS-582, Parts 1&2: 2020), ISO/IEC 80601-2-59: 2017 and by numerous health authorities worldwide for thermal scanner deployment and users' guidelines. These accolades and contributions to the global biomedical industry substantiate his international standing as a scholar and prove that his professional expertise and standards are aligned to leading scholars within the field. He was highly involved in the development of the Thermal-Scanner used for fever screening, especially during the SARS critical outbreak in 2003 as well as Covid-19. He co-led the first invention of thermal scanning for fever.

His book on "Application of Infrared to Biomedical Sciences, Springer Nature, 2017, 552 pages" with the monograph of 35k downloads, more than 100 citations, 80 mentions [8]. This book comprehensively analyses the latest update of IRPT case studies in 28 chapters. Also, his fever-screening related work has been published as 6 book chapters in other edited books such as "Medical Infrared Imaging: Principles and Practices", "The Biomedical Engineering Handbook", "Skin Anatomy & Physiology Research Developments", and "Recent Advances in Medical Image Segmentation and Registration Technologies". Additionally, he was invited for keynote speeches and lectures in various international conferences and workshops on fever scanners related topics. These include the 13th Quantitative InfraRed Thermography Conference, National Metrology Centre's Workshop [6], IEEE Conferences, Cambridge Conference on Medical Physiology and US-SPIE Conference Series in ThermoSense.

Under the SingHealth-NTU collaborative research grant in 2018, he worked on clinical study-based proofs-of-concept to screen patients for carotid artery diseases with IRPT technique. He also developed both passive static and active dynamic thermographic methods to detect abdominal aortic aneurysm from only midriff-skin surface isotherms and unique cardiac thermal-pulse [1-6]. This aneurysm detection technique was the first of its kind to open such proof-of-concept via systematic coupled CFD/CHT numerical methods, quantitative experimental prototype measurements and was archived in numerous top thermal science journals. Adopting a multi-directional and multidisciplinary approach to solve a research problem, he ensured that his research encompassed the following activities: computational studies, laboratory investigations, stringent CIRB ethics approval application, thermography-based data collection, primitive image processing methods and in-house built algorithms. Furthermore, he initiated local and overseas collaborations for sharing of knowledge and data for the testing of algorithms and setting up new experiments for scientific innovation and breakthroughs. In all, his dedicated interest and curiosity to explore advanced thermal imaging modalities and processing techniques have greatly contributed to research in IRPT and biomedical

sciences as demonstrated by his numerous technical disclosures, copyrights, and patents.

To conclude, as a non-intrusive, contactless, safe, and easy detection approach, IRPT imaging has shown numerous advantages to the medical field with early diagnosis potential as an adjunctive method to pre-emptively detect health problems [9,10].

### **Ongoing update of Ng's roles in IRPT**

Based on his expertise and track records in advancing the field of infrared imaging (such as unique cardiac thermal-pulse and tissue activities ratio formulation [1-6]), he is invited by the Editorial Office of IMR Press, an academic local open access company publishing biomedical and life sciences journals to be an Executive Editor. He is also invited by Dr. P.A. McCullough, EiC cum Cardiorenal Society of America to be the guest editor for a special issue of Reviews in Cardiovascular Medicine on "The Role of Thermography in Cardiovascular Diseases". The IRPT technique has many applications in biomedical sciences such as cardiovascular diseases. To create a healthier society through diagnosis in healthcare, we need to critically examine safe and non-invasive modalities with early detection potential as an adjunctive method to detect health problems. Currently, he is a guest editor for Sensors in Infrared for Biomedical Applications.

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# Hydrogen Gas production by Water Electrolysis

by Zhifeng Ren, Member EUAS



## Short Biography

*Zhifeng Ren is an M. D. Anderson Chair Professor at the Department of Physics and the Director of the Texas Center for Superconductivity at the University of Houston (TcSUH). He received his BS in 1984 from Sichuan Institute of Technology, MS in 1987 from Huazhong University of Science and Technology, and PhD in 1990 from the Institute of Physics, Chinese Academy of Sciences. His research focuses on thermoelectrics with high ZT, boron arsenide single crystals for high thermal conductivity and carrier mobility, nanomaterials for enhanced oil recovery, good catalysts for water splitting for H<sub>2</sub> generation, superconductor levitated vehicles for power, people, and goods transport, heated filters for catching and killing SARS-CoV-2 causing COVID-19 pandemic, carbon nanotubes, solar absorbers, flexible transparent conductors.*

## **Active Research Activities in Zhifeng Ren's group at the University of Houston, Texas, USA**

Professor Zhifeng Ren's group is currently carrying out a broad range of research projects involving fundamental and applied physics toward applications in the fields of materials, energy, electronics, *etc.* Among them, the most notable ones are:

1. Hydrogen gas production by water electrolysis.

Hydrogen is the best way to store the extra electrical power from solar, wind, and the electrical power grid when the supply is more than needed. The research deals with advanced catalysts for HER and OER for water electrolysis. We also study economical treatment to produce and sea water as the feedstock for the electrolysis. Up to now, multiple patent applications on new efficient catalysts and water treatment methods for water electrolysis have been filed and/or issued. These patents are owned by UH and being licensed to a company for large-scale hydrogen production.

2. A super superconducting levitated system for energy transport & storage and people & goods transport at speed up to 600 miles per hour. We study a superconducting levitated super system for electrical power transmission and storage over long distance without loss, liquid hydrogen storage and transport over long distance to avoid using trucks for long distance, and people and goods transport at speed up to 600 miles per hour through superconducting levitated vehicles. This system does not need to acquire new land, but use the existing highway system. A patent application has been filed for commercialization opportunities.
3. Nanofluid for enhanced oil recovery and cleaning.  
Nanoparticle fluid can drastically and permanently reduce heavy oil viscosity to make the heavy and extra heavy oils very flowable. The nanoparticle fluid generates multiple effects that are all beneficial to oil recovery and cleaning of oily surfaces. Oil field testing is being carried out at multiple oil fields. Multiple patents have been filed.
4. Heated high efficiency air filters.  
High efficiency particle air (HEPA) filters with heating capability was invented and are being manufactured for achieving cleaner air in schools, hospitals, hotels, convention centers, *etc.* These filters are ideal for cleaning the air for any closed space.
5. Thermoelectric materials and devices for conversion of heat into electrical power and also cooling.  
High performance thermoelectric materials have been discovered over the last twenty years in Ren's labs, and devices have been found efficient for both power generation and cooling. Multiple patents have been issued to UH and many more are being examined.
6. Future's semiconductors that are better than silicon.  
Over the last a few years, my group has made a huge progress on discovering a new semiconductor that is potentially better than the currently widely used silicon in our phones, computers, and many other electronics. We envisioned this new semiconductor will play a crucial role in the future electronics.

# Recent Research on Fluid Dynamics & Turbulence

by James Glimm, Member EUAS

## Short Biography

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Email: james.glimm@stonybrook.edu*

## **Professional Preparation**

*Columbia University, Engineering, BA, 1956  
Columbia University, Mathematics, Ph.D. 1956-1959*

## **Appointments**

*1999- Staff Member, Computational Science Center, Brookhaven National Laboratory  
1989- Distinguished Professor, SUNY at Stony Brook  
1982-89 Professor, Courant Institute, New York University  
1974-82 Professor, The Rockefeller University  
1968-74 Professor, Courant Institute, New York University  
1960-68 Professor, Associate Professor, Assistant Professor, MIT  
1959-60 Temporary Member, Institute for Advanced Study*

## **Professional Service**

*Advisory Committee of the Center for Computational Geoscience, Xi'an University, Xi'an PRC  
2007-2009 President American Mathematical Society*

## **Prizes, Awards, Fellowships**

*2002 National Medal of Science  
Member, National Academy of Sciences  
Member, American Society of Arts and Sciences  
1993 Steele Prize for a paper of fundamental importance (AMS)  
1980 Dannie Heineman Prize for Mathematical Physics (APS)  
1965-1966 Guggenheim Fellowship  
1963-1964 Guggenheim Fellowship  
1959-1960 National Science Foundation Fellowship*

## **Fields of Expertise**

*Nonlinear partial differential equations, Computational fluid dynamics, Stochastic partial differential equations, Mathematical physics, Quantum physics, Scientific computing, Quantification of uncertainty, Turbulence modeling, Computational electromagnetics, Turbulence modeling, Financial mathematics*

**James Glimm, Daniel Lazarev and Gui-Qiang Chen. Maximum entropy production rate as a necessary admissibility condition for the fluid Euler and Navier-Stokes equations. Nature Physics 2 (2021)**

## **Abstract.**

In a particle physics dynamics, we assume a uniform distribution as the physical measure and a measure-theoretic definition of entropy on the velocity configuration space. The dynamics is governed by an assumption of a Lagrangian formulation, with the velocity

time derivatives as the momenta conjugate to the velocity configurations. From these definitions and assumptions, we show mathematically that a maximum entropy production principle selects the physical measure as a solution of the fluid Navier-Stokes and Euler equations from among alternate measures on the configuration space.

The physical solution is shown to be a solution of the Navier-Stokes or Euler equations in the Lagrangian frame, but its transformation to an Eulerian frame is not established, and depends on the regularity of the solution, a property which is known to be difficult to establish.

### **James Glimm On the Nature of Turbulence, Proceedings of HYP2022, to appear.**

#### **Abstract**

Three main results are presented.

- (1) Physical solutions of the Navier-Stokes equation are characterized by an admissibility condition for the local space time maximization of entropy production relative to comparison solutions. These solutions are stochastic in the sense that they are realized by Young measures rather than by weak solutions of the Leray-Hopf class.
- (2) Renormalized perturbation theory, adapted to fluids from standard methods of quantum field theory, is shown to converge for the physical vacuum state and all higher multiparticle states. Using this convergence for the vacuum state alone, the Reynolds stress tensor is shown to converge to a constant in the limit as all cutoffs are removed.
- (3) The entropy minimizing solution mean is a classical weak (PDE) solution of the Leray-Hopf class and it is a smooth solution of the Navier-Stokes equation.

### **James Glimm, Jarret Petrillo and Min Lee, Smooth vs. Physical Solutions of the Navier-Stokes Equation. arXiv 2212.14734v3 [physics.flu-dyn]**

#### **Abstract**

Smooth solutions for the Navier-Stokes equations of the class considered by Leray and Hopf exist. They describe the mean state of a turbulent flow but do not describe a turbulent state itself. They fail the admissibility criterion of a maximum rate of entropy production. They have zero entropy, zero turbulent fluctuations and are laminar.

For the same general initial conditions, the physically admissible solution of the turbulent flow exists as a Young measure, with a stochastic formulation.

The proofs are supported by renormalized perturbation series, which is constructed as a modification of the renormalized perturbation series of quantum field theory. This expansion is shown to converge for the vacuum state and other physical states. It gives a statistical description of the lowest energy fully turbulent state, usually referred to as fully developed turbulence. This state is statistically stationary and translation invariant.

Topologically, the moments are interpreted in terms of energy and vorticity surfaces in  $R^3$  in the form of spheres and possibly knotted tori of arbitrary genus.

Considerations of phase transitions within turbulent flow lead to a conjectured unified picture of phase transitions within fluids, Yang-Mills fields with quarks and quantum general relativity.

**Min Lee and James Glimm, Axioms for Quantum Gauge Fields  
arXiv 2112.08575v1 [math-phys]**

**Abstract**

The purpose of this paper is to extend the classical axiom scheme for quantum field theory to include most of the known examples of quantum gauge theories. The axioms are developed in both the Euclidean and Minkowski metrics for space time. We demonstrate that the Euclidean axioms imply the Minkowski (Wightman) axioms.

We also prove the reconstruction theorem for Yang-Mills quantum fields as operator-valued tempered distributions with gauge transformation properties.

**Quantum Field Theory**

An extensive development of this subject was conducted in collaboration with Arthur Jaffe, Thomas Spencer and an extended group of collaborators. The main thrust of this work was to establish in full mathematical rigor the formal manipulations of quantum physicists, in the cancellation of divergences based on renormalized perturbation theory. These results depended on a restriction of the number of space time dimensions  $D$  to  $D = 2$  or  $D = 3$ , but did not allow  $D = 4$ .

I have been largely absent from this field for some 30 years . I am currently developing methods to address the case of  $D = 4$ . Also missing from the earlier work is the consideration of gauge fields, to be included in planned new activities.

**Numerical Methods**

I have developed numerical methods for the study of turbulent mixing of distinct fluids. A specialized code, called front tracking, has two distinguishing features, It prevents artificial (numerical) mixing of distinct fluids, beyond what is allowed by viscous diffusion at a level specified by physics. The method also includes subgrid models, dynamically adapted to the turbulent nature of the flow. Using this method, we achieved excellent agreement with experimental results for turbulent mixing.

The numerical method is described in the Handbook article

**Dan She, Ryan Kaufman, Hyunkyung Lim, Jeremy Melvin, Abigail Hsu and James Glimm, “Front-Tracking Methods” In::Handbook of numerical methods for hyperbolic problems 17 (2016) Elsevier.**

**Abstract**

Front Tracking is the use of surfaces or lower dimensional manifolds as computational degrees of freedom in a numerical algorithm. Its purpose is to improve the resolution of discontinuities or steep gradients in the solution variables or in the laws of physics which

describe them. Thermal or concentration discontinuities, and thermodynamic phase discontinuities, often poorly handled by Eulerian advection schemes, may benefit from the use of front tracking. Other examples include discontinuities or strong gradients in opacity, conductivity, permeability, and material strength.

We present the Front Tracking algorithm in a formulation which includes two important recent developments, namely (cell-by-cell) conservation and an application programming interface (API) for ease of insertion of tracking into client codes. Ongoing work to improve the late time robustness of the solution, still in progress, is outlined here.

We also present an overview of solved problems, based on the front tracking algorithm. We discuss in general terms the problem classes for which the algorithm is beneficial as well as those for which it seems to offer little benefit. This important distinction is the topic of ongoing research.

One sample (of many) of the numerical method used to model turbulent mixing experiments which excellent agreement to the experimental data is given below:

**James Glimm David H. Sharp, Tulin Kaman, and Hyun Kyung Lim, New Directions for Rayleigh-Taylor Mixing, Philosophical Transactions of the Royal Society A: 371, pp 183 (2013).**

#### **Abstract**

We study the Rayleigh–Taylor (RT) mixing layer, presenting simulations in agreement with experimental data. This problem is an idealized subproblem of important scientific and engineering problems, such as gravitationally induced mixing in oceanography and performance assessment for inertial confinement fusion. Engineering codes commonly achieve correct simulations through the calibration of adjustable parameters. In this sense, they are interpolative and not predictive. As computational science moves from the interpolative to the predictive and reduces the reliance on experiment, the quality of decision making improves. The diagnosis of errors in a multi-parameter, multi-physics setting is daunting, so we address this issue in the proposed idealized setting. The validation tests presented are thus a test for engineering codes, when used for complex problems containing RT features. The RT growth rate, characterized by a dimensionless but non-universal parameter  $\alpha$ , describes the outer edge of the mixing zone. Increasingly accurate front tracking/large eddy simulations reveal the non-universality of the growth rate and agreement with experimental data. Increased mesh resolution allows reduction in the role of key subgrid models. We study the effect of longwavelength perturbations on the mixing growth rate. A self-similar power law for the initial perturbation amplitudes is here inferred from experimental data. We show a maximum  $\pm 5\%$  effect on the growth rate. Large (factors of 2) effects, as predicted in some models and many simulations, are inconsistent with the experimental data of Youngs and co-authors. The inconsistency of the model lies in the treatment of the dynamics of bubbles, which are the shortest

# Aluminum-Copper Alloy Anode Materials for High-Energy Aqueous Aluminum Batteries

by Qing Jiang, Member EUAS



## Short Biography

*Qing Jiang is a Professor of the School of Materials Science and Engineering, Jilin University since 1992. He received his BSc and MSc in Materials Science from Jilin University of Technology (merged into Jilin University in 2000) in 1982 and 1984, respectively, and PhD in Chemistry from University of Stuttgart, Germany in 1990.*

*Dr. Jiang was elected as a Member of the EU Academy of Sciences in 2018, and an Academician of the Asia Pacific Academy of Materials in 2015. He is also a Fellow of The Institute of Physics (U.K.), and members of the editor board of several academic journals.*

*His current research interests include synthesis of nanomaterials as well as their applications in catalysis, energy storage and conversion (fuel cell, batteries, supercapacitors, and electrocatalysis), with focus on kinetics aspects of mass transfer and chemical reaction. He has published more than 750 papers in peer-reviewed journals, including Nat. Nanotechnol., Nat. Chem., Nat. Commun., Sci. Adv., Joule, Chem, Matter, etc. His publications have been cited more than 31,000 times with H-index = 88 (Web of Science).*

In 2022, he authored and coauthored 34 papers and several representative ones with their abstracts are listed below:

- 1. Qing Ran, Hang Shi, Huan Meng, Shu-Pei Zeng, Wu-Bin Wan, Wei Zhang, Zi Wen, Xing-You Lang,\* Qing Jiang,\* Aluminum-copper alloy anode materials for high-energy aqueous aluminum batteries, Nat. Commun., 2022, 13, 576.**

## **Abstract**

Aqueous aluminum batteries are promising post-lithium battery technologies for large-scale energy storage applications because of the raw materials abundance, low costs, safety

and high theoretical capacity. However, their development is hindered by the unsatisfactory electrochemical behaviour of the Al metal electrode due to the presence of an oxide layer and hydrogen side reaction. To circumvent these issues, we report aluminum-copper alloy lamellar heterostructures as anode active materials. These alloys improve the Al-ion electrochemical reversibility (e.g., achieving dendrite-free Al deposition during stripping/plating cycles) by using periodic galvanic couplings of alternating anodic  $\alpha$ -aluminum and cathodic intermetallic  $\text{Al}_2\text{Cu}$  nanometric lamellas. In symmetric cell configuration with a low oxygen concentration (i.e.,  $0.13 \text{ mg L}^{-1}$ ) aqueous electrolyte solution, the lamella-nanostructured eutectic  $\text{Al}_{82}\text{Cu}_{18}$  alloy electrode allows Al stripping/plating for 2000 h with an overpotential lower than  $\pm 53 \text{ mV}$ . When the  $\text{Al}_{82}\text{Cu}_{18}$  anode is tested in combination with an  $\text{Al}_x\text{MnO}_2$  cathode material, the aqueous full cell delivers specific energy of  $\sim 670 \text{ Wh kg}^{-1}$  at  $100 \text{ mA g}^{-1}$  and an initial discharge capacity of  $\sim 400 \text{ mAh g}^{-1}$  at  $500 \text{ mA g}^{-1}$  with a capacity retention of 83% after 400 cycles.

**2. Bo Li, Wang Gao,\* Qing Jiang, A universal picture for ejecting atoms on metallics, *Acta Mater.*, 2022, 228, 117792.**

#### **Abstract**

The surface-site stability of transition metals and alloys, which can be measured by the ejection energy, is essential in corrosion and electrocatalysis. However, the complex geometric and alloying effects of alloys prohibit the accurate estimation of ejection energies. Herein we introduce the geometric and electronic gradients and cohesive properties of surface sites to determine the ejection energy for transition metals, single-atom alloys, binary alloys, near-surface alloys, and high-entropy alloys. This predictive model reveals not only the electronic and geometric determinants of interatomic bonding in alloys but also the range-reaching characters of alloying and geometric variation, which outlines explicitly the commonality and difference between different alloys in bonding. Our model uncovers a novel physical picture for the interatomic bonding of alloys, provides a simple way to estimate the alloying effect, and is helpful for modulating the stability of alloy surfaces.

**3. Haibin Ma, Zhiwen Chen, Zhili Wang,\* Chandra Veer Singh,\* and Qing Jiang,\* Interface engineering of Co/CoMoN/NF heterostructures for high-**

**performance electrochemical overall water splitting, *Adv. Sci.*, 2022, 9, 2105313.**

#### **Abstract**

The development of low-cost and high-efficiency catalysts for both hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) in alkaline electrolyte is still challenging. Herein, interfacial Co/CoMoN heterostructures supported on Ni foam (Co/CoMoN/NF) are constructed by thermal ammonolysis of CoMoO<sub>x</sub>. In 1.0 M KOH solution, Co/CoMoN/NF heterostructures exhibit excellent HER activity with an overpotential of 173 mV at 100 mA cm<sup>-2</sup> and a Tafel slope of 68.9 mV dec<sup>-1</sup>. Density functional theory calculations indicate that the low valence state Co site acts as efficient water-dissociation promoter, while CoMoN substrate has favorable hydrogen adsorption energy, leading to an enhanced HER activity. The Co/CoMoN/NF heterostructures also achieve high OER activity with an overpotential of 303 mV at 100 mA cm<sup>-2</sup> and a Tafel slope of 56 mV dec<sup>-1</sup>. Using Co/CoMoN/NF heterostructures as the cathode and anode, the alkaline electrolyzer requires a low voltage of 1.56 V to reach the current density of 100 mA cm<sup>-2</sup> along with superior long-term durability. This study provides a new design strategy toward low-cost and excellent catalysts for water splitting.

**4. Zhe Meng, Jia-Xin Yao, Chang-Ning Sun, Xia Kang, Rui Gao, Hong-Rui Li, Bo Bi, Yong-Fu Zhu, Jun-Min Yan,\* Qing Jiang, Efficient ammonia production beginning from enhanced air activation, *Adv. Energy Mater.*, 2022, 12, 2202105.**

#### **Abstract**

Ammonia is considered to be a next-generation clean energy carrier, and thus the green synthesis of NH<sub>3</sub> is of great importance. In this work, non-thermal plasma oxidation is combined with electroreduction to achieve an efficient two-step NH<sub>3</sub> synthesis. A Ti bubbler is introduced in the first step of plasma activation of air to effectively produce nitrate/nitrite (NO<sub>x</sub><sup>-</sup>) in an absorption solution, and the production rate achieves the highest value of 55.29 mmol h<sup>-1</sup>; the obtained NO<sub>x</sub><sup>-</sup> aqueous solution is directly employed as catholyte for the second step of electroreduction with oxygen vacancy-rich

Co<sub>3</sub>O<sub>4</sub> nanoparticles as the catalyst. Density functional theory calculations reveal that the introduction of oxygen vacancies endows their adjacent Co atoms with improved activity, which promotes adsorption and hydrogenation of NO<sub>x</sub><sup>-</sup>, meanwhile suppressing the hydrogen evolution reaction. Thus the oxygen vacancy-rich Co<sub>3</sub>O<sub>4</sub> NPs present a significant NH<sub>3</sub> production rate of 39.60 mg h<sup>-1</sup> cm<sup>-2</sup>, high Faradaic efficiency of 96.08% and a large current density (376.48 mA cm<sup>-2</sup>), outperforming the previously reported ones including N<sub>2</sub> or NO<sub>x</sub><sup>-</sup> electroreduction.

**5. Huan Meng, Qing Ran, Tian-Yi Dai, Hang Shi, Shu-Pei Zeng, Yong-Fu Zhu, Zi Wen, Xing-You Lang,\* Wei-Tao Zheng, Qing Jiang,\* Surface-alloyed nanoporous zinc as reversible and stable anodes for high-performance aqueous zinc-ion battery, Nano-Micro Lett., 2022, 14, 128.**

#### **Abstract**

Metallic zinc (Zn) is one of the most attractive multivalent-metal anode materials in post-lithium batteries because of its high abundance, low cost and high theoretical capacity. However, it usually suffers from large voltage polarization, low Coulombic efficiency and high propensity for dendritic failure during Zn stripping/plating, hindering the practical application in aqueous rechargeable zinc-metal batteries (AR-ZMBs). Here we demonstrate that anionic surfactant-assisted in situ surface alloying of Cu and Zn remarkably improves Zn reversibility of 3D nanoporous Zn electrodes for potential use as high-performance AR-ZMB anode materials. As a result of the zincophilic Zn<sub>x</sub>Cu<sub>y</sub> alloy shell guiding uniform Zn deposition with a zero nucleation overpotential and facilitating Zn stripping via the Zn<sub>x</sub>Cu<sub>y</sub>/Zn galvanic couples, the self-supported nanoporous Zn<sub>x</sub>Cu<sub>y</sub>/Zn electrodes exhibit superior dendrite-free Zn stripping/plating behaviors in ambient aqueous electrolyte, with ultralow polarizations under current densities up to 50 mA cm<sup>-2</sup>, exceptional stability for 1900 h and high Zn utilization. This enables AR-ZMB full cells constructed with nanoporous Zn<sub>x</sub>Cu<sub>y</sub>/Zn anode and K<sub>z</sub>MnO<sub>2</sub> cathode to achieve specific energy of as high as ~ 430 Wh kg<sup>-1</sup> with ~ 99.8% Coulombic efficiency, and retain ~ 86% after long-term cycles for > 700 h.

# Force-Directed Graph Layouts Revisited: A New Force Based On The T-Distribution

by Oliver Deussen, Member EUAS



## Short Biography

### **Education and Professional Experience**

Mar 2003 – now	<b>Full Professor</b> Visual Computing, Konstanz University, Germany
Jun 2010 – Dec 2020	<b>Visiting Professor</b> Shenzhen Institute of Applied Technologies, Chinese Academy of Science, China
Jul – Sep 2006	<b>Visiting Researcher</b> Computer Graphics Group, Microsoft Research, Redmond
Mar 2004 – Sep 2005	<b>Head of Department</b> Computer and Information Science, Konstanz University, Germany
Sep 2000 – Feb 2003	<b>Associate Professor (C3)</b> Dresden University of Technology, Germany
Apr 1996 – Aug 2000	<b>Postdoctoral Researcher</b> Otto-von-Guericke University of Magdeburg, Germany
Mar 1996	<b>Graduation</b> Dr. rer nat, Karlsruhe Institute of Technology (KIT), Germany

### **Professional Activities**

Jan 2019 – now	<b>Speaker</b> Excellence Cluster “Centre for the Advanced Study of Collective Behaviour”, University of Konstanz (with Iain Couzin and Urs Fischbacher)
Jan 2019 – Dec 2020	<b>President</b> Eurographics Association
Jan 2012 – Dec 2015	<b>Editor in Chief</b> Computer Graphics Forum, Journal for Computer Graphics
Jul 2015 – now	<b>Vice Speaker</b> DFG Collaborative Research Center 161 Quantitative Methods for Visual Computing with Daniel Weiskopf, University of Stuttgart
March 2020 – now	<b>DFG Review Board</b> DFG Review Board 409-05 “Interactive and Intelligent Systems, Image and Language Processing, Computer Graphics and Visualization”
Ongoing	<b>Associated Editor, IPC-Member, Papers Chair etc.</b> ACM SIGGRAPH; IEEE Visualization; Eurographics; Pacific Graphics; Workshop on Computational Aesthetics in Graphics, Visualization and Imaging; Symposium on Non-Photorealistic

*Animation and Rendering; Vision Modelling Visualization; Informatik Spektrum; Sibgrapi; Sino-German Symposium on Visualization, Selection committees for Studienstiftung des Deutschen Volkes*

#### **Honors, Awards, Patents, Scientific Achievements**

2022	<i>Member of the Heidelberg Academy of Science</i>
2021	<i>Fellow of the German Association for Informatics</i>
2020	<i>Member EU Academy of Sciences</i>
2016	<i>awarded within the Guangdong leading Talents Plan (China)</i>
2014	<i>awarded within the 1000 Talents Plan (China)</i>
2014	<i>Nomination Technical Achievement Award for Xfrog Modelling Software</i>
2013	<i>Eurographics Fellow</i>
2007	<i>awarded Virtual earth academic collaboration of Microsoft Research, 35k USD</i>

#### **Important Publications**

**F. Zhong, M. Xue, J. Zhang, F. Zhang, R. Ban, O. Deussen, Y. Wang: Force-Directed Graph Layouts Revisited: A New Force Based On The T-Distribution, IEEE Transactions on Visualization and Computer Graphics, Volume: 29, January 2023**

In this paper, we propose the t-FDP model, a force-directed placement method based on a novel bounded short-range force (t-force) defined by Student's t-distribution. Our formulation is flexible, exerts limited repulsive forces for nearby nodes and can be adapted separately in its short- and long-range effects. Using such forces in force-directed graph layouts yields better neighborhood preservation than current methods, while maintaining low stress errors. Our efficient implementation using a Fast Fourier Transform is one order of magnitude faster than state-of-the-art methods and two orders faster on the GPU, enabling us to perform parameter tuning by globally and locally adjusting the t-force in real-time for complex graphs. We demonstrate the quality of our approach by numerical evaluation against state-of-the-art approaches and extensions for interactive exploration.

**M. Xue, Z. Wang, F. Zhong, Y. Wang, O. Deussen, Y. Wang: Taurus: Towards A Unified Force Representation And Universal Solver For Graph Layout, IEEE Transactions on Visualization and Computer Graphics, Volume: 29, January 2023**

Over the past few decades, a large number of graph layout techniques have been proposed for visualizing graphs from various domains. In this paper, we present a general framework, Taurus, for unifying popular techniques such as the spring-electrical model, stress model, and maxent-stress model. It is based on a unified force representation, which formulates most existing techniques as a combination of quotient-based forces that combine power functions of graph-theoretical and Euclidean distances. This representation enables us to compare the strengths and

weaknesses of existing techniques, while facilitating the development of new methods. Based on this, we propose a new balanced stress model (BSM) that is able to layout graphs in superior quality. In addition, we introduce a universal augmented stochastic gradient descent (SGD) optimizer that efficiently finds proper solutions for all layout techniques. To demonstrate the power of our framework, we conduct a comprehensive evaluation of existing techniques on a large number of synthetic and real graphs. We release an open-source package, which facilitates easy comparison of different graph layout methods for any graph input as well as effectively creating customized graph layout techniques.

**Mariana Rodriguez-Santiago, Paul Nührenberg, James Derry, Oliver Deussen, Fritz A Francisco, Linda K Garrison, Sylvia F Garza, Hans A Hofmann, and Alex Jordan. Behavioral traits that define social dominance are the same that reduce social influence in a consensus task. Proceedings of the National Academy of Sciences (PNAS), 117(31):18566–18573, 2020**

Dominant individuals are often most influential in their social groups, affecting movement, opinion, and performance across species and contexts. Yet, behavioral traits like aggression, intimidation, and coercion, which are associated with and in many cases define dominance, can be socially aversive. The traits that make dominant individuals influential in one context may therefore reduce their influence in other contexts. Here, we examine this association between dominance and influence using the cichlid fish *Astatotilapia burtoni*, comparing the influence of dominant and subordinate males during normal social interactions and in a more complex group consensus association task. We find that phenotypically dominant males are aggressive, socially central, and that these males have a strong influence over normal group movement, whereas subordinate males are passive, socially peripheral, and have little influence over normal movement. However, subordinate males have the greatest influence in generating group consensus during the association task. Dominant males are spatially distant and have lower signal-to-noise ratios of informative behavior in the association task, potentially interfering with their ability to generate group consensus. In contrast, subordinate males are physically close to other group members, have a high signal-to-noise ratio of informative behavior, and equivalent visual connectedness to their group as dominant males. The behavioral traits that define effective social influence are thus highly context specific and can be dissociated with social dominance. Thus, processes of hierarchical ascension in which the most aggressive, competitive, or coercive individuals rise to positions of dominance may be counterproductive in contexts where group performance is prioritized.

**Jörg Marvin Gülzow, Patrick Paetzold, and Oliver Deussen. Recent developments regarding painting robots for research in automatic painting, artificial creativity, and machine learning. Applied Sciences, 10(10):3396, 2020**

E-David (Electronic Drawing Apparatus for Vivid Image Display) is a system for controlling a variety of painting machines in order to create robotic paintings. This article summarizes the hardware set-up used for painting, along with recent developments, lessons learned from past painting machines, as well as plans for new approaches. We want to apply e-David as a platform for research towards improving automatic painting and to explore machine creativity. We present different painting machines, from small low-cost plotters to large industrial robots, and discuss the benefits and limitations of each type of platform and present their applicability to different tasks within the domain of robotic painting and artificial creativity research. A unified control interface with a scripting language allows users a simplified usage of different e-David-like machines. Furthermore, we present our system for automated stroke experimentation and recording, which is an advance towards allowing the machine to autonomously learn about brush dynamics. Finally, we also show how e-David can be used by artists “in the field” for different exhibitions.

**Deussen O., M. Spicker, Q. Zheng: Weighted Linde-Buzo-Gray Stippling, ACM Transactions on Graphics 36.6 (2017), P. 233:1-12**

We propose an adaptive version of Lloyd’s optimization method that distributes points based on Voronoi diagrams. Our inspiration is the Linde–Buzo–Gray–Algorithm in vector quantization, which dynamically splits Voronoi cells until a desired number of representative vectors is reached. We reformulate this algorithm by splitting and merging Voronoi cells based on their size, greyscale level, or variance of an underlying input image. The proposed method automatically adapts to various constraints and, in contrast to previous work, requires no good initial point distribution or prior knowledge about the final number of points. Compared to weighted Voronoi stippling the convergence rate is much higher and the spectral and spatial properties are superior. Further, because points are created based on local operations, coherent stipple animations can be produced. Our method is also able to produce good quality point sets in other fields, such as remeshing of geometry, based on local geometric features such as curvature.

**Ahmed, G., Perrier, H., Coeurjolly, D., Ostromoukhov, V., Guo, J., Yan, D., Huang, H., and Deussen, O.: Low-Discrepancy Blue Noise Sampling, ACM Transactions on Graphics (TOG) 35 (6), 247, 2016**

We present a novel technique that produces two-dimensional low-discrepancy (LD) blue noise point sets for sampling. Using one-dimensional binary van der Corput sequences, we construct two-dimensional LD point sets, and rearrange them to match a target spectral profile while preserving their low discrepancy. We store the rearrangement information in a compact lookup table that can be used to produce arbitrarily large point sets. We evaluate our technique and compare it to the state-of-the-art sampling approaches.

# First-Principles Multiscale Modeling of Mechanical Properties in Graphene/Borophene Heterostructures Empowered by Machine-Learning Interatomic Potentials

by Timon Rabczuk, Member EUAS

## Short Biography

*Prof. Dr.-Ing. at Bauhaus University Weimar, Chair of Computational Mechanics  
Former Director of the Institute of Structural Mechanics, Bauhaus University Weimar  
National High End Foreign Expert at Tongji University, Shanghai, China  
Listed in ISI Highly Cited 2014 and 2015 in 'Computer Science' and 'Engineering'  
ERC-CoG COMBAT*

*Coordinator of ITN-INSIST and IRSES-MULTIFRAC*

*Prof. Rabczuk is Full Professor at Bauhaus University Weimar and listed as highly cited researcher of Thomson Reuters/Clarivate Analytics in Computer Science and Engineering since 2014 (until now). The research focus of Prof. Rabczuk is Computational Solid Mechanics with emphasis on method development for problems involving fracture and failure of solids and fluid-structure interaction. He is currently developing deep energy methods and machine learning based approaches for the solution of PDEs, nonlocal operator methods and formulations based on Isogeometric Analysis. Another key research direction is Integrated Computational Material Engineering/Computational Materials Design with focus on polymer-matrix composites, batteries and recently phononic topological insulators.*

## **Professional Experience**

*02/1998-12/2001 Wissenschaftlicher Mitarbeiter (Scienti\_c co-worker) at the 'Institute of Concrete Structures and Materials Science' at the University of Karlsruhe with Prof. J. Eibl  
01/2002-02/2002 Wissenschaftlicher Mitarbeiter (Postdoctoral Fellow) at the Fraunhofer Institut für Kurzzeitdynamik-Fraunhofer (Ernst Mach) with Prof. K. Thoma  
01/2002 PhD-defense: Numerische Untersuchungen zum Fragmentierungsverhalten von Beton mit Hilfe der SPH-Methode (Numerical analysis of concrete fragmentation using SPH)  
02/2002-09/2005 Postdoctoral fellow at Northwestern University, Department of Mechanical Engineering, Group of Computational Mechanics, Evanston, Illinois, USA with Prof. T. Belytschko  
10/2005-01/2007 Wissenschaftlicher Mitarbeiter (Postdoctoral fellow) at the Chair of Computational Mechanics, Department of Mechanical Engineering, Technical University of Munich, Germany with Prof. W.A. Wall  
02/2007-02/2009 Senior Lecturer at the University of Canterbury, Department of Mechanical Engineering, Christchurch, New Zealand  
since 02/2009 Univ.-Professor at the Bauhaus University of Weimar, chair of Computational Mechanics, Institute of Structural Mechanics, Department of Structural Engineering, Weimar, Germany  
2010-2013 Director of the Institute of Structural Mechanics at Bauhaus University Weimar*

## **Membership and awards**

*07/2005 Awarded Marie-Curie Intra-European Fellowship (not used)  
Editorial Board member of several journals such as 'Computer Methods in Applied Mechanics and Engineering', 'Applied Physics A', 'Composite Structures', 'Computational Materials Science', 'Finite Elements in Analysis and Design', 'Computers & Structures', 'Theoretical and*

*Applied Fracture Mechanics', 'Engineering with Computers', 'Mechanics of Advanced Composite Structures' or 'Journal of Computational Design and Engineering (JCDE)'*

*2008 Second IMACS 2008 Most Successful Papers Award 1*

*since 01/2015 Executive Editor of 'Frontiers of Structural and Civil Engineering' (Journal of the Chinese Academy of Engineering)*

*since 09/2016 Associate Editor of 'International Journal of Impact Engineering'*

*since 03/2018 Editor-in-chief of 'Computers, Materials & Structures' (CMC)*

*since 01/2021 Associate Editor of 'Applied Physics A'*

*since 01/2022 Associate Editor of 'International Journal of Mechanics and Materials in Design'*

*since 04/2022 Associate Editor for 'Underground Space'*

*since 05/2022 Associate Editor for 'Defense Technology'*

*2014-2021 Listed as ISI-Highly Cited Researcher in the categories 'Computer Science' and 'Engineering'*

*since 2014 Member of the Modeling Market Place (MMP) Working Group of the European Materials Modeling Council (EMMC)*

*since 2015 Member of the EU Academy of Sciences*

#### **Professional Services**

*Reviewer for more than 50 journals (such as Journal of the Mechanics and Physics of Solids since 10/2017, Advanced Materials since 07/2016, ACS*

*Nano since 07/2015, Scientific Reports since 04/2015, Nano Letters since 03/2013, International Journal for Numerical Methods in Engineering since 02/2002, Engineering Fracture Mechanics- since 05/2008, Journal of Computational Physics- since 09/2008, Computer Methods in Applied Mechanics and Engineering since 11/2009, Composite Structures since 02/2011)*

*Reviewer, organizer of mini-symposia and session chair for several conferences since 06/2007*

*Transfer of Knowledge projects to some software companies such as DIFFPACK (InnuTech, Germany), SIMPLAS (Antikythera Systems Lda, Portugal), the research unit at Bosch GmbH and GeoFBA (China) and other companies (Open-Source software-development and application), e.g. Geolink (Germany), ENSCO (Vietnam), 'Korean Expressway Corporation' (Korea), Golden Base Construction JSC (Vietnam) or SMI Huangpu River Upper Reach Raw Water Co., the largest water supplier in China.*

*since 10/2009 Reviewer for the German Research Foundation (DFG)*

*2009 Organizer and host of the 'International Workshop: Technology and Society: Simulation Methods-Extreme Events: Modeling, Analysis and Prediction', 7.10-9.10, Weimar*

#### **Mortazavi, B., Silani, M., Podryabinkin, E.V., (...), Zhuang, X., Shapeev, A.V.: First-Principles Multiscale Modeling of Mechanical Properties in Graphene/Borophene Heterostructures Empowered by Machine-Learning Interatomic Potentials, Advanced Materials, 33(35), 2102807, 2021**

Density functional theory calculations are robust tools to explore the mechanical properties of pristine structures at their ground state but become exceedingly expensive for large systems at finite temperatures. Classical molecular dynamics (CMD) simulations offer the possibility to study larger systems at elevated temperatures, but they require accurate interatomic potentials. Herein the authors propose the concept of first-principles multiscale modeling of mechanical properties, where ab initio level of accuracy is hierarchically bridged to explore the mechanical/failure response of macroscopic systems. It is demonstrated that

machine-learning interatomic potentials (MLIPs) fitted to ab initio datasets play a pivotal role in achieving this goal. To practically illustrate this novel possibility, the mechanical/failure response of graphene/borophene coplanar heterostructures is examined. It is shown that MLIPs conveniently outperform popular CMD models for graphene and borophene and they can evaluate the mechanical properties of pristine and heterostructure phases at room temperature. Based on the information provided by the MLIP-based CMD, continuum models of heterostructures using the finite element method can be constructed. The study highlights that MLIPs were the missing block for conducting first-principles multiscale modeling, and their employment empowers a straightforward route to bridge ab initio level accuracy and flexibility to explore the mechanical/failure response of nanostructures at continuum scale.

**Mortazavi, B., Podryabinkin, E.V., Novikov, I.S., (...), Zhuang, X., Shapeev, A.V.: Accelerating first-principles estimation of thermal conductivity by machine-learning interatomic potentials: A MTP/ShengBTE solution, Computer Physics Communications 258,107583, 2021**

Accurate evaluation of the thermal conductivity of a material can be a challenging task from both experimental and theoretical points of view. In particular for the nanostructured materials, the experimental measurement of thermal conductivity is associated with diverse sources of uncertainty. As a viable alternative to experiment, the combination of density functional theory (DFT) simulations and the solution of Boltzmann transport equation is currently considered as the most trusted approach to examine thermal conductivity. The main bottleneck of the aforementioned method is to acquire the anharmonic interatomic force constants using the computationally demanding DFT calculations. In this work we propose a substantially accelerated approach for the evaluation of anharmonic interatomic force constants via employing machine-learning interatomic potentials (MLIPs) trained over short ab initio molecular dynamics trajectories. The remarkable accuracy of the proposed accelerated method is confirmed by comparing the estimated thermal conductivities of several bulk and two-dimensional materials with those computed by the full-DFT approach. The MLIP-based method proposed in this study can be employed as a standard tool, which would substantially accelerate and facilitate the estimation of lattice thermal conductivity in comparison with the commonly used full-DFT solution.

**Mortazavi, B., Podryabinkin, E.V., Roche, S., (...), Zhuang, X., Shapeev, A.V.: Machine-learning interatomic potentials enable first-principles multiscale modeling of lattice thermal conductivity in graphene/borophene heterostructures, Materials Horizons 7(9), pp. 2359-2367, 2020**

One of the ultimate goals of computational modeling in condensed matter is to be able to accurately compute materials properties with minimal empirical information. First-principles approaches such as density functional theory (DFT) provide the best

possible accuracy on electronic properties but they are limited to systems up to a few hundreds, or at most thousands of atoms. On the other hand, classical molecular dynamics (CMD) simulations and the finite element method (FEM) are extensively employed to study larger and more realistic systems, but conversely depend on empirical information. Here, we show that machine-learning interatomic potentials (MLIPs) trained over short *ab initio* molecular dynamics trajectories enable first-principles multiscale modeling, in which DFT simulations can be hierarchically bridged to efficiently simulate macroscopic structures. As a case study, we analyze the lattice thermal conductivity of coplanar graphene/borophene heterostructures, recently synthesized experimentally (*Sci. Adv.*, 2019, **5**, eaax6444), for which no viable classical modeling alternative is presently available. Our MLIP-based approach can efficiently predict the lattice thermal conductivity of graphene and borophene pristine phases, the thermal conductance of complex graphene/borophene interfaces and subsequently enable the study of effective thermal transport along the heterostructures at continuum level. This work highlights that MLIPs can be effectively and conveniently employed to enable first-principles multiscale modeling *via* hierarchical employment of DFT/CMD/FEM simulations, thus expanding the capability for computational design of novel nanostructures.

**Mortazavi, B., Novikov, I.S., Podryabinkin, E.V., (...), Shapeev, A.V., Zhuang, X.: Exploring phononic properties of two-dimensional materials using machine learning interatomic potentials, Applied Materials Today 20,100685, 2020**

Phononic properties are commonly studied by calculating force constants using the density functional theory (DFT) simulations. Although DFT simulations offer accurate estimations of phonon dispersion relations or thermal properties, but for low-symmetry and nanoporous structures the computational cost quickly becomes very demanding. Moreover, the computational setups may yield nonphysical imaginary frequencies in the phonon dispersion curves, impeding the assessment of phononic properties and the dynamical stability of the considered system. Here, we compute phonon dispersion relations and examine the dynamical stability of a large ensemble of novel materials and compositions. We propose a fast and convenient alternative to DFT simulations which derived from machine-learning interatomic potentials passively trained over computationally efficient *ab-initio* molecular dynamics trajectories. Our results for diverse two-dimensional (2D) nanomaterials confirm that the proposed computational strategy can reproduce fundamental thermal properties in close agreement with those obtained via the DFT approach. The presented method offers a stable, efficient, and convenient solution for the examination of dynamical stability and exploring the phononic properties of low-symmetry and porous 2D materials.

**Mortazavi, B., Javvaji, B., Shojaei, F., (...), Shapeev, A.V., Zhuang, X.: Exceptional piezoelectricity, high thermal conductivity and stiffness and promising photo-catalysis in two-dimensional MoSi<sub>2</sub>N<sub>4</sub> family confirmed by**

**first-principles, Nano Energy 82,105716, 2021**

Chemical vapor deposition has been most recently employed to fabricate centimeter-scale high-quality single-layer  $\text{MoSi}_2\text{N}_4$  (*Science*; 2020;369; 670). Motivated by this exciting experimental advance, herein we conduct extensive first-principles based simulations to explore the stability, mechanical properties, lattice thermal conductivity, piezoelectric and flexoelectric response, and photocatalytic and electronic features of  $\text{MA}_2\text{Z}_4$  (M = Cr, Mo, W; A = Si, Ge; Z = N, P) monolayers. The considered nanosheets are found to exhibit dynamical stability and remarkably high mechanical properties. Moreover, they show diverse electronic properties from antiferromagnetic metal to half metal and to semiconductors with band gaps ranging from 0.31 to 2.57 eV. Among the studied nanosheets, the  $\text{MoSi}_2\text{N}_4$  and  $\text{WSi}_2\text{N}_4$  monolayers yield appropriate band edge positions, high electron and hole mobilities, and strong visible light absorption, highly promising for applications in optoelectronics and photocatalytic water splitting. The  $\text{MoSi}_2\text{N}_4$  and  $\text{WSi}_2\text{N}_4$  monolayers are also predicted to show outstandingly high lattice thermal conductivity of 440 and 500 W/mK, respectively. For the first time we show that machine learning interatomic potentials trained over small supercells can be employed to examine the flexoelectric and piezoelectric properties of complex structures. As the most exciting finding,  $\text{WSi}_2\text{N}_4$ ,  $\text{CrSi}_2\text{N}_4$  and  $\text{MoSi}_2\text{N}_4$  are found to exhibit the highest piezoelectric coefficients, outperforming all other-known 2D materials. Our results highlight that  $\text{MA}_2\text{Z}_4$  nanosheets not only undoubtedly outperform the transition metal dichalcogenides family but also can compete with graphene for applications in nanoelectronics, optoelectronic, energy storage/conversion and thermal management systems.

# The Virtual Hospital is an Essential Building Block of the Hospital of the Future

by Pascal Verdonck, Member EUAS



## Short Biography

Pascal Verdonck was born in 1963 in Gent, Belgium. He graduated as Master of Science Civil Engineering in 1986 from the Ghent University. He obtained his diplomas in Master of Business Administration (1989), Master of Science Biomedical Engineering (1993) and PhD (1993) from the Ghent University. He is married with Nathalie Van Peteghem and has two children Simon (°1993) and Charlotte (°1995)

### **Professional activities and relevant experience**

- Assistant (1987-1992), post-doctoral researcher (1993-1995), assistant professor (1996-2002) and full professor "cardiovascular mechanics and biofluid dynamics "at the Ghent University since 2002
- Visiting professor University of Groningen, Groningen , the Netherlands (2001-2007)
- Visiting professor Imperial College, London (2004-2008)
- Tenured professor at the International Faculty for Artificial Organs, Bologna, Italy
- Head of the Department of Civil Engineering of the Ghent University (1998-2006)
- Ombudsman of the Faculty of Applied Sciences of the Ghent University (1993-2003)
- Chairman bachelor programs of the Faculty of Applied Sciences of the Ghent University (2003-2006)
- Scientific secretary of the Institute Biomedical Technology of the Ghent University (1997-2006)
- Visiting professor University Paris XII (1997)
- Visiting Socrates professor TU Kosice (2000-2004) and Julich (2000-2010)
- Member Board European Society for Engineering and Medicine (2002-2004)
- Member of the Board of Trustees of the International Society for Artificial Organs ISAO (1999-2003)
- Member of the Board of the ESAO European Society for Artificial Organs (2004-2011)
- Vice Chairman of the alumni of the engineers studied at the Ghent University (1995-2003)
- Vice Président "Société Biomécanique" (2000-2002) , Président "Société Biomécanique" (2002-2004)
- Member evaluation commission Belgium for " medical devices" and "active medical devices " (2001-2007)
- Chairman of the Board of Directors start-up "FluidDA" (2007- 2009)
- Member of the Board of Directors AZ Maria Middelaes hospital Gent (2000-2007)
- CEO of private hospital "AZ Maria Middelaes" Gent (2007- 2015) ([www.azmmsj.be](http://www.azmmsj.be))
- Senior full professor "MedicalTechnology" Ghent University (2007-) ([www.ugent.be](http://www.ugent.be))
- Visiting Professor "biomedical engineering" Catholic University Leuven, Belgium (2009-)
- Chairman National Committee Biomedical Engineering (2001-) ([www.ncbme.be](http://www.ncbme.be))
- Member of the Royal Flemish Academy of Belgium for sciences and arts (2009-)
- Member of the Board of Directors OLV Aalst Hospital (2012-) ([www.olvz.be](http://www.olvz.be))
- Member of the Board of Directors Acerta (2013) ([www.acerta.be](http://www.acerta.be))
- Vice chairman of the Board of Directors Artevelde University College Gent (2005-) ([www.arteveldehs.be](http://www.arteveldehs.be))
- Vice Chairman Belgian Association Hospital Directors (2013-) ([www.ziekenhuisdirecteurs.be](http://www.ziekenhuisdirecteurs.be))
- Member of the Board of Directors Voka Flanders chamber of commerce and industry (2015-)
- Chairman of the Board of Directors AZ Maria Middelaes hospital Gent (2015-) ([www.azmmsj.be](http://www.azmmsj.be))
- CEO MedTech Flanders ([www.medtech.flanders.be](http://www.medtech.flanders.be)) (2015-)

- *Member of the board of Directors Sint-Vincentius Deinze Hospital ((2017-)*
- *Member of the board of Directors Jan Yperman Hospital Ieper ((2019-)*
- *Board Member European Association Hospital Managers (2019-) (www.eahm.eu.org)*
- *Member of the board of Directors Medvia (2022-) (www.medvia.be)*

#### **Actual academic courses**

- *“Biosystems”, 2<sup>nd</sup> year bachelor engineering sciences @Ghent University*
- *“BioFluid Mechanics”, 2nd year master biomedical engineering sciences @Leuven University*
- *“Leadership in Healthcare”, 2nd year master biomedical engineering sciences @Ghent University*
- *“Engineering project in a hospital”, 2nd year master biomedical engineering sciences @Ghent University*

#### **Research and innovation**

*His scientific research has spanned numerous fields of biomedical engineering sciences : experimental and numerical modeling of the cardiovascular system, haemodynamics and transport phenomena in extracorporeal circulation and artificial organs, computational biodesign and medical device technology. He is an active advisor for the MedTech Start & Scale-up Ecosystem.*

## **The virtual hospital is an essential building block of the hospital of the future**

### **Abstract**

Value-based, connected and integrated healthcare are gaining momentum in the healthcare landscape. Industry 4.0 is transforming nowadays rapidly healthcare into a data-driven sector. Data and innovation create future value. Based upon the concept of a human-centered, health data-driven ecosystem a future proof virtual hospital can be built as part of the hospital of the future . This requires a performant data process/ framework : collection, currency, transmission and intelligence all protected within a shell of security. Realizing this framework in a safe, compliant and secure way is an essential legal step that determines the possibility for health care professionals to use it in an accountable way. Only then the virtual hospital will fully become available for an individual.

### **Keywords**

Healthcare ecosystem, value-based care, connected care, integrated care, hospital of the future, the future of health, mHealth, eHealth, digital therapy

### **Background**

The hospital of the future is mainly focused on improving patient outcomes and experiences through a combination of innovative technology, data driven healthcare , and (inter)national & regional collaboration. As these trends continue to evolve, hospitals will play an increasingly important role in shaping the future of health. So the “hospital of the future ” is closely tied to the “future of health”.

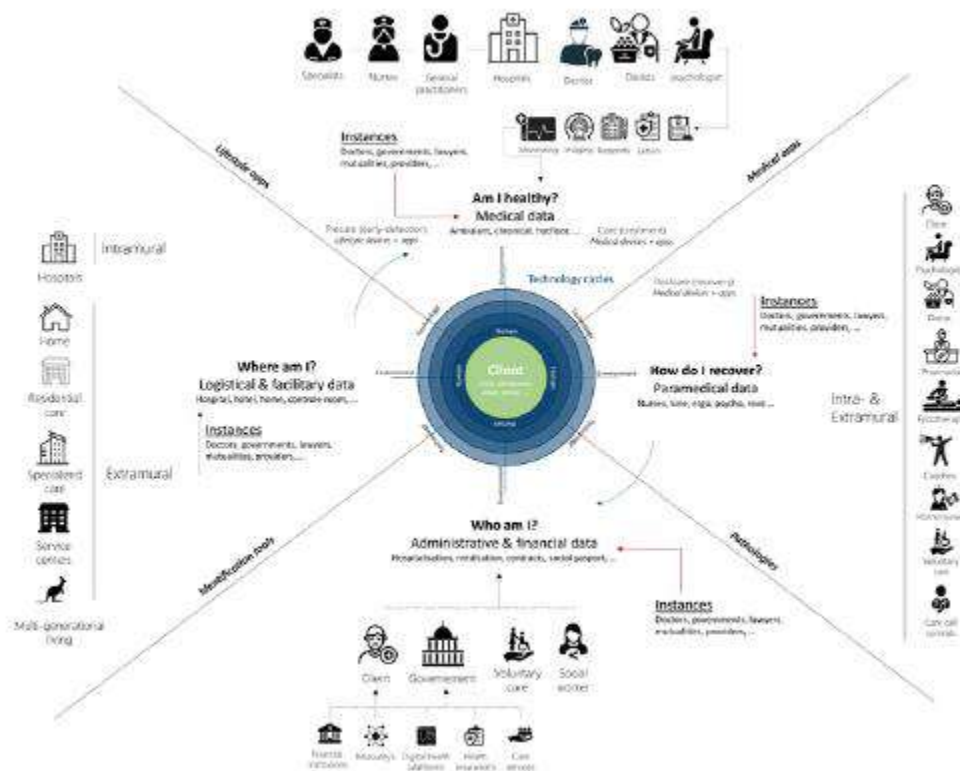
Healthcare globally evolves in this digital era towards a connected, integrated and value-based care. But it is our vision that you only can integrate care around the patient permanently if you are connected with the patient in order to realize value based healthcare.

However at this point the current way of implementing connected and integrated care is still a patchwork of different data platforms without coherent legal proof solutions. The fact that data is stored in different locations and requested upon from other location causes no general data overview, non-uniform data structures, a decrease in patient-value and legal issues.

**A human- centered, health-data-driven ecosystem**

We published a unique data model to tackle these problems. The model describes data sources in the form of technologies, humans and environments in four data quadrants (financial and administrative, logistical and facility, medical and paramedical). Collection, transmission, processing, interpretation and security are needed as elementary steps between the data source and end-user, to make data usable in the day-to-day practice. This human-centered, health-data- driven ecosystem consists out of four different quadrants (Q). Each of these quadrants contain a specific data domain used in care. Each quadrant has a defining question that can be answered by the data generated within the quadrant itself. We defined the following quadrants (see figure 1):

Q1. 'Who am I?': administrative and financial  
 Asking 'Who am I?' will generate administrative and financial data containing the client's personal info, historical medical data, medication schemes, social passports, etc. The data sources are the client himself, the government, voluntary caretakers and social workers. Typically administrative data is data collected at every encounter with the care system, through the entire lifetime of the client, going from birth over youth, adolescence, grown-up, elderly until passing away. The data is to be supplemented with data from financial institutions, mutuality's, digital health data platforms, health insurances and care services.



**Figure 1:** schematic representation in four quadrants of a human- centered, health-data-driven ecosystem

**Q2. 'Where am I?': logistics and facility services data**

The second question 'Where am I?' will generate the logistics and facility services data of the client. This data can be related to the centered client but also to the internal stakeholders. It describes where a client resides and from which environment the client originates. In order to facilitate the connection from the client to the health care professional and vice versa in order to organize remote monitoring, provide chronic disease management, supply elderly care, prevent readmission and provide personal care, the location and physical environment of the patient is an important aspect for the continuity of care. In the logistical and facility domain we define two different groups of environments: intramural and extramural.

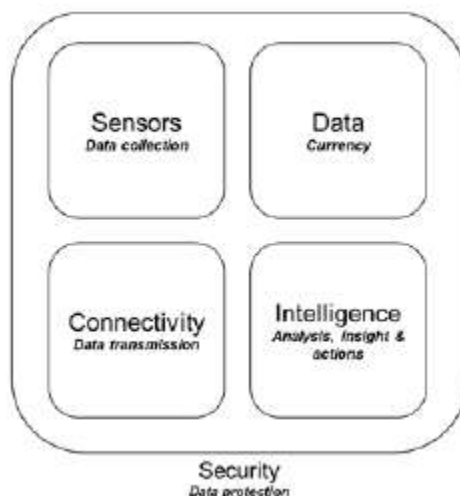
**Q3. Am I healthy?: medical data**

The third questions, 'Am I healthy?', generates the medical data. It finds its origin in exams (policlinic or technical), lab tests, imaging modalities, operations, etc. The content of the data is related to medico-technical, ambulant, chronic and hot floor treatments. Chronologically in the care path of the client the third quadrant contains the early-detection of possible pathologies. In this part, data coming from lifestyle applications and devices of the second quadrant are processed, analysed and added to the digital environments of the care-actors of the third quadrant. This information provides early insight into the question 'is the client healthy?'. During the diagnosis and treatment of the client a lot of data will be gathered. Written reports of care actors, lab results, data from static monitoring devices, information from imaging, referral letters, et all need to be taken into account. Human actors involved in this quadrant can be located in many different environments ranging from a hospital, a general practitioners office, a juvenile care institution to a rehabilitation center, etc. A third part of information of medical data in this third quadrant will be the medical applications and wearable devices.

**Q4: How do I recover?: paramedical data**

The fourth quadrant is where the paramedical data is being generated. Here all paramedic actors involved to the recovery and post-care of a client are localized. These will generate data that needs to be accessible for all internal stakeholders to close the loop of the ecosystem and lead to a full recovery. The main sources will be intra- and extramural care takers and the clients themselves who generates data through their wearables, medical applications or eHealth platforms used in their recovery process. A close feedback loop over the first and second quadrant to the actors of the third quadrant exists. The goal of this feedback loop is to closely connect as many caretakers with the follow-up of the recovery or post care of their clients.

Figure 2 represents the essential components of a data process/ framework : collection, currency, transmission and intelligence all protected within a shell of security. Realizing this framework in a safe, compliant and secure way is an essential legal step that determines the possibility for health care professionals to use it in an accountable way. Only then the virtual hospital will fully become available.



**Figure 2:** The needed data framework

## The virtual hospital of the future

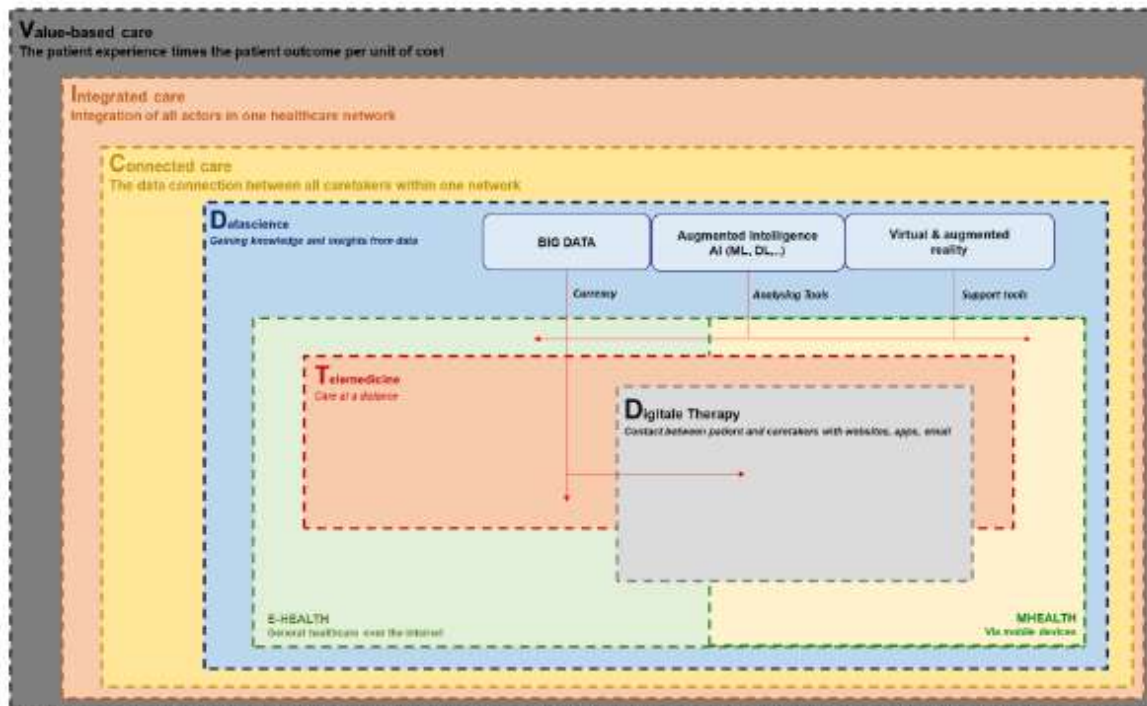
In the near future, hospitals may be designed with more emphasis on telemedicine and digital technology, incorporating features such as remote monitoring, artificial intelligence, and virtual and augmented reality. At the same time, they will still need to maintain physical spaces for procedures, equipment, and staff to deliver in-person care. Some healthcare services still require in-person visits and physical facilities, such as surgery, interventions, diagnostic tests, and emergency care. Therefore, a hybrid model that combines both physical and virtual elements is likely to be the most effective approach.

The vision starts with focus on value based healthcare. But to create value we have to connect 24/7 with the client/patient to integrate care around the patient if necessary. Therefore we integrate the available health data around the patient (zero-line). E-health, also known as digital health or telehealth, refers to the use of digital technologies and electronic communication to support and improve healthcare delivery and outcomes. E-health encompasses a wide range of applications, including telemedicine, mobile health (mHealth).

Data sciences and data analytics is the process of examining large and varied data sets using statistical and computational methods to uncover useful information, patterns, and insights. It involves collecting, cleaning, processing, and analyzing large amounts of data to extract meaningful and actionable insights (big data, AI, VR, AR, ...). Data sciences is thus a supporting tool and in fact the crucial hinge to connect the healthcare vision with real virtual health.

Telemedicine is one of the most common forms of e-health, which involves the delivery of healthcare services remotely through video conferencing, messaging, or other electronic means. This allows patients to receive medical care from the comfort of their own homes (home care and home hospitalisation). M-health, also known as mobile health or telehealth, refers to the use of mobile devices such as smartphones, tablets, and wearable devices to support and enhance healthcare services. M-health solutions enable healthcare providers to remotely monitor and manage patients' health conditions, deliver medical information, provide preventive care, and offer consultations through mobile devices.

Digital therapy, also known as e-therapy, refers to the use of digital technologies such as web-based platforms, mobile apps, and virtual reality to provide psychological interventions for mental health conditions. Digital therapy aims to provide accessible, affordable, and convenient mental health care to individuals who may have difficulty accessing traditional face-to-face therapy.



**Figure 3:** A synthesis of a future proof virtual hospital

## Conclusion

Overall, a hybrid approach to future proof healthcare is likely to provide patients with the best of both worlds: the convenience and flexibility of virtual care, combined with the expertise and resources of traditional hospitals. In order to realize this an accelerated collaboration of different stakeholders is essential to realize in a safe, compliant and secure way the data-information backbone. Only then we will be able to integrate the care efficiently around an individual and being able to deliver health value permanently.

# Investigations of the Atomic Structure and the Novel Properties of a New Class of Solids, the so called Nanoglasses

by Herbert Gleiter, Member EUAS

## Short Biography

*Herbert Gleiter received his Ph.D. in Physics and was a Post Doctoral Fellow at Harvard University and MIT. In 1973, Gleiter became Chair Professor of Materials Science and founded in 1988 today's Leibniz Institute of New Materials at Saarbruecken, Germany. In 1994, he was appointed President of Research and Technology of the Research Center Karlsruhe, Germany, and 4 years later, he became the Founding Director of the Center's Institute of Nanotechnology. In 2012 the University of Nanjing founded the "Herbert Gleiter Institute of Nanoscience" and appointed him as the Institute's Founding Director. In 2019 the Chinese Academy of Science decided to set up a new research laboratory at Shenyang working on Nanomaterials. This laboratory - named Herbert Gleiter International Laboratory - will be managed and guided by scientists from China, Germany and the US.*

*Prof. Gleiter received more than 40 prizes. Among them, the most highly reputed awards in Germany, the Leibniz and the Max Planck Research Prize and the Cothenius Medal, the most prestigious award of the German National Academy of Sciences. The Alexander von Humboldt Foundation honored him by selecting him in 2006 for the Humboldt Medal and in 1999 for Werner Heidsieck Medal. Seven Universities from Germany, Hong Kong, Switzerland and China awarded him Honorary Doctor degrees. He is a Member of 12 Academies/National Academies of Science and/or Engineering: Three Academies in the US, one in Germany, in UK, in Belgium, in Austria, in Greece, and three Academies/National Academies in India. Among them are the National Academy of Engineering, the American Academy of Arts and Sciences, the National Academy of Inventors, the European Academy of Arts and Sciences, the Academia Europaea, the EU Academy of Sciences, the Indian National Academy of Sciences and the Indian National Academy of Engineering..*

*By the end of the 70's he and his research group pioneered to a new kind of materials, called today nano-crystalline materials. In fact, the first publication on nanocrystalline materials has been cited today more than 3400 times and this area of Materials Science has been cited up to now in total over 150 000 times and about 6 to 8 international conferences on nano-materials are organized every year. His first paper pioneering nano-crystalline materials has been cited so far more than 3500 times.*

*In recent years, Herbert Gleiter expanded the field of Materials Science by developing nanostructured non-crystalline materials. They are called today nano-glasses. Nano-glasses opened the door to non-crystalline materials with new atomic and electronic structures and/or with chemical compositions that cannot be generated in the form of the glassy materials we have today. For example, they permit the production of new kinds of alloys (e.g alloys of silica and metals), new magnetic materials, new medical applications etc. In other words, nano-glasses may open the way into a "glass age" that would be based on the new properties of nano-glasses.. The significance of this contribution was recently acknowledged by electing him (together with the Nobel Laureates Haensch and zur Hausen) as the first member from Germany in the the US National Academy of Inventors and by appointing him to be the "Researcher of the Year 2020.*

The studies performed during the period of time covered by this report (January 1 2022 to December 31 2022) were focused on investigations of the atomic structure

and the novel properties of a new class of solids, the so called nanoglasses.

Nanoglasses represent a new kind of non-crystalline materials consisting of nanometer-sized glassy regions that are connected by interfacial regions with a new kind of atomic structure that differs structurally from the two atomic arrangements that were known up to now: The structurally periodic atomic arrangements on crystalline solid and the atomic arrangements in glasses characterized by short range order.

This new type of atomic arrangements in the interfaces of nanoglasses results in new properties differing drastically from the properties of the glassy as well as of the crystalline state of materials with the same chemical composition. By utilizing these new features of nanoglasses a new age of new technologies (a glass age) based on these new kinds of non-crystalline materials (i.e. nanoglasses) may be initiated.

Concerning the new atomic structure, the new properties and the novel applications in technology, medicine etc. of nanoglasses that have been reported so far, we refer to some of the recently published review articles: H. Gleiter in *Small* 22 2016 2225; Si Lan et al, in *nature materials letters* doi .org/10.1038; R.Baughman, *Science* 308, 2005 63).

Based on the obvious potential of this new kind of non-crystalline materials - the nanoglasses – the Chinese Liaoning Academy Materials Science has decided to set up a new research center in China located at Shenyang, China with the name of Herbert Gleiter International Institute (HGII) . This laboratory will be one of the largest laboratories of the Chinese Academy of Sciences. Its research will focus on a wide spectrum of studies in the area of nanoglasses extending from new kinds of materials by means of nanoglass alloys to the proliferate cell growth on nanoglasses and its applications in implantation medical treatments and to the production of single atom transistors.

These studies are planned to be performed at the newly founded research HGII center at Shenyang in direct cooperation with research groups from more than 15 Universities located in China as well as abroad.

In 2022 I have been appointed by the Liaoning Academy Materials Science to be

the Director of the new Herbert Gleiter International Institute (HGII). In that function I will be able to determine the research directions of the HGII, to supervise its research activities and to recruit its researchers and technicians.

The close multi-disciplinary cooperation of the HGII with research institutions covering a wide spectrum of research methods in experiment as well as in theory, the HGII will be able to contribute in many ways to the rapid development of the new fields of nanoglasses and by utilizing the new features of nanoglasses technologically a age of new technologies (a glass age) based on these new kinds of non-crystalline materials (i.e. nanoglasses) may be initiated. Obviously, in this new field the HGII will have the potential to become one of internationally leading centers in the age of new technologies (a glass age) based on these new kinds of non-crystalline materials.

### **Award of the Stookey Prize of Discovery in combination with the Stookey Lecture of Discovery**

**The contributions** based on the discovery and the investigations of **the new atomic structure** and the **novel properties of** a new class of solids, the so called **nanoglasses** were recognized in 2022 by the *American Ceramic Society* by selecting me for one of their most highly recognized awards, the **2022 Stookey Award of Discovery in combination with the Stookey Lecture of Discovery**.

This lecture and the presentation of the **2022 Stookey Award of Discovery** was scheduled at the Glass and Optical Materials Division Section of the Annual Meeting of *the American Ceramic Society* held on May 22 – 26, 2022 at Baltimore, MD USA.

## New Aspects in Molecular Quantum Mechanics

by Henry F. Schaefer, Member EUAS

### Short Biography

Henry F. Schaefer III was born in Grand Rapids, Michigan. He attended public schools in Syracuse (New York), Menlo Park (California), and Grand Rapids (Michigan), graduating from East Grand Rapids High School. In 2018 Professor Schaefer received the Alumnus/Alumna of the Year Award from East Grand Rapids High School. He received his B.S. degree in chemical physics from the Massachusetts Institute of Technology and Ph.D. degree in chemical physics from Stanford University. For 18 years he served as a professor of chemistry at the University of California, Berkeley. During the 1979-1980 academic year he was also Wilfred T. Doherty Professor of Chemistry and inaugural Director of the Institute for Theoretical Chemistry at the University of Texas, Austin. Dr. Schaefer is currently Graham Perdue Professor of Chemistry and Director of the Center for Computational Quantum Chemistry at the University of Georgia. He is simultaneously Professor of Chemistry, Emeritus, at the University of California at Berkeley. His other academic appointments include Professeur d'Echange at the University of Paris (1977), Gastprofessur at the Eidgenössische Technische Hochschule (ETH), Zürich (1994, 1995, 1997, 2000, 2002, 2004, 2006, 2008, 2010), David P. Craig Visiting Professor at the Australian National University (1999), and Visiting Professor at the Ludwig Maximilians University (LMU) Munich (2012, 2013, 2014, 2015, 2016, 2017, 2018, 2019).

Schaefer is the author of more than 1700 scientific publications, with a large majority appearing in the *Journal of Chemical Physics*, *Journal of the American Chemical Society* or the *Journal of Physical Chemistry*. A total of 300 scientists from 35 countries gathered in Gyeongju, Korea for a six-day conference in February, 2004 with the title "Theory and Applications of Computational Chemistry: A Celebration of 1000 Papers of Professor Henry F. Schaefer III." In May 2010, the University of California at Berkeley hosted a large international conference in Professor Schaefer's honor, the title of the conference being "Molecular Quantum Mechanics: From Methylene to DNA and Beyond." Simultaneous with the Berkeley conference was published the book *Selected Papers of Henry F. Schaefer III*, Edited by R. J. Bartlett, T. D. Crawford, M. Head-Gordon, and C. D. Sherrill. In May 2014 the Peking University Graduate School sponsored a large conference in honor of Professor Schaefer and Professor Leo Radom in Shenzhen, China. In August 2019, the American Chemical Society Division of Physical Chemistry held a five-day symposium titled "Computational Quantum Chemistry: from Promise to Prominence," in honor of Dr. Schaefer in San Diego, California. A symposium in Professor Schaefer's honor in December 2021 at the International Chemical Congress of Pacific Basin Societies (PACIFICHEM) in Honolulu, Hawaii.

Critical to Professor Schaefer's scientific success has been a brilliant array of students and coworkers; including 82 undergraduate researchers who have

published papers with him, 133 successful Ph.D. students (plus 14 in progress), 55 postdoctoral researchers, and 81 visiting professors who have spent substantial time in the Schaefer group. A number of his students have gone on to positions of distinction in industry (Accelrys, Adesis, ALTANA, American Cyanamid, AstraZeneca, AT&T, Avaya, Bicerano and Associates, Castle Hill Gaming, Chemical Abstracts, Clariant, Computational Geosciences, Coraid, DeNovaMed, Deutsche Bank, Dow Chemical, ELANTAS, Electronic Arts, Endress-Hauser, EnerDel, First Source Research, GAUSSIAN, Goodrich, Google, Henkel, Hewlett-Packard, Hughes Aircraft, IBM, ICON, Komag, Locus Pharmaceuticals, Lonza Pharma & Biotech, Materials Design, McKesson Corp, Mobil Research, Molecular Simulations, Monsanto, Nimble Storage, OpenEye, OSI Software, PartnerRe, Pfizer, Pharmaceutical Research Associates, Polaroid, Proctor & Gamble, Q-CHEM, Reagens Deutschland, Ricoh, RWDC Bioplastics, Schroedinger, SciCo, Sugan, Treventis, Universal Display Corporation, VALIS, WaveSplitter Technologies, Xcellence LLC, and Xenon Pharmaceuticals). Four of his graduated Ph.Ds have started their own companies.

Several of Schaefer's former students have gone on to successful careers in government laboratories, including the Australian National University Supercomputer Center, Environmental Protection Agency (EPA), Joint Institute for Laboratory Astrophysics (JILA), Lawrence Berkeley National Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Molecular Sciences Software Institute, NASA Ames, National Cancer Institute, National Center for Disease Control, National Institute of Environmental Health Sciences, National Institutes of Health (Bethesda), National Research Council of Canada (Ottawa), Naval Research Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, Pittsburgh Supercomputing Center, Sandia National Laboratories, and the Savannah River National Laboratory. Charles Blahous went directly from his Ph.D. studies with Dr. Schaefer to the position of American Physical Society Congressional Scientist Fellow, and eventually to positions of significant importance in the U.S. political system (chief of staff for Senator Alan Simpson of Wyoming and later for Senator Judd Gregg of New Hampshire; and Executive Director of President George W. Bush's Bipartisan Committee to Strengthen Social Security; see *Wall Street Journal* article April 22, 2005). Dr. Blahous is currently Research Fellow at the Hoover Institution, Stanford University, and J. Fish and Lillian P. Smith Chair at the Mercatus Center, George Mason University. He was appointed by President Barack Obama to the Board of Trustees for Social Security and Medicare.

Many of Dr. Schaefer's students have accepted professorships in universities, including the University of Alabama at Birmingham, University of Arizona, Beijing Normal University, Budapest University (Hungary), University of California at Merced, City University of New York, University of Concepcion (Chile), Duke University, Emory University, Fatih University (Istanbul, Turkey), Georgia Tech, University of Georgia, University of Giessen (Germany), University of Girona

(Spain), University of Grenoble (France), University of Guelph (Ontario), Hacettepe University (Ankara), University of Heidelberg (Germany), University of Illinois-Chicago, University of Illinois-Urbana, Indian Association for the Cultivation of Science (Calcutta), Indiana University-Purdue University at Indianapolis, Johns Hopkins University, Keio University (Japan), University of Kentucky, Lehigh University, University of Manchester (England), University of Marburg (Germany), University of Massachusetts, University of Memphis, University of Michigan, University of Mississippi, National Tsing Hua University (Taiwan), University of North Dakota, Ohio State University, Osaka University (Japan), University of Ottawa (Canada), University of Paris - Sud (France), Pennsylvania State University, University of Pittsburgh, Pohang Institute of Science and Technology (Korea), Portland State University, Rice University, Rikkyo University (Tokyo), Scripps Research Institute, University of South Florida, St. Andrew's University (Scotland), St. Petersburg State University (Russia), Stanford University, University of Stirling (Scotland), University of Stockholm (Sweden), University of Tasmania (Australia), Technical University of Munich (Germany), Texas A&M University, the University of Texas at Arlington, University of Trondheim (Norway), University of Tübingen (Germany), Ulsan National University of Science and Technology (Korea), and Virginia Tech.

Dr. Schaefer has been invited to present plenary lectures at more than 300 national or international scientific conferences. He has delivered endowed or named lectures or lecture series at more than 60 major universities, including the Kenneth S. Pitzer Memorial Lecture at Berkeley, the Israel Pollak Distinguished Lectures at the Technion - Israel Institute of Technology, Haifa, the C. V. Raman Memorial Lecture in Calcutta, India, the Per-Olov Lowdin Lectures at the University of Uppsala, Sweden, and the Jan Almlöf/Odd Gropen Lectures in Norway. He is the recipient of 31 honorary degrees. He served as Editor-in-Chief of the London-based journal *Molecular Physics* for ten years (1995-2005). He is currently Associate Editor for the journal *Physical Chemistry Chemical Physics*. He was also the longest serving President of the World Association of Theoretical and Computational Chemists, from 1996 to 2005. His service to the chemical community includes the chairmanship of the American Chemical Society's Subdivision of Theoretical Chemistry (1982) and Division of Physical Chemistry (1992). At the 228th National Meeting of the American Chemical Society (Philadelphia, August, 2004) the Division of Computers in Chemistry and the Division of Physical Chemistry co-sponsored a four-day "Symposium in Honor of Henry F. Schaefer's 60th Birthday." The book *Theory and Applications of Computational Chemistry: The First Forty Years* (1308 pages, Elsevier) was published in 2005 in honor of Professor Schaefer.

Professor Schaefer's major awards include the American Chemical Society Award in Pure Chemistry (1979, "for the development of computational quantum chemistry into a reliable quantitative field of chemistry and for prolific exemplary calculations of broad chemical interest"); the American

Chemical Society Leo Hendrik Baekeland Award (1983, “for his contributions to computational quantum chemistry and for outstanding applications of this technique to a wide range of chemical problems”); the Schrödinger Medal (1990); the Centenary Medal of the Royal Society of Chemistry (London, 1992, as “the first theoretical chemist successfully to challenge the accepted conclusions of a distinguished experimental group for a polyatomic molecule, namely methylene”); the American Chemical Society Award in Theoretical Chemistry (2003, “for his development of novel and powerful computational methods of electronic structure theory, and their innovative use to solve a host of important chemical problems”). In 2003 he also received the annual American Chemical Society Ira Remsen Award, named after the first chemistry research professor in North America. The Remsen Award citation reads “For work that resulted in more than one hundred distinct, critical theoretical predictions that were subsequently confirmed by experiment and for work that provided a watershed in the field of quantum chemistry, not by reproducing experiment, but using state-of-the-art theory to make new chemical discoveries and, when necessary, to challenge experiment.”

*The Journal of Physical Chemistry* published a special issue in honor of Dr. Schaefer on April 15, 2004. In 2009 and 2010, the journal *Molecular Physics* published seven separate issues in honor of Professor Schaefer. He was elected a Fellow of the American Academy of Arts and Sciences in 2004. He was the recipient of the prestigious Joseph O. Hirschfelder Prize of the University of Wisconsin for the academic year 2005-2006. He became a Fellow of the Royal Society of Chemistry (London) in 2005. He was among the inaugural class of Fellows of the American Chemical Society, chosen in 2009. He earlier became a Fellow of the Alfred P. Sloan Foundation, John S. Guggenheim Foundation, American Physical Society, and American Association for the Advancement of Science. In April 2011 he received the Ide P. Trotter Prize of Texas A&M University. Recent recipients of this prestigious award have included Nobelists Charles Townes, William Phillips, Francis Crick, Steven Weinberg, and Roald Hoffmann. In 2012 he received the Alexander von Humboldt Award. In March 2012 Professor Schaefer received the \$20K SURA Distinguished Scientist Award, given to the outstanding scientist in any field in the southern USA, from Missouri to Texas to Florida to Virginia. In April 2013, at the Chemical Heritage Foundation in Philadelphia, Dr. Schaefer received the Chemical Pioneer Award of the American Institute of Chemists. In January 2014 he was named by *The Best Schools* as one of “The 50 Most Influential Scientists in the World Today.” In March 2014 he received the American Chemical Society Peter Debye Award in Physical Chemistry. In February 2016 he was elected an Honorary Fellow of the Chemical Research Society of India. In May 2019, he received the Gold Medal of the American Institute of Chemists. Seven of the previous 14 recipients of the AIC Gold Medal received the Nobel Prize. Also in May 2019 Dr. Schaefer received the ACS Charles H. Stone Award.

For 40 years Professor Schaefer has been one of the most highly cited scientists in the world. The Science Citation Index reports that his research had been cited more than 81,000 times. Professor Schaefer's Thomson-Reuters H-index is currently 123. He has published 173 Citation Classic Papers. His research involves the use of state-of-the-art computational hardware and theoretical methods to solve important problems in molecular quantum mechanics.

# Cancer Immunotherapy by Tumor Membrane Vesicles conjugated to Potent Immunostimulatory Molecules

by Dong Moon Shin, Member EUAS



## Short Biography

**Dong Moon Shin, MD, FACP, FAAAS**

**Professor of Medical Oncology and Francis Kelly Blomeyer Chair in Cancer Research  
Emory University School of Medicine**

*Dr. Dong Moon Shin is currently Professor of Medical Oncology, Otolaryngology and Biomedical Engineering, and holds Frances Kelly Blomeyer Distinguished Endowed Chair in Cancer Research in the Department of Hematology and Medical Oncology at Winship Cancer Institute of Emory University. He graduated from Yonsei University College of Medicine and trained for Residency in Internal Medicine at Cook County Hospital, Chicago, IL and fellowship of Medical Oncology at the University of Texas M. D. Anderson Cancer Center, Houston, TX.*

*He has served as a faculty member in the Department of Thoracic/Head and Neck Medical Oncology at M. D. Anderson Cancer Center and University of Pittsburgh as Professor and Director of Head and Neck Cancer Program before he joined Emory University. He has been consecutively selected for last 18 years as a Best Doctor from Best Doctors in America since he was elected first in year 2003 and he has been also consecutively selected one of the Top Doctors from Castle Connolly Medical Ltd. and Atlanta Magazine for last 16 years since he was elected first in year 2005. Distinguished Leadership Award for Cancer Research from American Biographical Institute, Georgia Cancer Coalition Distinguished Scholar Award, the 2009 Yonsei University's Medicine Grand Prize Award, Honorary Professor at Central South University, China, the Frances Kelly Blomeyer Distinguished Endowed Chair in Cancer Research, and the 18th KBS Global Korean Award (in the category of Science and Technology). And he was also bestowed for Fellow of American Association of Advancement of Science (FAAAS) and many others.*

*Dr. Shin has also chaired numerous peer-review committees, including but not limited to the American Head and Neck Society, American Association of Cancer Research and the American Society of Clinical Oncology. He has also served as a member of many study sections at the National Cancer Institute, NIH and on the editorial boards (more than 15 scientific journals) including the Journal of Clinical Oncology, Clinical Cancer Research, Cancer Prevention Research, Molecular Cancer Therapeutics, International Journal of Oncology and others. He has published more than 360 articles in peer-reviewed journals (H-index of 70 and more than 27,000 citation numbers as of January 2021) in addition to more than 370 other publications including meeting abstracts, books, book chapters and monographs.*

*Dr. Shin's research has been well funded through funding from NIH/NCI (R01s, U01s, R21, etc.) and other funding agencies. Specifically he has been Principal Investigator of Emory University's Head and Neck Cancer SPORE program (Specialized Programs of Research Excellence), which*

*was awarded to Emory in 2007 by the National Cancer Institute (NCI). Another area of his interest has been nanotechnology based anti-cancer drug delivery in collaboration with several other investigators including biomedical engineers, chemists, material scientists, imaging experts and animal scientists.*

**In the 2023 annual report** I would like to highlight on immune based therapy for cancer, particularly, in the therapeutic tumor vaccine development for head and neck squamous cell carcinoma (HNSCC) in collaboration with several other investigators, specifically, basic immunologists (Drs. Periasamy Selvaraj and Ramireddy Bommireddy) and animal scientists.

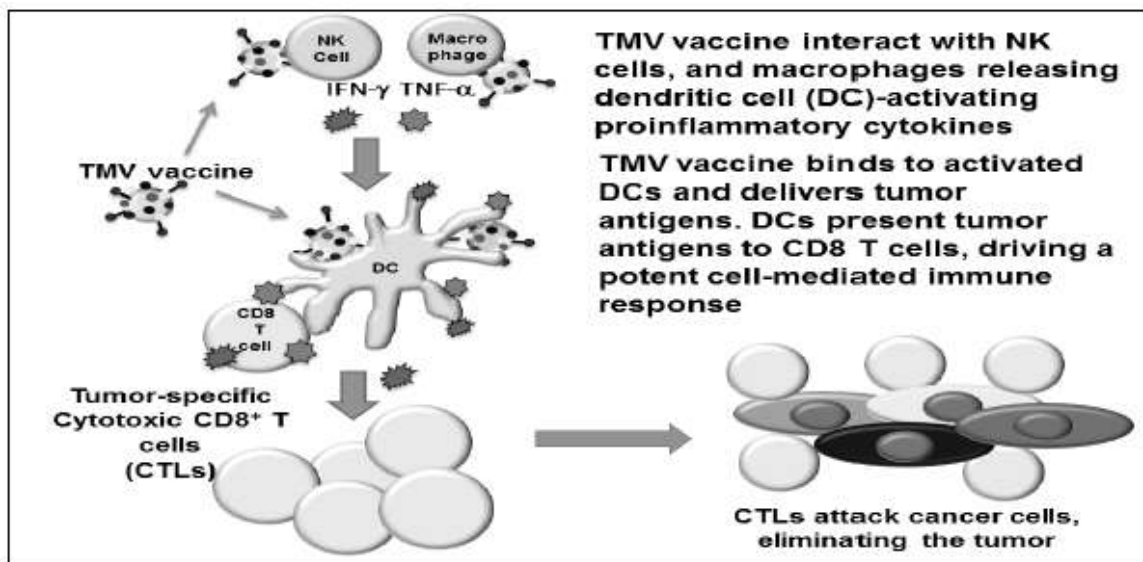
The standard of care for surgically resectable HNSCCs consists of surgery followed by radiation therapy (RT) or concurrent chemoradiation therapy (CRT). However, tumor recurrence and/or metastasis frequently occur after definitive treatment for locally advanced HNSCC, and survival for patients with recurrent and/or metastatic disease is very poor (1). Recently, immune checkpoint inhibitors (ICI), pembrolizumab, nivolumab (anti-PD-1 antibody) and others have been approved by the U.S. FDA for the treatment of recurrent and/or metastatic HNSCC and made significantly improve of the survival of patients compared with single or combination cytotoxic chemotherapy as the first or second line of the treatment (2,3,4). More recently, ICIs are being tested for initial treatments combined with CRT or in an adjuvant setting for locally advanced HNSCC (5,6). Since ICIs act via pre-existing anti-tumor T cell immunity, the lower response rate of HNSCC patients to anti-PD-1 antibody suggests that either the majority of HNSCC patients do not have pre-existing anti-tumor T cell immunity (innate resistance) or their tumors use other escape mechanisms (adaptive resistance). One possible way to induce de novo anti-tumor immunity is through vaccination with potent adjuvants to further enhance anti-tumor immunity in HNSCC (5).

Although therapeutic cancer vaccines have shown promising results in animal models, they have failed in human clinical trials including HNSCC over the years (6). The major reasons for failure of these approaches include: a) lack of strategies to include patient-to-patient variation in target tumor antigens, b) poor adjuvants and c) immunosuppression (5). For example, many of the previous vaccine approaches employed genetically modified allogeneic tumor cell lines, cell lines developed from patients, single tumor antigens or antigen-specific peptides as vaccine sources (7-10). These approaches induced anti-tumor immunity in patients, but the clinical benefit was limited because the tumors might have escaped immune attack due to their heterogeneous nature, as the vaccines did not represent all the variations found in each patient's tumor. To address these limitations, personalized vaccine immunotherapy approaches that include patient-specific tumor antigens with highly promising results are being developed. These include the use of patient-specific neoepitope peptide vaccines and whole tumor lysate pulsed dendritic cell (DC) adoptive cell therapy approaches (11). This suggests that the use of patient-specific antigens is critical in developing efficacious therapeutic cancer vaccines. In this context, we have developed a personalized autologous vaccine immunotherapy approach that is easy to prepare, store and administer, and importantly includes a patient-specific antigenic signature.

In fact, our group is currently developing membrane-based vaccine approach which is autologous vaccine immunotherapy using a novel protein transfer technology to incorporate glycosyl phosphatidylinositol (GPI)-anchored forms of immunostimulatory

molecules (GPI-ISMs) such as GPI-B7-1 and GPI-IL-12 onto tumor membrane vesicles (TMVs) (12-16). TMVs are derived from the patient's surgically excised frozen tumor tissues by homogenizing the tumor tissue and then centrifuging it over a sucrose gradient to isolate TMVs. Therefore, these TMVs are representing tumor heterogeneity with all kinds of different clones of various molecular characteristics from the patients' tumors. These TMVs will be further modified to incorporate membrane-anchored ISMs by a protein transfer process to produce TMV vaccine. Since the TMV contains the unique antigenic profile of each different clones of the given patient tumor, this personalized approach can provide an effective immunotherapy for HNSCC, wherein the target antigens will vary from patient-to-patient. Our TMV vaccine simultaneously delivers the patient's unique tumor antigen signature along with potent ISMs to the immune system to induce effective anti-tumor immunity. It is possible that GPI-B7-1 and GPI-IL-12 incorporated onto tumor cell membranes by protein transfer will enhance the delivery of TMVs to immune cells such as DCs, NK, and macrophages and activate them, resulting in a robust anti-tumor T cell immunity (**Figure 1**). These TMVs are uniform in size (300 to 500 nm) and are suitable for uptake and processing by antigen presenting cells, such as DCs (14-16). Further, IL-12 may provide a third signal for T cell proliferation. The TMVs are cellular plasma membrane vesicles and distinct from secreted immunosuppressive tumor exosomes

Although most immunostimulatory molecules and cytokines are not GPI-anchored, it is possible to convert them to GPI-anchored proteins using recombinant DNA techniques. The GPI anchor consists of a glycosylated moiety attached to phosphatidylinositol which contains two fatty acid tails, anchoring the protein to the cell membrane lipid bilayer (14).



**Figure 1.** Interaction of TMV vaccine with NK cells, macrophages and dendritic cells

Naturally occurring GPI-anchored proteins are widely distributed in mammalian cells. Studies by Dr. Selvaraj's laboratory have shown that purified GPI-anchored proteins can be spontaneously incorporated onto tumor cell membranes (13-15). This technique of incorporating purified GPI-anchored proteins onto live cell surfaces or isolated membrane vesicles is referred to here as protein transfer. This property of GPI-anchored molecules

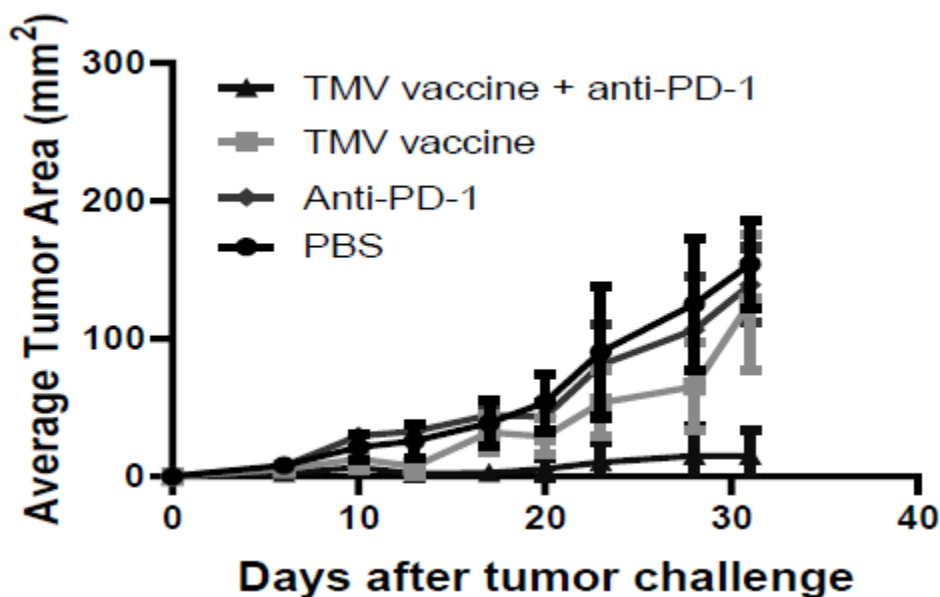
permits the manipulation of TMVs to display desired ISMs without the use of gene transfer (13-15). Tumor cells or TMVs expressing such modified GPI-ISMs are capable of inducing protective anti-tumor immunity (12-16). However, T cell marker CD3 and B cell marker CD19 are undetectable in the TMVs.

Based on these scientific premises, we hypothesize that membrane-based patient-specific vaccines such as our TMV vaccine either alone or in combination with ICIs will induce anti-tumor immunity against HNSCC and improve the overall survival of the patients. Our preclinical studies to test this hypothesis in murine HNSCC models show that immunization of mice with TMV vaccine induced immune infiltrates in the tumor and inhibited metastasis. In our recent study to determine whether mice immunized with TMV vaccine are protected (or no tumor growth) from tumor challenge (prophylactic setting), C3H/HeJ mice were administered with TMV vaccine every week for 4 doses and then challenged with SCC VII tumor cells after the last dose of vaccine administration. We have observed that SCC VII tumor growth is delayed in mice vaccinated with TMV vaccine compared to control PBS treated mice (17). In order to determine whether TMV vaccine induces anti-tumor antibody response, plasma was isolated and analyzed for antibody using SCCVII cells as target and FITC-conjugated anti-mouse IgG as secondary antibody by flow cytometry. However, interestingly, we did not observe any antibodies in the plasma collected after two doses of TMV vaccine. To test whether TMV vaccine inhibits tumor growth in a therapeutic setting, SCC VII tumor-bearing mice administered with TMV vaccine (100 µg/dose) every week (2 or 4 doses) starting 3 days after tumor cell challenge on the left flank. The data suggest that tumors in all five mice in the PBS control group grew fast while two doses of TMV vaccine failed to inhibit the tumor growth, however, four doses of TMV vaccine inhibited tumors in 2 mice, delayed tumor growth in 1 mouse and no effect in 2 mice. Tumor-free mice that survived for more than 60 days were rechallenged with SCC VII tumor cells and tumor growth was monitored. While all the control naïve mice developed tumors, none of the protected mice in the anti-PD1 mAb group and TMV vaccine therapy group developed secondary tumor growth suggesting a long lasting protective anti-tumor memory response induced by the TMV vaccine, and further the data represent the TMV vaccination works as dose dependent manner as we observed in breast cancer model (18,19).

We also tried to determine whether TMV vaccine inhibits oral SCC tumors in mice and have tested the efficacy of TMV vaccine on murine oral cancer (MOC) cell lines MOC1 and MOC2. MOC1 is a murine oral cancer cell line derived from a DMBA carcinogen induced tumor from C57BL/6 mouse. MOC1 is a slow growing tumor with infiltration of CD4+ and CD8+ T cells and is partially responsive to anti-PD-L1 mAb (17). MOC2 is also a murine oral cancer cell line derived from a DMBA carcinogen induced tumor in CXCR3 knockout C57BL/6 mouse. MOC2 is a highly aggressive metastatic model with negligible or no T cell infiltration in the tumors and is thus termed a cold tumor. MOC2 does not respond to anti-PD1 alone or the combination of anti-PD-1 + anti-CTLA-4 antibody therapy, indicating it as a representative model for patients who do not respond to ICI immunotherapy.

In our experiments, in order to see whether TMV vaccine is also effective against murine oral cancer (MOC) models, we have prepared TMV vaccine from tumors grown in C57BL/6 mice. TMV vaccine was administered 3 days after tumor challenge and anti-PD-1 antibody (clone RMP1-14, BioXCell) was administered starting day10 after tumor cell

challenge. The data suggest that while TMV vaccine or anti-PD1 antibody alone inhibits minimally MOC2 tumor growth, the combination of both agents significantly reduces tumor growth suggesting an additive effect in tumor growth inhibition in these mice (**Figure 2**). Combination therapy also significantly increased the survival of tumor bearing mice and eliminated tumors in 40% (2/5) of the mice. In the different experiment, the tumor free mice in the combination group were rechallenged with MOC1 tumor cells after 100 days of primary challenge to confirm the long-lasting anti-tumor immunity in vaccinated mice (17).



**Figure 2.** Tumor growth inhibition study for PBS control, TMV vaccine, anti-PD-1 anti-body, and combination of TMV vaccine with anti-PD-1 antibody in MOC2 mice study.

Therefore, our eventual goal is to induce anti-tumor immunity in HNSCC patients using the patient's own tumor tissue as the multi-antigen source which may prevent or treat recurrent and/or metastatic diseases thus increasing the survival of the patients. We may also try to determine the TMV vaccine efficacy in humanized mice using patient-derived xenograft (PDX) tumor tissue and autologous PBMC and to investigate biomarkers of anti-tumor response to predict the efficacy of treatment using genomics approaches from the humanized mouse studies.

We also plan to conduct early phases of clinical trial of TMV-based immunotherapy alone and/or in combination with ICI for recurrent and/or metastatic diseases in patients with HNSCC and other malignancies (20-23). We believe that completion of the proposed ongoing studies will advance a novel, personalized vaccine immunotherapy approach for patients with recurrent/metastatic HNSCC and possibly other solid tumors.

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# A Novel Frequency-free Movable Test Vehicle for Retrieving Modal Parameters of Bridges: Theory and Experiment

by Yeong-Bin Yang, Member EUAS

## Short Biography

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Dr. Yeong-Bin Yang received his Ph.D. degree from Cornell University in 1984. He is a member of Chinese Academy of Engineering, EU Academy of Sciences, European Academy of Sciences and Arts, and foreign member of Austrian Academy of Sciences. Currently, he is Honorary Dean of Civil Engineering, Chongqing University, and Professor Emeritus of National Taiwan University (NTU). Also, he is Editor-in-Chief of *International Journal of Structural Stability and Dynamics*, former President of Asian-Pacific Association of Computational Mechanics, and former Chairman of International Steering Committee of East Asia-Pacific Conference on Structural Engineering and Construction.

Previously, he was President of National Yunlin University of Science and Technology (Yuntech), Dean of NTU College of Engineering, Chairman of NTU Civil Engineering Department, and President of four societies in Taiwan: Institute of Engineering Education Taiwan (IEET), Chinese Institute of Civil and Hydraulic Engineering (CICHE), Society of Theoretical and Applied Mechanics (TAM), and Chinese Society of Structural Engineering (CSSE). He has published over 280 referred journal papers, focused on the following areas: structural nonlinear theory and analysis, vehicle-bridge interaction dynamics, train-induced wave propagation, and vehicle scanning method for bridges. In each area he has also published a monograph. He has a Google citation of 14777 times and H index of 60.

In 2022, Dr. Yang and his group have published the following papers:

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Typically, the Abstract for Ref. [3] is as follows:

### **A novel frequency-free movable test vehicle for retrieving modal parameters of bridges: Theory and Experiment**

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**Abstract:** Vehicle frequency and pavement roughness are two factors that used to adversely affect the vehicle scanning method for bridges. To tackle these at once, this study proposes the use of a novel frequency-free test vehicle in parked state for bridge measurement. In terms of measurement speed and data quality, the proposed technique is a trade-off between the moving vehicle and fixed sensor techniques, which has the advantage of movability. A test vehicle (single-axle) is considered frequency-free if its frequency is made far larger than those of the bridge of interest. The test vehicle will also

be free of pavement roughness if it is used in the parked (non-moving) state. Firstly, based on the bridge-vehicle transmissibility, a test vehicle is designed to have a frequency far beyond those of the bridge of concern, thereby enhancing the bridge frequency peaks. Secondly, lab tests were conducted for two axle-wheel assemblies under ambient vibration. Of interest is that the axle with PU tires shows a favorable random, small and even spectral distribution with no self frequency up to 20 Hz. The PU tires was then assembled as a part of the test vehicle that is self balanced in entity. Finally, the self-made test vehicle was calibrated on a benchmarked bridge and applied to the Xiamen Bus Rapid Transit system. Taking a three-span girder bridge of the system as an example, it was demonstrated that the frequencies, mode shapes and damping ratios of the first four modes of the bridge (flexural or torsional) can be well detected by the frequency-free test vehicle. Compared with the direct measurement, the proposed technique is equally accurate, but more competitive in efficiency and movability.

**Keywords:** bridge modal parameters; test vehicle; frequency-free; design; vehicle scanning method; vehicle-bridge interaction.

The Abstract for Ref. [8] is:

### **Internal Instability of Thin-Walled Beams under Harmonic Moving Loads**

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**Abstract:** Frequent resonance may result in excessive vibrations and endanger the safety of bridges. Firstly, the governing equations of motion are derived for the vertical, lateral and torsional vibrations of a mono-symmetric thin-walled box beam under a harmonic moving load. Then the resonance conditions are derived by letting the denominator of the response of concern equal to zero. For the mono-symmetric beam, the vertical resonance is uncoupled, but the torsional and lateral resonances are coupled. When in *vertical* resonance, the vertical motion of the beam will *diverge* by *growing to a maximum* during the acting period of the moving load. Similar phenomenon exists for the torsional-flexural resonance. A specific case occurs when the above two resonance frequencies coincide, for which the *critical length* of the beam can be determined. The phenomenon of simultaneous resonance is a kind of *internal instability* featured by the fact that the beam can transform repetitively from the vertical mode to the torsional-flexural mode, and vice versa, with no additional energy input. To avoid the inherent internal instability, a beam should be designed with a length *not equal* or *close* to the *critical length* presented in this paper. All the aforementioned resonances have been extensively studied for cases involving both harmonic and random moving loads and validated by the finite element analysis.

**Keywords:** dynamic instability, moving load, resonance, thin-walled beam, torsional-flexural resonance.