

Last April, the AIChE organized the 8th World Congress on Particle Technology in Orlando, Florida. We amassed over 100 poster presentations, 630 oral presentations, five plenary speakers, and over 25 keynote speakers covering 14 different topics in Particle Technology. Our overarching theme for this congress was "Expanding Boundaries," which may sound like a cliché, but it's really not. This conference focused on expanding boundaries regarding the topics, training, and even the meeting format. The topic areas spanned all aspects of particle technology with additional considerations for pharmaceuticals, environmental impact, sustainable energy, and safety. Furthermore, topic areas ranged from fundamental research in particle design, classification, interactions, and hydrodynamics to industrial applications in granular flow systems, separations, conveying and reaction processes.

However, that was not the only boundaries we encroached. We changed the meeting functionality itself. Most topic areas kicked-off with keynote speakers and presentation durations were dependent on topic area and determined by the area chairs. Realizing some topics needed to be covered in 15-minute presentation whereas others may require more time, areas had different presentations lengths. We were concerned that moving from topic to topic would be more challenging; but, each topic area could now present their material in a time frame that best supports their needs.

We also added lots of break-out areas and discussion space within the WCPT VIII conference space with the goal of stimulating discussion or just having a place to collect your thoughts from a recent presentation. Likewise, poster sessions were at the forefront of the conference. One poster session highlighted student research with a competitive "best poster" award while the other provided a venue for those last minute revelations.

With all of this, we hoped to stimulate discussion on not only where particle technology has been but also where it needs to go. The results were a success. Not once did I hear that the presentations were too short or too long or that a mixed schedule impeded jumping from one technical area to another. To be honest, at many of the conferences that I attend, most papers don't start on time anyway.

The break-out areas were also a success judging by how full they were during coffee breaks. Having the training sessions, poster sessions and the exhibit integrated into these space also revealed significant benefits. Poster sessions were well attended, and the exhibitor space also showed substantial and focused activity. Training sessions were never too far from all this excitement.

Hence, it is my biased opinion that the WCPT VIII was a good, value-added conference. The AIChE Team, led by Stéphanie Orvoine-Couvrette, made this easy. Ilia Killeen and Michelle Marsnick made sure the hotel delivered on what they promised, which was not an easy task. The WCPT VIII Advisory Board provide four years of support and guidance to ensure we had the right preliminary speakers, topic-relevant keynote speakers, and a schedule that was functional.

Finally, I have to thank our sponsors who made all this possible. With AIChE's Evan Flach coordinating sponsorship, we had notable companies such as CPFD-Software, Chevron, IFPRI, LUM, PSRI, Siemens, ANSYS, Corteva, ExxonMobil, PSE, SABIC, Bioconjugate Chemistry, ACS SyntheticBiology, GranuTools, NETL, and Elsevier provide the funding we needed. The result was a reasonable registration cost that included coffee, tea, etc. during breakouts, lunch during posters sessions, and allowed us to finish the conference with a dinner under the stars listening to zydeco music.

Five months after the conference, all that is left is publishing key WCPT VIII papers into a special issue of *Powder Technology*. We have 55 papers in the queue, and I am thankful for another group of colleagues, my reviewers. They are now volunteering their valuable time to ensure we have a special issue that meets and exceeds all peer-reviewed publications for "Expanding Boundaries."

So, would I do this again? I would, but with the knowledge that is having the right team and a proactive and effective meeting organizer is paramount in making you want to do this again. Thank you, everybody, for all your help, suggestions, and guidance. World Congress in Particle Technology IX will be in Spain in 2022!

#### **Editorial:**

#### Importance of Volunteerism

The foundation of every successful organization or an organized event is an army of unsung volunteers who contribute their time, effort and intellect towards its success. The spirit of volunteerism is imbibed in our personal and professional identities, and our sense of belongingness to this technical community. We should think of it as a way to *Pay Forward*. For the more "seasoned" members, it is a way to share their wisdom, experience and knowledge while the "upcoming" generation can bring enthusiasm, energy and creative ideas to the table.

Volunteerism should be fun and rewarding so each of us must figure out and seek our own niche. No effort or contribution is insignificant if it is executed in the right spirit. At the end, we must leave our technical community better and stronger than what we inherited. *PTF needs you...* 

Shrikant Dhodapkar, Newsletter Editor

Fellow, The Dow Chemical Company

# In this issue...

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- WCPT9 Announcement
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- ♦ PTF Elections
- ♦ PTF Organization

# PTF Executive Committee Elections

Executive Committee members act as a liaison to the PTF and play an important role in improving PTF via activities such as recruiting new members/officers, judging posters at the annual meetings and helping in other PTF standing committees.

You can cast your vote online.

More information on candidates...

# **Recap - World Congress on Particle Technology 8**



The 8<sup>th</sup> World Congress on Particle Technology, held April 22-26, 2018 at the Orlando World Center Marriott in Orlando, FL, brought together nearly 900+ attendees from around the globe. With over 600 papers and presentations, 25 keynotes and 5 featured plenary speakers, the technical program stimulated discussions on the forefront of research in particle science and technology. The conference was chaired by Ray Cocco, President and CEO of Particulate Solid Research, Inc. (PSRI) and organized by AIChE.

		600+ Oral Presentations
900+ Attendees	Ē	25+ Keynotes
		5 Plenaries
Traveled from <b>34 countries</b>	·	80+ Poster Presentations
		22 Exhibiting Companies



Program summaries, video interviews, photos, proceedings and more are available on www.wcpt8.org.

# **Recap - World Congress on Particle Technology 8**

### **PLENARIES**

Plenary speakers highlighted the 8<sup>th</sup> World Congress on Particle Technology. Clockwise from top left: Heinrich Jaeger (University of Chicago) spoke about contact charging in granular materials. At the final plenary, Karl Jacob (The Dow Chemical Company) delivered "An Industrial Perspective on the Future Needs in Solids Processing Research and Education." Jinghai LI (Chinese Academy of Sciences) discussed mesoscience as a new paradigm of particle technology. Marc-Olivier Coppens (University College London) proposed nature-inspired chemical engineering as a pathway to particle technology innovation. Alissa Park (Columbia University) spotlighted novel nanoscale particulate systems for carbon capture and conversion.



## STUDENT POSTERS AWARD WINNERS

Congratulations to the winners of the World Congress on Particle Technology Student Poster Competition, supported by Corteva Agriscience<sup>™</sup>, agriculture division of DowDuPont<sup>™</sup>.

**1st Place:** Atomically Deposited Sintering Aids: Assessing the Effects of Alumina Particle ALD on the Sintering and Performance of SOFC Electrolytes and Dental Ceramics, Rebecca O'Toole, *University of Colorado at Boulder* 

**2nd Place:** Systems Integration for Dry Granulation Based Continuous Pharmaceutical Tableting, Sudarshan Ganesh, *Purdue University* 

**3rd Place:** Understanding Phase Transition of Acetaminophen in the Bulk and Surface of Acetaminophen, Hanane Abouhakim, *University of Leeds* 



# **Roving Camera...**









www.aicheptf.org

# WCPT8 - Organizing Committee

Special thanks to the organizing committee...

# **Conference Chair**

Ray Cocco President & CEO Particulate Solid Research, Inc. (PSRI)

# **Advisory Board**

Alissa Park, Columbia University Benjamin Amblard, IFPEN Tim Bell, DowDuPont Ron Breault, National Energy Technology Laboratory David Craig, Jenike & Johanson, Inc. Rajesh Davé, New Jersey Institute of Technology Shrikant Dhodapkar, The Dow Chemical Company Thierry Gauthier, IFPEN



Matt Hankosky, Particulate Solid Research, Inc. Karl Jacob, The Dow Chemical Company Mayank Kashyap, SABIC George Klinzing, University of Pittsburgh Gary Liu, DuPont Raffaella Ocone, Heriot-Watt University Stéphanie Orvoine-Couvrette, AIChE Eric Shen, ExxonMobil Al Weimer, University of Colorado at Boulder

# Area Chairs

Area	Chairs		
Applications for Sustainable Energy & Environment	Eric Shen	Alissa Park	
Applications of Particle Technology for Pharmaceuticals	Chi-Hwa Wang	Brenda Remy	
Applications of Solids Processing Unit Operations	Haim Kalman	Bruce Hook	
Combustible Dust Safety – co-sponsored with 14th GCPS	Konaur Manjauth		
Education	Mayank Kashyap	George Klinzing	
Fluidization & Multiphase Flow	S.B. Reddy Karri	Tony Bi	
Handling & Processing of Granular Systems	David Craig	Shrikant Dhodapkar	
Particle-Based Separations: Fundamentals & Applications	Ben Freireich	Alvaro Ramirez Gomez	
Particle & Bulk Powder Characterization	Al Weimer	Younjune Park	
Particle Classification	JunWu Wang	Benjamin Amblard	
Particle Design	Mark Jones	Yongsheng Han	
Particle Interactions	Stefan Heinrich	Shuji Matasusaka	
Particle & Nanoparticle Functionalization	Fanxing Li	Allan Issangya	
Special Topics in Particle Technology	Muhdu Kodam	Paola Lettieri	
Poster Sessions	Tim Bell	Ray Cocco	

# 9<sup>th</sup> World Congress on Particle Technology

The World Congress on Particle Technology (WCPT) is the world's major scientific congress for particle and bulk solids technology. It is an international forum for research, technological development and innovation in new technologies. Research advances presented and discussed in every edition of WCPT have found many industrial applications in different fields (chemical, pharmaceutical, food production, mining, agricultural, energy ...). Held every four years since its inception in 1990, it is intended to stimulate discussions on the forefront of research in particle science and technology. Each WCPT edition is celebrated in a different continent, the previous one (WCPT8) was celebrated in Americas, in Orlando (Florida) on April 22-26, 2018. WCPT8 counted with over 900 participants (speakers, chairs, exhibitors...), 630 oral presentations and over 100 posters, more than 25 keynote lectures, and 5 plenary lectures. Participants attended from 34 countries, and there were present 22 exhibiting companies.

The next World Congress on Particle Technology (WCPT9) will be celebrated in Europe in Madrid (Spain). It will be organized by the Spanish Association of Chemists and Chemical Engineers (ANQUE) with the support of the European Federation of Chemical Engineering (EFCE), the Spanish Chemist Industry Federation (FEIQUE), the Society for Chemical Engineering and Biotechnology (DECHEMA) and the Spanish Forum of Chemistry and Society (FQS).

This has been possible due to a bottom-up and integrative initiative of eight working parties from the European Federation of Chemical Engineers (EFCE) (WP Agglomeration, WP Comminution and Classification, WP Characterization of Particulate Systems, WP Crystallization, WP Drying, WP Mechanics on Particulate Solids, WP Mixing and WP Multiphase Fluid Flow) which started in 2015, in Nice (France), during the celebration of the 10<sup>th</sup> European Congress of Chemical Engineering (ECCE10). There, the III International Symposium on Handling and Hazards of Particulate Industry (HANHAZ2015) was organized as a joint event and as an incipient collaboration of 3 WPs of Materials in EFCE (WP Characterization of Particulate Systems, WP Crystallization and WP Mechanics on Particulate Solids). This effort was fruitful and during the celebration of the 10<sup>th</sup> World Congress on Chemical Engineering (WCCE10) in 2017, Barcelona (Spain) another joint event, the I International Conference on Processing, Handling and Characterization of Particulate Materials (PARMAT2017), was organized by 8 EFCE-WPs, strengthening the links between these WPs specialized in different areas of particle technology. For WCPT9, Prof. Carlos Manuel Negro Álvarez (Congress Chair), from the Complutense University of Madrid, Prof. Álvaro Ramírez-Gómez (Scientific Chair), from the Technical University of Madrid and Dr. Hermann Feise (International Advisory Committee Chair) from BASF, together with 8 EFCE-WPs will define the strategy that will aim to promote the inclusiveness of the industry and the academia as in previous WCPT editions. The main aim will be to engage the whole community on particle technology in the different continents and their countries through an outreach and promotion program specifically designed for this purpose.

# Join us in Madrid!

For further information please contact: **Prof. Carlos Manuel Negro Álvarez** (<u>cnegro@ucm.es</u>) **Prof. Álvaro Ramírez-Gómez** (<u>alvaro.ramirez@upm.es</u>) **Dr. Hermann J. Feise** (<u>hermann.feise@basf.com</u>)



# WCPT8 Plenary Lecture: Prof. Marc-Olivier Coppens

# Nature-Inspired Chemical Engineering – A Pathway to

# **Innovation in Particle Technology**

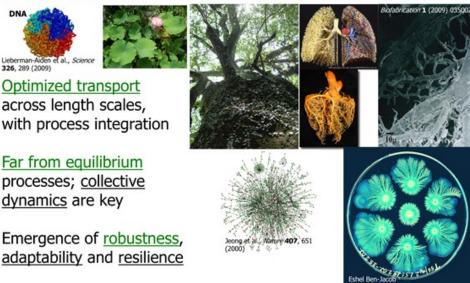
**Marc-Olivier Coppens** 

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Some of our most challenging problems in manufacturing, energy, sustainability and healthcare relate to particle technology. The field remains highly empirical, with many unsolved technical and scientific problems, due to the complexity of particle structures and dynamics, with nonlinear interactions that include a wide range of time and length scales. The latter extend from interparticle pores, to grains, aggregates, and vessels, where fluid-particle interactions often add to the multiscale complexity. Innovation is required to provide step-change solutions to such complex problems, especially to be applicable in the practical context of industrial production, product design and use. We propose **nature-inspired chemical engineering (NICE)** as a pathway to such innovation.

A principal reason is that nature holds a treasure trove of ideas to inspire solutions to technological problems, because of the similarities of key requirements in technology (like process scalability, efficiency, and robustness) to those in nature, where solutions have evolved that differ greatly from those currently employed in technical applications, with properties that are exceptionally more advanced. Examples include the scalable growth of trees, the hierarchical architecture that makes our lungs so efficient (minimum loss of metabolic energy during breathing), and the self-organising principles that render bacterial communities resilient or lead to remarkably regular patterns in the sand by the pulsating action of the wind, despite of (or embracing!) the complexity of these systems. Figure 1 illustrates the multiscale architecture and dynamics of nature, and some of its associated, emerging properties.



### Scalable architecture: molecules - cells - organ - organism/system

Figure 1: The architecture and dynamics of nature – and associated, emerging properties.

However, learning from nature is not straightforward. Typically, nature's best solutions to a problem extend beyond first appearances and superficial similarities, and, so, observing nature in search of solutions should go beyond mimicking – "biomimetics," in a narrow sense. Gaining inspiration from nature is most effective in solving technical problems when we have sufficient fundamental understanding, which can then be appropriately translated within the context of an application. As in any product and process design, the real power of nature-inspired design requires moving beyond imitation, and appreciating the technical, industrial or societal context.

While out-of-the-box thinking is desired to drive innovation, and observing nature can spur creative thought, a systematic methodology is required to guide us from nature to technology. Core to the NICE approach is the mechanistic, methodological translation of fundamental principles underpinning desirable properties in natural systems to technology, by extracting fundamental **concepts** (e.g., what makes the lung so efficient, scalable and robust?) to inform nature-inspired **designs** (e.g., a fractal, branching distributor with a finite scaling range, and optimised length and diameter ratios of its channels, similar to the lung) that are not blindly adopted, but **adapted** to the context of a practical application (e.g., in fluidization, catalysis or in fuel cell technology). Those steps involve experimentation and computation, but also understanding of the design context: the time scales, available materials and other available resources, as well as economics and other constraints. **Implementation** is increasingly enabled by immense progress in materials science and engineering, additive manufacturing, computational speed, and advanced control systems. Thus, NICE introduces creativity by virtue of its methodology, together with scientific fundamentals and technical engineering,

This step-wise methodology (from observation to concept, design and implementation with adaptation) renders practicality to the NICE approach for problem solving, but, to make the approach truly versatile (beyond isolated, *ad hoc* solutions), we also need to know *how* we "observe nature" and extract those interesting principles. This is why we advocate a **thematic** approach, one that builds on ubiquitous fundamental mechanisms – a bit like a nature guide. Without guide, we might look, but we do not see what is hidden in the rainforest. There are many ways to look, but we will use engineering eyes, since we aim to solve engineering problems. These eyes go beyond purely descriptive biology or geology, but include the mechanistic foundations of physics, with the sense of scale and solution-oriented systems perspective that is the cornerstone of engineering.

Three prominent mechanisms that underpin three corresponding themes in the NICE approach are: (T1) **Hierarchical transport networks**, (T2) **Force balancing** and (T3) **Dynamic self-organisation** [1]. More could be added, but these three are remarkably prevalent. Figure 2 illustrates the NICE approach on the basis of these themes, and the systematic methodology, from concept to design and implementation. The examples in Figure 2 are illustrative for the themes and breadth of application areas.

The first example, related to (T1) is a lung-inspired fuel cell [2]. A self-similar, scalable, fractal branching airway tree links the trachea to the bronchioles. There are 14-16 levels of self-similarity in an adult human lung, in which the cube of the diameter of each mother branch is the sum of the cubes of the two daughters. Deeper down the airway tree lies a uniform distribution of alveoli in the acini, which exchange oxygen and CO<sub>2</sub> with the blood stream. Remarkably, this specific hierarchical cascade leads to minimum entropy production (or a minimal loss of metabolic energy during breathing). The transition from fractal to uniform happens just where the Péclet number, Pe~1, thus convective flow transitions to diffusion as the dominating transport mechanism for air. In earlier NICE work, we had already used the fractal concept of the branching architecture of lungs and botanical trees to design a scalable, branching fluid injector, immersed in fluidized beds, hereby reducing the bubble size, promoting local particle-fluid contact and mixing, facilitating scalability, and increasing overall efficiency in catalytic fluidized bed reactors [1,3]. We also designed and synthesised hierarchically structured porous catalysts with an optimal pore size distribution, including wide pore channels with optimised size, apart from the nanopores where most of the catalysis occurs, and thus minimise diffusion limitations, similar to what is observed in alveoli or leaves [1,4]. Now, demonstrating the versatility of the NICE approach, we use the same mechanism of an optimised, scalable hierarchical transport network employed in lungs to address transport limitations and scalability issues in fuel cells [2]. To translate the described concept into a design for fuel cells, an optimised fractal architecture of flow channels in the fuel cell's flow plates is realised using additive manufacturing, while an optimal porous electrocatalyst architecture can be synthesised, using progress in materials chemistry. Both steps are guided by computational optimisation, using the parametric relationships learnt from the optimal structure of the lung. The result is a scalable fuel cell design with highly increased current density (A/cm<sup>2</sup>) and, for PEM fuel cells, Pt catalyst utilisation (kW/g Pt).

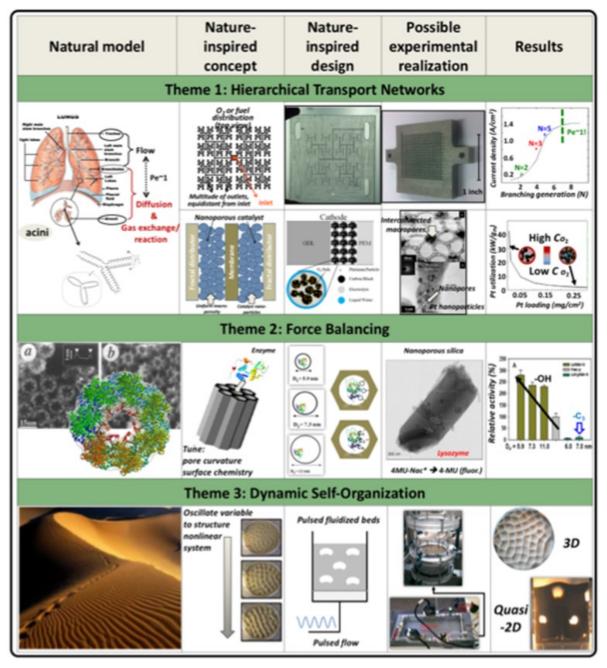


Figure 2: The NICE approach applied to particle technology, and beyond.

The second example relates to **(T2)**, addressing problems of *catalyst performance* (activity, selectivity and stability) by utilising *nano-confinement* effects observed in chaperones. The latter are complexes found, e.g., in *E. coli*, which help to fold proteins –bringing enzymes in their three-dimensional shape important for catalysis. These supramolecular complexes act thanks to spatial confinement in a nanochannel, barely wider than the enzyme, but also electrostatic interactions. It is the subtle balancing of forces that leads to the stabilisation of the enzyme inside the cavity. At a large scale, balanced mechanical forces provide superior robustness of trees and bones, and serve as inspiration for architects, while, at the micro– and nanoscale, other forces, like capillarity, electrostatics or polarisation, come into play, which are often subtly balanced with superior cooperative effects, such as in the chaperone. By designing mesoporous silica with a tuned pore size, enzymes (but also other catalytic complexes) could be stabilised on the curved pore surface, avoiding their denaturing by combining steric confinement with electrostatic interactions. Like in chaperones *both* the steric effects (fitting nano-size) and the electrostatics matter [1]. In Figure 2, this is illustrated via the activity of stably immobilised lysozyme within ordered mesoporous silica SBA-15, which, when both effects come into play (a function of pH), leads to increased activity, above that even of free lysozyme in solution for a hydrolysis

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reaction, while the activity would decrease for a propylated, hydrophobic surface [4,5]. Such effects can be utilised for healthcare applications as well, for example for porous particle hosts used in controlled, targeted drug delivery [6].

The third example in Figure 2, related to (T3), demonstrates a way to intensify the operation and "structure" fluidized bed reactors, by using a pulsating gas flow. Regular patterns form on the surfaces of dunes and sandy beaches, as a result of the perturbations caused by gusty wind or crashing waves. Such perturbations structure the complex granular dynamics to create ordered patterns, a form of dynamic self-organisation that results from energy dissipation, due to drag and friction. Similarly, when oscillating the gas flow in a bubbling fluidized bed, there is a window of amplitudes and frequencies that transform the chaotic bubble flow to a regular one: square and other regular patterns in shallow 3D beds, and triangular tessellations of rising bubbles in deep, quasi-2D beds [1,3,7-9]. The physics of pattern formation have been extensively explored in the context of vibrated granular matter, but in fluidized beds, we have only very recently started to build some understanding on the exact nature of pattern initiation and propagation in this inherently multiphase system [7-9]. The patterns relate to the mesoscopic physics of the system, which oscillates between fluid-like and solid-like when the fluid flow periodically rises and drops. Such viscoplastic behaviour is notoriously difficult to simulate, and current formulations of two-fluid models (TFM) are not yet able to reproduce the experimentally observed regular bubble patterns, while discrete element methods combined with computational fluid dynamics (CFD-DEM) can [7]. The bubble size could even be manipulated by changing amplitude and frequency of pulsation. Universal behaviour was discovered in the threshold for pattern formation for a broad range of Geldart B particles [8]. The regular pattern formation can thus be used as a fingerprint for multiphase computational modelling approaches, as many traditional approaches that could predict average bubble size or distribution fail the "fingerprint" of pattern formation [7]. Thus, new fundamental insights are obtained that guide model development for fluidized bed operation and design [9]. In addition, pulsation may avoid flow maldistribution and facilitate scale-up by structuring the fluidized bed hydrodynamics [10].

In **conclusion**, the NICE approach draws lessons from nature to guide innovation in particle technology. Its power stems from its fundamental mechanistic basis, as well as its systematic step-by-step methodology, which allows the practitioner to translate mechanistic insights underpinning desirable properties in nature to concepts and designs. It does this whilst appreciating the different context of a technological application and the original natural environment. By being thematically organised according to omnipresent fundamental mechanisms (hierarchical transport networks, force balancing, and dynamic self-organisation), it is exceptionally versatile. Validation of the NICE approach in a number of examples thus serves as a basis for new applications in other areas. Hence, the opportunities of NICE, like the infinite wonders of nature, are vast – and thus we advocate to take nature as our guide to help us develop more sustainable solutions for technology.

#### Further reading:

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# WCPT8 Plenary Lecture: Prof. Jinghai LI

### Mesoscience – Opening a New Paradigm of Particle Technology

Jinghai Ll

**Professor and President** 

National Natural Science Foundation of China



Professor Jinghai LI delivered his plenary lecture entitled "Mesoscience – Opening a New Paradigm of Particle Technology" in the 8th World Congress on Particle Technology (WCPT8) 2018. Prof. LI received his B.S. from the Department of Thermal Engineering of the Harbin Institute of Technology in 1982, where he entered a master's degree program in the same year. He obtained his Ph.D. from the Institute of Process Engineering (IPE), Chinese Academy of Sciences (CAS) in Beijing in 1987. From 2004 to 2016, he was a vice president of CAS in charge of strategic study and member election. In February 2018, he was appointed the president of National Natural Science Foundation of China (NSFC). He established the Energy-Minimization Multi-Scale (EMMS) model, which has been successfully applied for multiphase flow systems in wide areas of industry processes. Currently, he is devoted to promoting the concept of mesoscience based on the EMMS principle of compromise in competition as a transdisciplinary science.

The plenary lecture by Prof. Jinghai LI started with the common challenges, i.e., the mesoscales in mesoregimes, followed by case studies on both material and reactor levels encountered in particle technology and relevant research areas, then he pointed out the possible common principle to meet the challenges, the EMMS principle of compromise in competition, finally, he highlighted two outputs based on such principle, one is the virtual reality featuring real-time simulation and the other is the mesoscience as a transdisciplinary science.

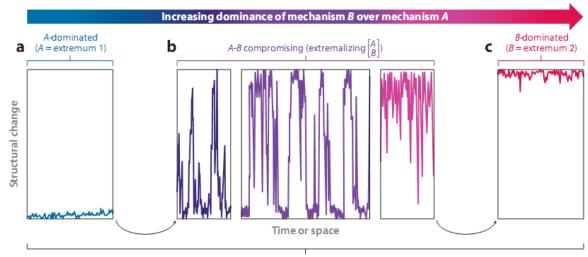
Mesoscale phenomena exist in between "unit" scales and "system" scales at different levels of the real world. For particle technology, such levels mainly refer to the material and reactor levels. Understanding of complex processes at the mesoscales, e.g., interphase drag and mass transfer, characterized by spatiotemporal dynamic structures, is a common challenge.

Initiated by recognizing the importance of clusters of particles in a fluidized bed, Prof. Jinghai LI reviewed the three decades of research on mesoscales of particulate systems at IPE-CAS, which was exemplified by the EMMS model specific for gas-solid fluidization, where he established the stability condition or variational function for particle clustering phenomenon. The EMMS model finds its wide application especially after being integrated into computational fluid dynamics (CFD). In extending the EMMS model to many different complex systems, such as gas-liquid, turbulence, gas-liquid-solid, emulsion, material preparation, protein, and catalysis systems, covering many industrial processes, to mention but a few, maximizing iso-paraffins (MIP), methanol to olefins (MTO), polyethylene and so on, he proposed the EMMS principle generally for different complex systems, featuring compromise in competition between different dominant mechanisms in physics and formulated as multi-objective variational problem in mathematics.

Prof. LI addressed that all meso-scale problems or processes are dominated jointly by at least two mechanisms, e.g., mechanism A = extremum 1 and mechanism B = extremum 2, for simplicity of discussion. The A- and B-dominated states coexist in an alternating manner with respect to both time and space in the mesoregime. Therefore, the variational criterion for the system can be physically expressed as compromise in competition between dominant mechanisms, and can be mathematically formulated into a multi-objective variational problem, that is, the EMMS principle.

The EMMS principle bridges variables and processes at different scales and reflects the consistency of underlying logic and structural features among the problem (complex systems), modeling (multi-objective variational optimization), computer hardware and software. As a result, the EMMS principle can facilitate the realization of EMMS diagram with high accuracy, high speed, and large scale in applications. This EMMS paradigm has two main features: similarity between logic and structure, and a computation strategy of "first globally, then regionally, and finally, locally in detail." These two features enable the optimization of the accuracy, speed, and scalability of computation and thus lay the foundation to realize the virtual process engineering (VPE). According to the EMMS paradigm, a platform for the demonstration of VPE was constructed at IPE-CAS. Over this platform, one can perform realtime computation and control experiment simultaneously, enabling online comparison between them, thus, providing a very powerful tool for future research and development.

In the last section of his lecture, Prof. LI summarized the rationale for mesoscience: the common physical principle, i.e., the compromise in competition, the unified mathematical formulation, in terms of multi-objective variational problem, together with the huge potential in application. These three aspects are believed to drive the EMMS principle a leap to the mesoscience. This new transdisciplinary science is not only for chemical science but bridge the missing links in the logic and landscape of current knowledge system. NSFC launched the major research plan on mesoscience in recognition of the critical importance and rapid development over this new field. In perspective, Prof. Li summarized two directions in urgent demand in this new field of R&D: first, the effects of mesoscale structure on transport and reactions, with examples of catalytic mechanism, crystallization process, change of states, energy storage etc.; second, the common principle of mesoscience in both physics and mathematics. Although a general framework for mesoscience is on the horizon in Prof. Li's presentation, he also stressed several common issues to be confirmed: 1. Number of dominant mechanisms, whether we can have more than two mechanisms? 2. Level specific physical expression of the dominant mechanisms. 3. Interaction at interfaces. 4. Solution of multi-objective variational problems. 5. Regime transitions which are critical to distinguish multiple extremum compromise and single extremum dominance. In the concluding remarks, Prof. LI highlighted the mesoscience as an alternative way to cope with complexity and stressed again that the traditional approaches are not sufficient. We are on the horizon of the new era of R&D.



#### - Prof. Wei Wang and Dr. Fei Li

#### **Regime-specific behavior**

Figure 1 Three regimes occur successively as the relative dominance of mechanism B over mechanism A changes: (a) A-dominated: If A = extremum 1 plays a dominant role and B = extremum 2 is suppressed, B has little influence on the structure of the system. (b) A and B display compromise in competition in the mesoregime: With increasing dominance of B = extremum 2 over A = extremum 1, there is a critical condition at which A loses its absolute dominance over B and must compromise with B. This leads to the alternate appearance of a B-dominated-like state and an A-dominated-like state [not necessarily fully dominated with respect to time and space, giving rise to complex dynamic changes at the mesoscale of a system. (c) B-dominated: When the dominance of B reaches another critical value, A will be completely suppressed, losing its influence on the structure, whereas B is fully realized. (Li et al., 2016)

# WCPT8 Plenary Lecture: Prof. Alissa Park

### Towards Sustainable Energy and Materials: Carbon Capture and Conversion using Novel Liquid-like Nanoscale Hybrid Particulate Systems

A.-H. Alissa Park Director, Lenfest Center for Sustainable Energy Department of Earth and Environmental Engineering Columbia University



The atmospheric concentration of  $CO_2$  has naturally fluctuated on the timescales of ice ages. Concerns, however, stem from the recent dramatic increase in  $CO_2$  concentration, which coincides with global industrial development. This rise is mainly due to the high use of fossil fuels during power generation and chemical production. In order to meet the ever-increasing global energy demands while stabilizing the  $CO_2$  level in the atmosphere, the development of carbon capture, utilization and storage technologies is one of the critical needs.<sup>1</sup> In particular, there has been significant efforts to develop  $CO_2$  capture solvents and some have shown very promising results. For example, amine-based aqueous solvents can effectively and selectively capture  $CO_2$  from flue gas of coal-fired power plants. Unfortunately, the energy requirement for the current aqueous solvent systems is still considered to be too high leading to the estimated 30% reduction in the power plant efficiency. Thus, efforts have been focused on the development of second and third-generation  $CO_2$  capture solvents which are often water-free or water-lean.

#### Design and Synthesis of Novel Nanoscale Hybrid Particulate Systems for CO<sub>2</sub> Capture

There are a number of water-lean and waterless solvent options,<sup>2</sup> such as ionic liquids (ILs), CO<sub>2</sub>-triggered switchable solvents (i.e., CO<sub>2</sub>-binding organic liquids and reversible ILs), and nanoparticle organic hybrid materials (NOHMs) that are currently being developed to reduce the high parasitic energy challenge with novel materials design for CO<sub>2</sub> capture. NOHMs and ILs have promising properties, such as negligible vapor pressure and high chemical tunability but they are still being investigated in a lab-scale. For any of these CO<sub>2</sub> capture materials to be successful they must deliver: (1) high CO<sub>2</sub> capacity and selectivity, (2) low energy and water consumption, (3) low costs, (4) minimal environmental impacts, and (5) high degree of process intensification as well as scale-ability and adaptability for a wide range of very different applications.

Liquid-like NOHMs<sup>3-5</sup> (Nanoparticle Organic Hybrid Materials) are an emerging class of self-suspended nanoparticles with high CO<sub>2</sub> capture capacity, particularly when functionalized with amines or other bases. NOHMs comprise a polymeric canopy tethered to surface-modified nanoparticles (Figure 1)<sup>3</sup> and have great thermal stability and negligible vapor pressure. NOHMs can be designed with unique nanoscale structures to shape the way CO<sub>2</sub> is incorporated into the NOHMs via entropic effects.<sup>3-5</sup> A wide range of nanocores (e.g., SiO<sub>2</sub>, TiO<sub>2</sub>, magnetic nanoparticles) and polymers have been used to synthesize NOHMs with the maximum grafting density of polymers at around 3.8 chains/nm<sup>2</sup>. As shown in Figure 2, NOHMs can be designed with high CO<sub>2</sub> capture capacity as increasing the amount of amine functional groups.

While their CO<sub>2</sub> capture efficiency and selectivity are great, like other anhydrous CO<sub>2</sub> capture solvents, NOHMs

suffer from high viscosity. NOHMs' viscosity (300-10000 mPa  $\bar{s}$ ) is orders of magnitude higher than aqueous amine solvents.<sup>6</sup> Thus, there has been a number of innovative studies to reduce the viscosity of water-lean CO<sub>2</sub> capture solvents or overcome the mass transfer limitation caused by the high viscosity.

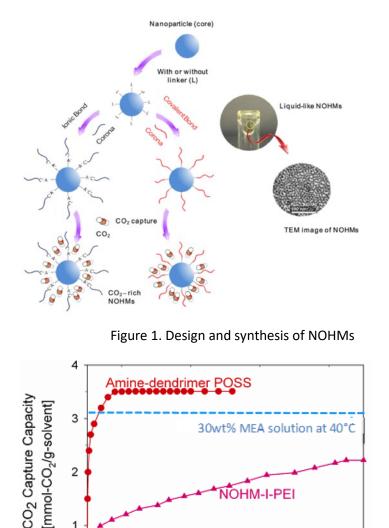


Figure 2. CO<sub>2</sub> capture using NOHMs with different amine loading

40

Time [hour]

20

**NOHM-I-PEI** 

NOHM-I-tPE

80

60

#### Microencapsulation of Water-lean CO<sub>2</sub> Capture Solvents with High Viscosity

2

0 0

There are three main viscosity control strategies that are currently being studied: encapsulation, H<sub>2</sub> bond control<sup>7</sup> and equilibrium shifting. Encapsulation of CO<sub>2</sub> capture solvents within a gas permeable polymer shell is a physical means of overcoming the viscosity challenge and microencapsulation of aqueous carbonate solutions and ILs has recently been reported.<sup>8</sup> As shown in Figure 3, we have developed a unique 3-D structured microfluidic device that can effectively produce the NOHMs-based capsules without internal coating needed for wetting control. NOHMsbased capsules exhibited a remarkable thermal stability and good compatibility with a wide range of humidity conditions, which would enable their application in flue gas capture with thermal regeneration (up to 150 °C). It was interesting to find that the mass transfer resistance through the shell layer was minimal even at the shell thickness of 60 μm. An optimal core size was determined based on the mass transfer kinetics as a function of NOHMs concentration and it was 380 µm for 10 wt.% NOHMs capsules. In this case, the CO<sub>2</sub> absorption rate was improved by 30 times compared to the bulk aqueous NOHMs. The microencapsulation of NOHMs provided an innovative approach to water-lean CO2 solvents with high viscosity combining the benefits of both liquid solvents and solid sorbent into one system.

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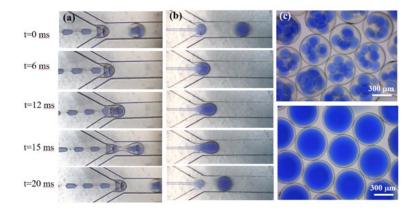
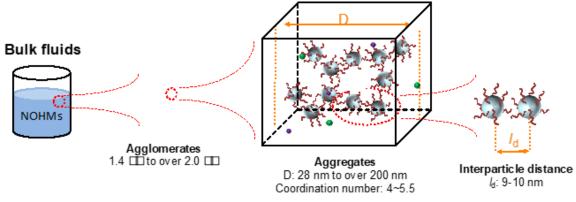


Figure 3. Encapsulated liquid particulate systems produced using a microfluidic device

#### Combined Carbon Capture and Conversion-to-Chemicals and Fuels using Renewable Electrons

Another interesting discovery that has recently been made on NOHMs is that it exhibits uniquely enhanced conductivity compared to untethered polymers. As the cost of renewable energy rapidly drops and intermittency of its supply starts to limit market penetration, the production of chemicals and fuels from  $CO_2$  using renewable energy becomes economically feasible and useful for load balancing and energy storage. Thus, various reaction pathways to convert  $CO_2$  to chemicals and fuels are currently being developed including the electrochemical reduction of  $CO_2$  to chemicals. One of the less studied issues associated with the electrochemical pathway is the low solubility of  $CO_2$  in aqueous electrolyte. Thus, the development of novel electrolytes with high  $CO_2$  solubility is desired.

Initially, it was suspected that NOHMs-based fluid would exhibit a lower conductivity compared to a binary fluid with untethered polymer since the main difference between two systems is solid nanoparticles in the NOHMs-based system. Interestingly, NOHMs-based electrolyte showed enhanced conductivity and even reduced viscosity. This result was indicative of a more effective pathway of ion transport in NOHMs-based fluids than in polymer-based fluids. Thus, we hypothesized that there may exist unique multi-scale structures, enabling an enhanced ion transport in the NOHMs-based fluids. In order to investigate this hypothesis, ultra-small-angle X-ray scattering (USAXS) technique at Argonne National Lab was used to construct the structures of NOHMs morphology in secondary fluids, from agglomerates at large scale (1 ~ 2 mm) to aggregates at mid-scale (20 ~ 200 nm), and to the interparticle distance at small scale (9 ~ 10 nm). As shown in Figure 4, interesting hierarchical structure was observed in NOHMs-based systems and this provided ions unique channels and pathways to migrate, resulting in the surprising conductivity enhancement. The enhanced transport behavior induced by multi-scale hierarchical structures suggest that NOHMs can be designed with interesting electrolyte properties which may allow the CO<sub>2</sub> capture to be pulled by the in-situ CO<sub>2</sub> conversion reactions.





#### Summary

A novel water-lean nanoscale hybrid solvent system has been developed for carbon capture with a potential to host its subsequent conversion to chemicals and fuels. The insight into the chemistry and structures of this hybrid solvent system is not only beneficial to the advancement in carbon capture and conversion, but it is also enlightening for the interdisciplinary development of various areas involving nanoscale hybrid materials. It is particularly interesting as NOHMs was encapsulated to create a particulate system that combines properties of liquid solvents and solid sorbent. Synchrotron studies have revealed unique hieratical structures that provides enhanced transport behaviors in systems even at high nanoparticle concentrations. This study illustrates how the fundamentals of particle technology are important in novel materials development and why they should be considered even during the early research stage for different applications.

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## The election is now open and will close on October 20, 2018.

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#### Ah-Hyung (Alissa) Park

### **Candidates for Academic Positions:**

**Kingsly Ambrose** is an Associate Professor of Agricultural and Biological Engineering at Purdue University. Kingsly earned his Ph.D. in Agricultural and Biological Engineering, studying caking of bulk solids, from Purdue University. His research interests are in particle and powder characterization, particle modeling, particle design, safety during powder handling, and grain drying. He has authored/co-authored 65 peer-reviewed journal articles and 5 book chapters. Kingsly has contributed in 118 conference presentations. His current research sponsors/collaborators include USDA, US Department of Labor, US DOE, The Andersons, CNH Industrial, National Grain and Feed Association, and Anton Paar.

**Bodhi Chaudhuri** is an Associate Professor of Pharmaceutics, Chemical Engineering and Materials Science at UConn. He got his PhD in Mechanical Engineering from NJIT after obtaining his MS and BS both in Chemical Engineering from IISc, Bangalore and Jadavpur University respectively. He performed postdoctoral research in Chemical Engineering at Rutgers and has 3 years of industrial experience. He has published more than 60 journal articles, book chapters, conference proceedings and delivered 30 invited talks in industry/academia in US/abroad. He is an editorial board member of several international journals including Advanced Powder Technology. He and his colleagues have garnered 9M of federal/industrial funding for research. He consulted to several pharmaceutical and engineering companies. He actively participates in activities of AIChE as PTF-session chair/co-chairs whilst organizing several international conferences. He received Young Investigator Award from FDA amongst several awards. Congressman Joe Courtney applauded his group's research efforts in US-Congressional Report in 2011.

**Heather Emady** is an Assistant Professor at Arizona State University, with research interests in granule formation and granular heat transfer. She has degrees from the University of Arizona (B.S., 2007) and Purdue University (Ph.D., 2012). Heather did postdoctoral work at P&G, as well as at Rutgers University. She joined ASU in January 2015, and won the Bisgrove Scholar Award (and appeared on a local PBS TV program to explain the importance of particle technology research to the general public). Heather has been active on the AIChE Women's Initiatives Committee since 2012, and currently serves as Past Chair. She has been a member of the PTF since 2011, and was an invited speaker at the 2016 FPST hosted by the PTF. Heather served on the PTF awards evaluation committee for the Best PhD Award for the past two years, and is very interested in getting more involved with the PTF.

Jae W. Lee is the department Head and a Professor of Chemical and Biomolecular Engineering at Korea Institute of Science and Technology in Korea. He obtained his BS/MS in Chemical Engineering at Seoul National University. He worked at S-oil Company for five years before getting his Ph.D. degree at Carnegie Mellon University. After his postdoc research as an Alexander Humboldt Fellow at Aachen Technical University, Jae joined the City College of New York and was promoted to a Full Professor in 2010. His main research interests include CO2 conversion to carbon nano-particles, chemical looping combined with CO2 utilization and methane hydrates. He has served in various international advisory

committees at AIChE. His CO2 conversion research was highlighted as an important technology transfer success by the Korean Ministry of ICT and Sciences and selected as 100 R&Ds of Korean National Academy of Engineering for the Year of 2025.

**Aaron J. Moment** is the Professor of Practice of the Department of Chemical Engineering at Columbia University. Prior to joining Columbia University in 2018, Prof. Moment worked at Merck & Co. for eighteen years as a Chemical Engineer and involved in the development of commercialized drugs including Januvia (diabetes) and Belsomra (sleep disorder). His research focuses on the synthesis and purification of small pharmaceutical molecules with emphasis on reaction thermodynamics, mechanisms, kinetics and process safety. The current efforts include chiral separation via crystallization, solid state chemistry of hydrated crystals, power ultrasound for particle engineering, and innovative reaction control and chemical safety. Moment received a number of professional honors including Merck Research Lab NJ Award for Risk Taking related to implementation of novel synthetic route to HCV pro-drugs involving organocatalysis to set chiral phosphorous center (2016). Prof. Moment received his B.S. at RPI and Ph.D. at MIT, both in Chemical Engineering.

#### **Candidates for Industrial Positions:**

**Willie Hendrickson** is the founder and CEO of the AVEKA Group. AVEKA was founded in 1994 as a spin off from 3M with 3 people and one site. Currently, the AVEKA Group comprises 5 manufacturing sites and 250 people for industrial, chemical, food and pharmaceutical contract manufacturing and process development of particulate materials. Prior to starting AVEKA, Willie worked at 3M as the Technical Manager for Particle Processing in 3M's Corporate Research Facility. Willie received his Ph.D. from the University of Florida in organometallic synthesis. He is currently the President of the International Fine Particle Institute and is an Adjunct Professor at the University of Minnesota's Department of Food Science. He has authored or coauthored over 20 technical papers or book chapters and is the current holder of 50 issued or applied for US patents.

Madhu Kodam is the Solids Processing Technology Leader in Corteva Agriscience<sup>™</sup>, the agricultural division of Dow-DuPont providing technical support for both manufacturing and R&D in various solids processing technologies. He has been with Dow for almost eight years. He is involved in solving a wide variety of problems related to particle technology, ranging from caking and flowability of bulk solids to pneumatic conveying, fluidization, and other twophase flow problems. He received his PhD in mechanical engineering from Purdue University, where he developed novel contact-detection algorithms for true pharmaceutical tablet shapes and different attrition mechanisms. His research interests include continuum modeling of bulk solid flows and the application of fundamentals for solving bulk solid flow problems. As part of AIChE, Dr. Kodam served as the Co-Chair and is currently the Area Chair of the Area 3C, Solids Processing and Handling.

**Michael J. Molnar**: Michael Molnar [B.S. Chemical Engineering, Carnegie Mellon University (1995), M.S.E. Chemical Engineering, The University of Michigan (2000)] began his professional career in 1995. Michael has worked in multiple research and manufacturing support roles within The Dow Chemical Company, Dow Corning Corporation, and Hemlock Semiconductor, where he has specialized in reaction engineering and thermodynamics, fluidization and solids processing, and pilot plant research. Most notably, Michael worked on the development of size reduction and classification technologies for high purity polysilicon and a fluidized bed chemical vapor deposition process to produce silicon granules. Michael is a recognized inventor with nine granted patent families. He is a senior member of AIChE and active within Group 3B of the Particle Technology Forum, where he has frequently served as session chair at the Annual Meeting. In 2015, he was selected by the National Academy of Engineering to participate in the China-America Frontiers of Engineering Symposium (CAFOE).

**Satish Nune**, Ph.D.: Dr. Satish K. Nune is a senior scientist in Applied Functional Materials Group at Pacific Northwest National Laboratory (PNNL). He is internationally known as an innovator in the development of porous nanomaterials for chemical transformations, water management, low temperature geothermal applications, and energy storage. Dr. Nune has over 60 peer-reviewed publications including 4 reviews, 1 book chapter and 12 patents (4 US patents and 5 Japan patents issued; 3 US patents filed). His research work is highly regarded with numerous citations (>2400) from research groups worldwide and has h-index 23. Dr. Nune has organized and co-organized multiple symposiums at AICHE-PTF. He is the topic area, Nanoparticles (3D) chair at 2018 AICHE meeting. Dr. Nune recently accepted to be on editorial board for NATURE SCIENTIFIC REPORTS. As a candidate for the position of Executive Committee (EC) for PTF, my main aim is to bring the PTF vision into an exciting reality.

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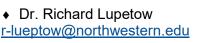
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