The PTF Newsletter

Letter from the "Chair"

With a sincere note of thanks to Rajesh Dave who led the PTF activities last two years as the chair, Jim Gilchrist from Lehigh University, the next chair-elect, and I are excited to carry on the PTF tasks with help from rest of the team of volunteers.

2019 has another exciting year of PTF activities in store. I hope that you all enjoyed the AIChE Annual Meeting and are recharged from your holiday break. I would like to thank George Klinzing for his assistance in selecting such a beautiful venue for our banquet last fall. The windows and glass fixtures and woodwork were truly stunning and an awesome history as well. And to thank all of those who helped with the programming for last fall's meeting.

This year we continue with the Student Travel Award Initiative begun last year. Based on the criteria established last year by the EC, our new PTF Vice Chair, Jim Gilchrist, will set up an award committee for these awards, as well as the others. The PTF Awards nominations are quickly coming up on us. Please note the deadline of May 19th for the nomination packages. There is a specific notice later in the newsletter about the award nomination process. As with last year, we will have a single round of nominations and the award committees with select from those prepared. There are many awards and I am sure many deserving candidates for these awards so please do your part and nominate someone! If you have any questions or concerns regarding the requirements, please feel free to contact Jim or I for clarifications as well as special requests or exceptions. We are here to help.

There is also more emphasis on diversity among our selection committees. While there has been significant diversity on the selection committees in the recent past, additional calls for diversity by many corporations and the AIChE itself have prompted this new emphasis. While I don't believe we should set any quotas, since that would be discriminatory, it is proper to keep this topic in mind while nominating and selecting candidates. As always, we want to select the best possible candidates for our awards each year.

I look forward to particularly great 2019. I hope yours is also.

Regards,

Bruce D. Hook, The Dow Chemical Co.
Chair, Particle Technology Forum

With this issue, I finish my four year term as the editor of the PTF Newsletter. Our newsletter continues to be the primary channel for our membership to stay abreast of key PTF activities, initiatives, share ideas and recognize the accomplishments of our peers. I have experimented with many ideas and formats, and strived to make each newsletter useful and informative. I hope that I succeeded to some extent.

My sincere thanks to the editorial advisory committee (Ray Cocco, George Klinzing, Pat Spicer, Reza Mostofi & Raj Dave) for their advice, ideas and encouragement.

Starting with the next issue, Mayank Kashyap will be taking over as the new editor. I am sure that he will bring new ideas and energy to this effort. I wish him the best...

Shrikant Dhodapkar, Dow Chemical
Editor, PTF Newsletter

In this issue...

2018 PTF Lifetime Achievement Award Lecture

Particles Are Forever

Sotiris E. Pratsinis
ETH Zurich, Switzerland

Particles are everywhere, in our iPhone, in the air we inhale, the bread, salt and pepper on the dinner table, in every pill we take, in the tires we drive on, the cement of bridges and driveways, the paint on the walls and so on. What is really new with particles, however, is the superior understanding we rapidly develop at the nano-scale, the new size limit in applied sciences and, in particular, for electronics and life sciences. This can only be compared to the excitement with the micro-scale in the mid-19th century. So with today's state-of-the art computational tools and diagnostics this understanding facilitates a much better connection between product performance and particle characteristics[1]. As a result, the design for their process scale-up is placed on a firm scientific basis and, most importantly, this understanding drives innovation! This creates new excitement with particles and a wave of new applications and opportunities (e.g., Figure 1)

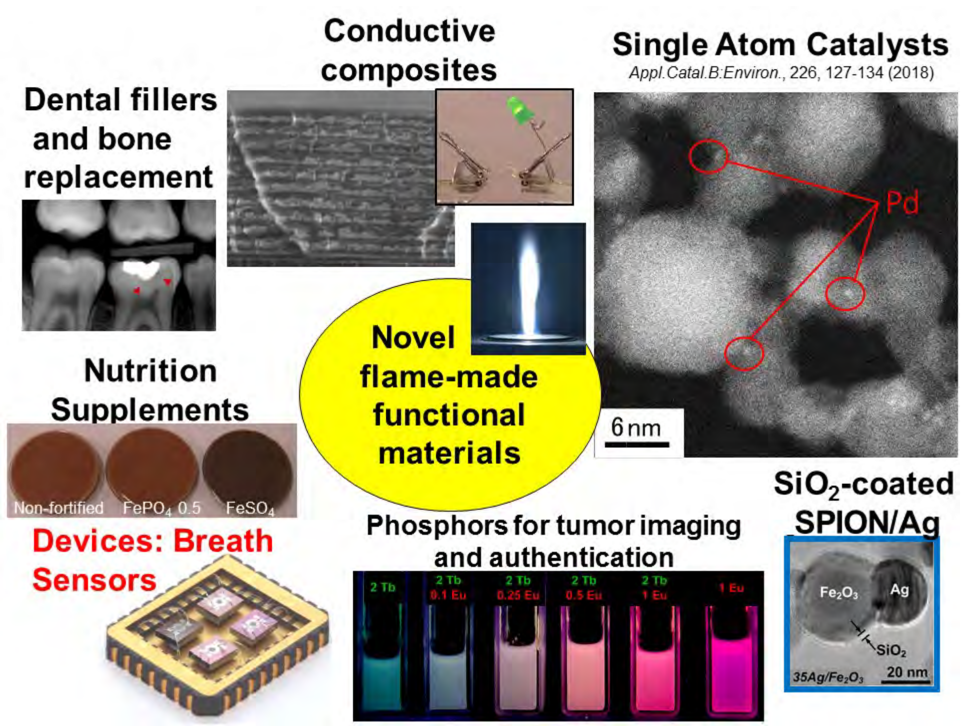


Figure 1. *Besides nanosilver[2] and carbon-coated biomagnetic cobalt nanoparticles[3] in the market already, a number of promising materials are made by flame aerosol particle technology: a). dental (radiopaque but transparent Ta_2O_5/SiO_2) composites, b) multi-layer and multifunctional (conductive, phosphorescent, magnetic & bactericidal) polymer composites[6], c) single Pd atoms on TiO_2 photocatalysts, d) $FePO_4$ nutritional supplements, e) SnO_2, WO_3, TiO_2 and ZnO gas sensor arrays[7], f) Y_2O_3-based phosphors and g) SiO_2-coated Janus-like plasmonic nanosilver - iron oxide nanoparticles (SPION) for theranostics[8].*

Today, for example, various pricy nanomaterials can be readily produced at kg/h with closely controlled size, composition and morphology, even at university laboratories capitalizing on the above understanding through multi-scale process design[4]. This facilitates the creation of spinoffs for niche markets like nanofluids, smart clothing and biomaterials to name a few. The dynamics of the mesmerizing and omnipresent fractal-like structures of particles (esp. when made in mass e.g., fumed silica) are better understood so now we can systematically design and operate their manufacturing units[5]. For example, novel computational schemes reveal that power laws govern the evolution from physically-bonded soft-agglomerates to chemically- or sinter-bonded hard-agglomerates (or aggregates) regardless of composition and polydispersity[5]. Understanding is rapidly advancing also at the surface and sub-particle level (molecular or atomistic) with clever algorithms and hardware. This facilitates the development of process design correlations from first principles that are tested rigorously with data[4]. New techniques such as tandem mass-mobility measurements not only quantify the morphology of above agglomerate structures but give the size of constituent particles when interfaced with the above power laws. That way the particle size, a key performance characteristic, is given online rather than from tedious offline microscopic or adsorption measurements that can hinder efficient manufacturing[5].

This understanding now facilitates the creation of sophisticated devices[1] containing particles with closely controlled characteristics such as gas sensors[7] that were not available with conventional technologies. For example, industrial prototypes of gas sensors that can selectively detect breath acetone, a tracer for fat burning, are developed. That way, such sensors could show when a gym workout is burning undesirable body fat or the effectiveness of a prescribed diet to control obesity. Frankly there are great opportunities for particle technology in life sciences that can be materialized by close interaction of particle scientists with medical doctors as we have seen with the undisputable impact of particle technology in pharmacy in recent years.

These successes and potential, however, should not let us overlook opportunities in connection to better understanding the *health impact of particles* to consumers and even us, the practitioners. After all, together with our students we are the first to handle such particles! Today the public is far more cautious with scientific discoveries demanding guarantees for human health! For example, just a few years ago the U.S. EPA had been petitioned to label nanosilver[2] (silver nanoparticles) as pesticide, the kiss to death of any consumer product, for its impact on aquatic life. Sound particle technology[2], however, clearly differentiated the role of silver ions from particles contributing to the safe use of nanosilver making it today the largest engineered nanomaterial in the market after the classics, carbon black and fumed oxides.

How can we keep up with all these advancements and be part of the innovation magic? A major enemy for innovation is fear, fear of the unknown. To overcome it you need knowledge~~,~~ and training. To stress the need for methodical effort with my students rather than mindless heroics, I frequently quote the classic Tina Turner song "…we don't need another hero...". So one of the three pre-requisite movies in ETH's course catalog for my research-oriented classes (in addition to standard physics, chemistry, math, thermo & transport) is "Chasing Mavericks". This is the true story of how Jay Moriarity (a surf legend) systematically learns to hold his breath for, at least, five minutes before trying to ride the Mavericks, the 40-feet high waves off the coast. It will take just about that long to come back to the surface when a Maverick takes down a surfer, according to the surfing aficionados….

Chasing Mavericks (2012)

Perseverance is the second asset for innovation. I exemplify it to my students with another class pre-requisite movie, the 2014 "Unbroken" by Angelina Jolie. This is the true story of Olympian Louis Zamperini surviving an airplane crash and 47 days on a raft in the Pacific Ocean followed by two years in a POW camp!

The commitment to do something truly great is the third and most important asset for innovation. Again, a class pre-requisite movie "The Salt of the Earth" drives this point. This is the story of photographer Sebastiao Salgado. After taking news photographs in all his professional life from the Rwanda genocide, war in Yugoslavia, famine in Ethiopia etc., he gets so depressed and quits his job. He recovers only when he commits to and initiates the reforestation of Amazon's Atlantic forest that had been decimated effectively to a barren area by excessive overlogging.

The Salt of the Earth

(2014)

Particle technology (as most scientific fields) is a contact sport. Whenever you have time, why not attend a seminar even on topics that you may know little about? Seek the inspiration. I love going to conferences and frequently take my students there. This is a great opportunity to refresh ideas, views, and, most importantly, take the pulse of the worldwide community. One will hardly get this by surfing the net. Conferences like AIChE attract researchers from all over the world. When young engineers see what the world does and cares about, they truly sense what needs to be done. That is a learning experience. When students see how colleagues from the rest of the world perform and present their research, they are motivated to perform as well, if not better. After all, an engineer's degree is a passport to the world. Just compare the worldwide job opportunities of this degree to more coveted ones from law and medical schools.

Lastly let me stress that even though we still have a lot to learn about particles, enough is already known to keep making an impact to the needs of the society[1] for sustainable living, energy and quality of life. We live in a great time for particle technology innovation.

Selected articles, perspectives & reviews of new aerosol-driven particle technology processes & products

1. From Functional Materials to Devices through Core Chemical Engineering, *AIChE J.*, **56**, 3028-3035 (2010).
2. G.A. Sotiriou, S.E. Pratsinis, Engineering nanosilver as an antibacterial, biosensor and bioimaging material, *Curr. Opinion Chem. Eng.* **1**, 3-10 (2011).
3. A. Schätz, R.N. Grass, W.J. Stark, O. Reiser, TEMPO Supported on Magnetic C/Co-Nanoparticles: A Highly Active and Recyclable Organocatalyst, *Chem. Eur. J.* **18**, 8262-8266 (2008).
4. B. Buesser, S.E. Pratsinis, Design of Nanomaterial Synthesis by Aerosol Processes, *Annual Rev. Chem. Biomol. Eng.,* **3**, 103–27 (2012).
5. M.L. Eggersdorfer, S.E. Pratsinis, Agglomerates and Aggregates of Nanoparticles made in the Gas Phase, *Adv. Powder Technol.* **25**, 71-90 (2014).
6. C.O. Blattmann, S.E. Pratsinis, Nanoparticle filler content and shape in polymer nanocomposites. *KONA Powder Part. J.* **36**, 3-32 (2019).
7. M. Righettoni, A. Amman, S.E. Pratsinis, Breath analysis by nanostructured metal oxides as chemo-resistive gas sensors, *Mater. Today,* **18**, 63–171 (2015).
8. F.H.L. Starsich, I.K. Herrmann, S.E. Pratsinis, Nanopartices for Biomedicine: Coagulation during Synthesis and Applications, *Annual Rev. Chem. Biomol. Eng.,* **10**, in press (2019).

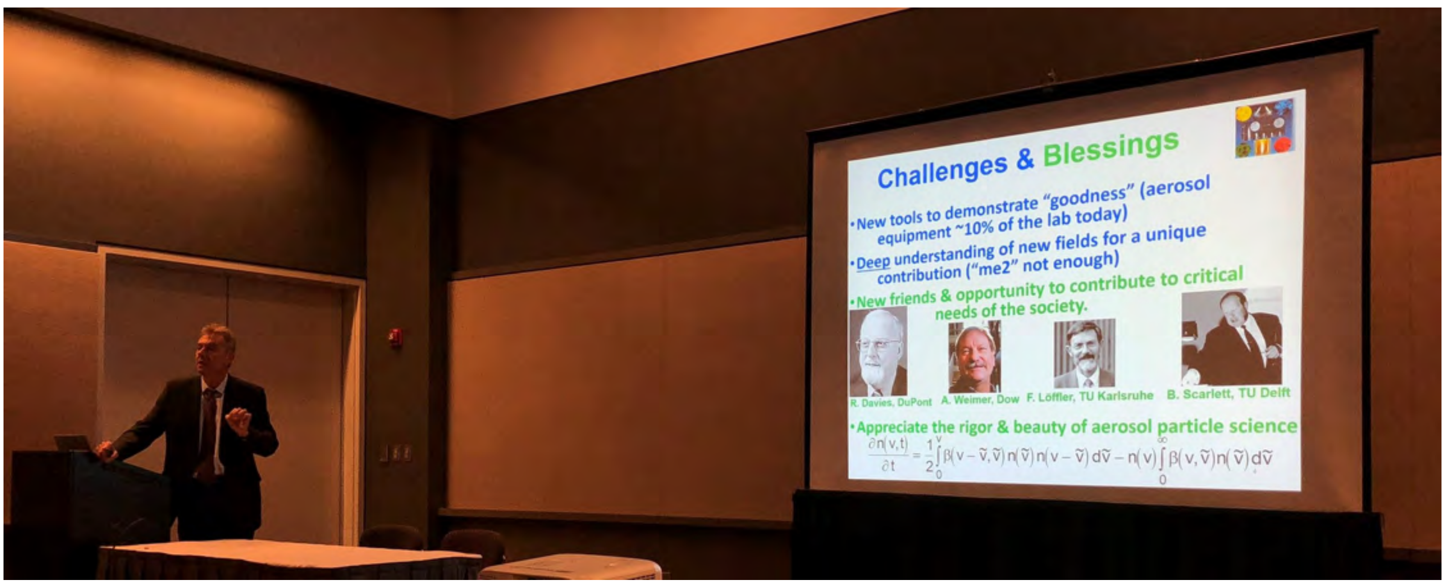
PTF Lifetime Achievement Award Winners

Sotiris Pratsinis **2018**	**Alan Weimer** **2017**	**Darsh Wasan** **2016**
John Carson **2015**	**Karl Jacob** **2014**	**Dimitri Gidaspow** **2013**
John Grace **2012**	**Ralph Nelson** **2012**	**Daniel Rosner** **2011**
Joachim Werther **2010**	**Ted Knowlton** **2009**	**Liang-Shih Fan** **2008**
Liang-Tseng Fan **2007**	**Douglas Fuerstenau** **2006**	**Joerg Schwedes** **2005**
George Klinzing **2004**	**Chi Tien** **2003**	**Brian Kaye** **2002**

ELSEVIER

Sponsor of the Lifetime Achievement Award

PTF Award Lecture



2018 Thomas Baron Award Lecture

Particle Technology
From Fundamentals to Translational Pharmaceutical and Energy Applications

Chi-Hwa Wang

Department of Chemical and Biomolecular Engineering,
National University of Singapore, Singapore, 117585
http://cheed.nus.edu.sg/stf/chewch/index.htm

This talk was focused on the fundamentals of fluid-particle flows and their corresponding translational applications in the biomedical, pharmaceutical, energy and environmental fields. The presentation started with an elucidation of dynamic behaviors of granular flow under shear, gravity, vibration and pneumatic conveying through a combination of simulation (computational fluid dynamics CFD) and experimental works (electrical capacitance tomography and electrostatics characterization). The concept of flow instability was then applied to micro- and nano-particle fabrication and drug encapsulation techniques for pharmaceutical applications. These "therapeutic" particles were used in drug delivery systems for the treatment of brain tumors in conjunction with CFD analysis to predict the transport and reaction phenomena of drug molecules respectively with the goal of achieving optimal drug delivery efficacy in an *in vivo* model. At the end of the talk, some applied particle technology principles in energy and environmental processes were reviewed. For instance, the development of gasification technology for the conversion of solid waste to energy and resource was reviewed along with the development of modular gasifier integration packages for processing mixed feedstock of biomass and sewage sludge to produce energy. The resulting gasification solid residue (fly ash and bottom ash) can be further processed in the forms of catalyst, biochar, and activated carbon for a variety of renewable energy and environmental applications.

1. Dynamic of Particulate Systems

Instabilities in Granular Flows & Pneumatic Transport Systems: Early in his career, Chi-Hwa Wang recognized that instabilities are important in the characterization of the dynamics of particle-fluid flow. For example, inelastic collisions lead to density and surface waves observed in granular flows in various flow geometries, such as shear flow, gravity-driven flow, and motion under vertical vibrations [*J. Fluid Mechanics*, 342, 179-197 (1997); *Chem. Eng. Sci.*, 53(22), 3803-3819 (1998); *J. Fluid Mech*., 435, 217-246 (2001); *J. Fluid Mechanics*, 492, 381- 410 (2003)] This phenomenon was predicted by linear stability analysis, and simultaneously measured by particle image velocimetry and phase Doppler interferometry [*Phys. Fluids*, 15(12) 3718-3729 (2003)]. In a series of publications dealing with pneumatic conveying, his group had investigated particle flow metering using electrical capacitance tomography [*Ind. Eng. Chem. Res.* 40(20) 4216-4226 (2001); *Chem. Eng. Sci.* 58(18) 4225-4245 (2003)], electrostatic charge generation and characterization [*Chem. Eng. Sci.*, 59(15) 3201-3213(2004); *Ind. Eng. Chem. Res., 43*, 7181-7199 (2004); *Chem. Eng. Sci.* 61, 7889 - 7908 (2006); *AIChE Journal*, 52 (11) 3775-3793 (2006)], particle attrition [*Chem. Eng. Sci.*, 61, 3435 – 3451, (2006); *Chem. Eng. Sci.*, 61, 3858 – 3874 (2006)], and CFD-DEM modeling [*AIChE Journal*, 52, 496-509 (2006); *Ind. Eng. Chem. Res.* 46, 1375-1389 (2007)]. His proof-of-concept studies on the use of single-plane and twin-plane correlations of electrical capacitance tomography data represent powerful non-intrusive measurements of particle concentration distribution and velocity in both horizontal and vertical conveying of granular solids.

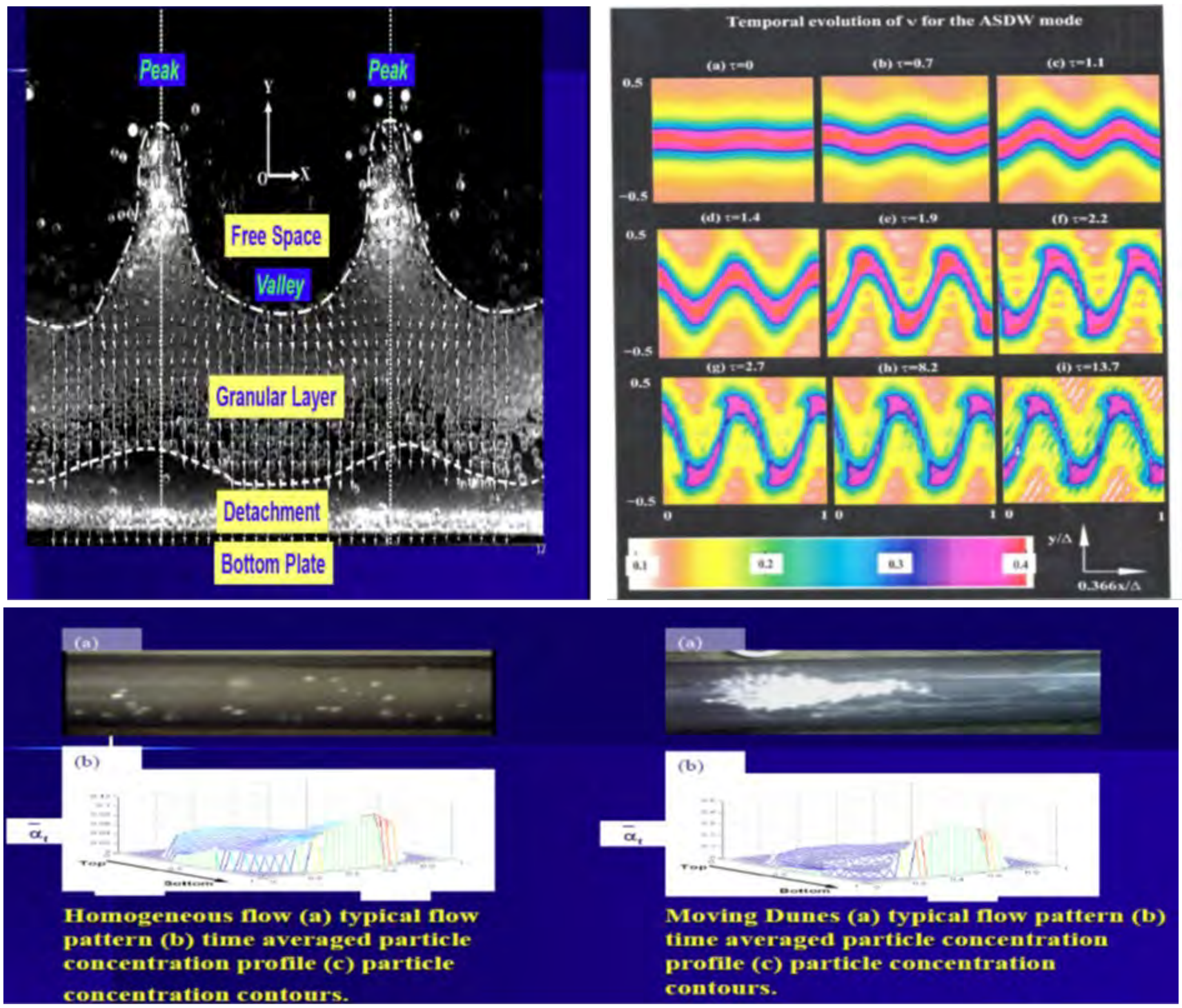


Figure 1. Density waves of granular material under (a) vertical vibration [Phys. Fluids, 15, 3718-3729 (2003)], (b) gravity flow [J. Fluid Mech., 435, 217-246 (2001)], (c) Electrical capacitance tomography image of horizontal conveying of granular materials [Ind. Eng. Chem. Res. 40, 4216-4226 (2001)].

2. Pharmaceutical and Biomedical Applications of Particles

Chi-Hwa Wang's group has successfully produced monodisperse, micro- and nano-particles using electrohydrodynamic atomization (EHDA) process, with precise control of layer thickness with a core-and-shell configuration. These studies have not only expanded our fundamental understanding of these processes, but have also led to advances in practical particle synthesis technologies and application of CFD for the modeling and optimization of drug delivery to brain tumors. His current work addresses the scale-up of these particle fabrication processes and applications in particle and cell deposition.

Micro- and Nano- Particle Fabrication Techniques for Pharmaceutical and Biomedical Applications: Through a combination of theoretical, simulation and experimental works, Chi-Hwa Wang has studied flow instabilities in EHDA systems [*Biomaterials,* 27, 3321-3332 (2006); *AIChE Journal*, 57, 57-78 (2011)] and jet breakup in supercritical systems [*Journal of Controlled Release,* 125, 96-106 (2008)], and has applied the associated phenomena to the fabrication of pharmaceutical particles. Chi-Hwa Wang's group has successfully produced monodisperse nano-particles using the supercritical antisolvent (SAS) method and the EHDA process, with precise control of layer thickness with a core-and-shell configuration [*AIChE Journal*, 63, 12, 5303-5319 (2017)]. These studies have not only expanded our fundamental understanding of these processes, but have also led to advances in practical particle synthesis technologies. For instance, the core-and-shell configuration has been applied in the delivery of therapeutic agents (anticancer and antiangiogenic agents) to treat brain tumors [*Biomaterials*, 34, 5149-5162 (2013)], and the delivery of growth factors and antibiotics for bone regeneration in dental [*Biomaterials* 34, 9990-9997 (2013)] and orthopedic applications [*Biomaterials,* 30,892-901(2009)]. The transport phenomena associated with drug release profile in the porous interstitial tissue space were simulated by Chi-Hwa's group using CFD and validated with both *in vitro* and *in vivo* drug delivery experiments [*J. Controlled Release*, 271, 74-87 (2018)]. His current work addresses the scale-up of these particle fabrication processes and application to particle and cell deposition patterns for 3D printing applications.

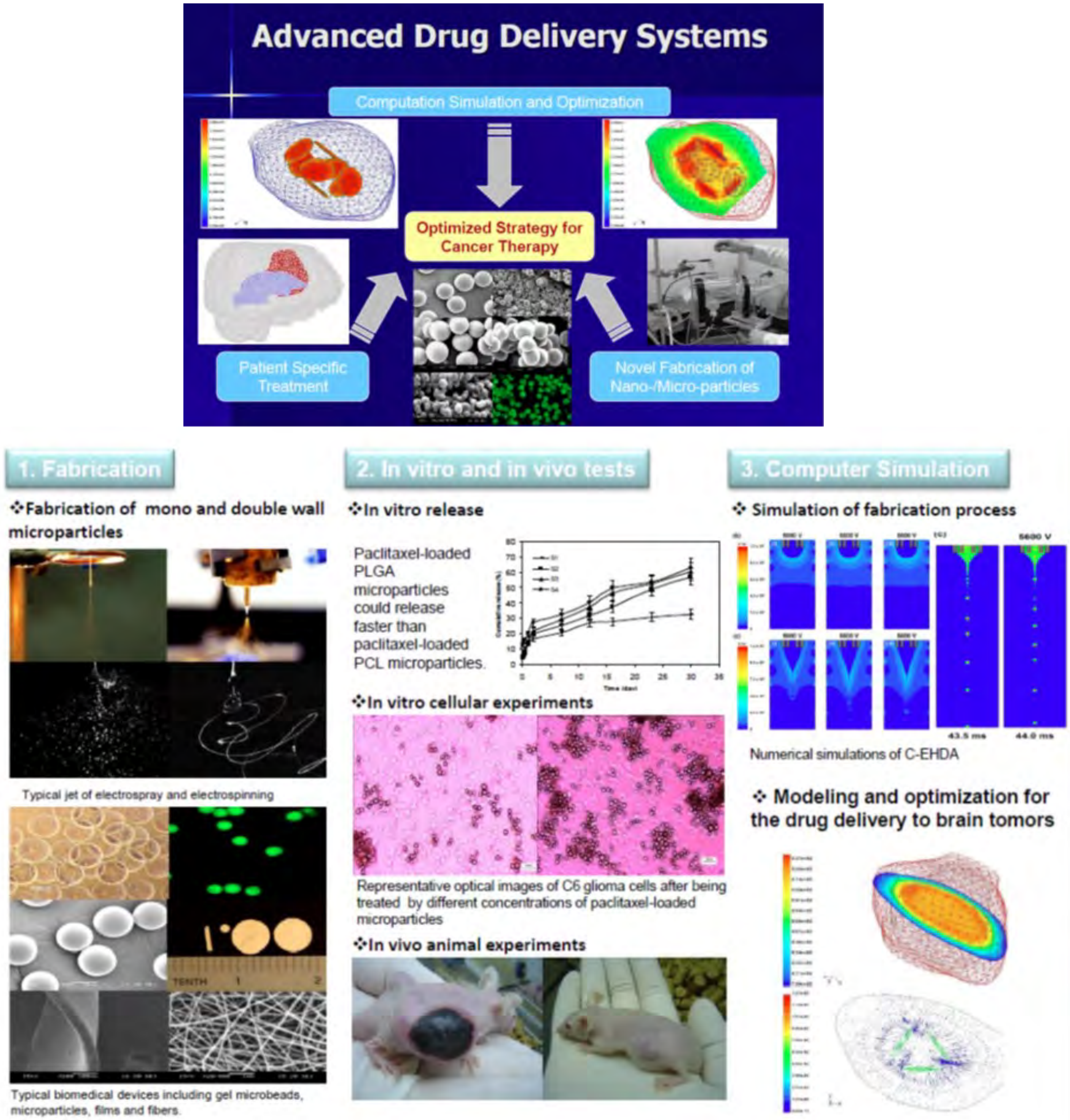


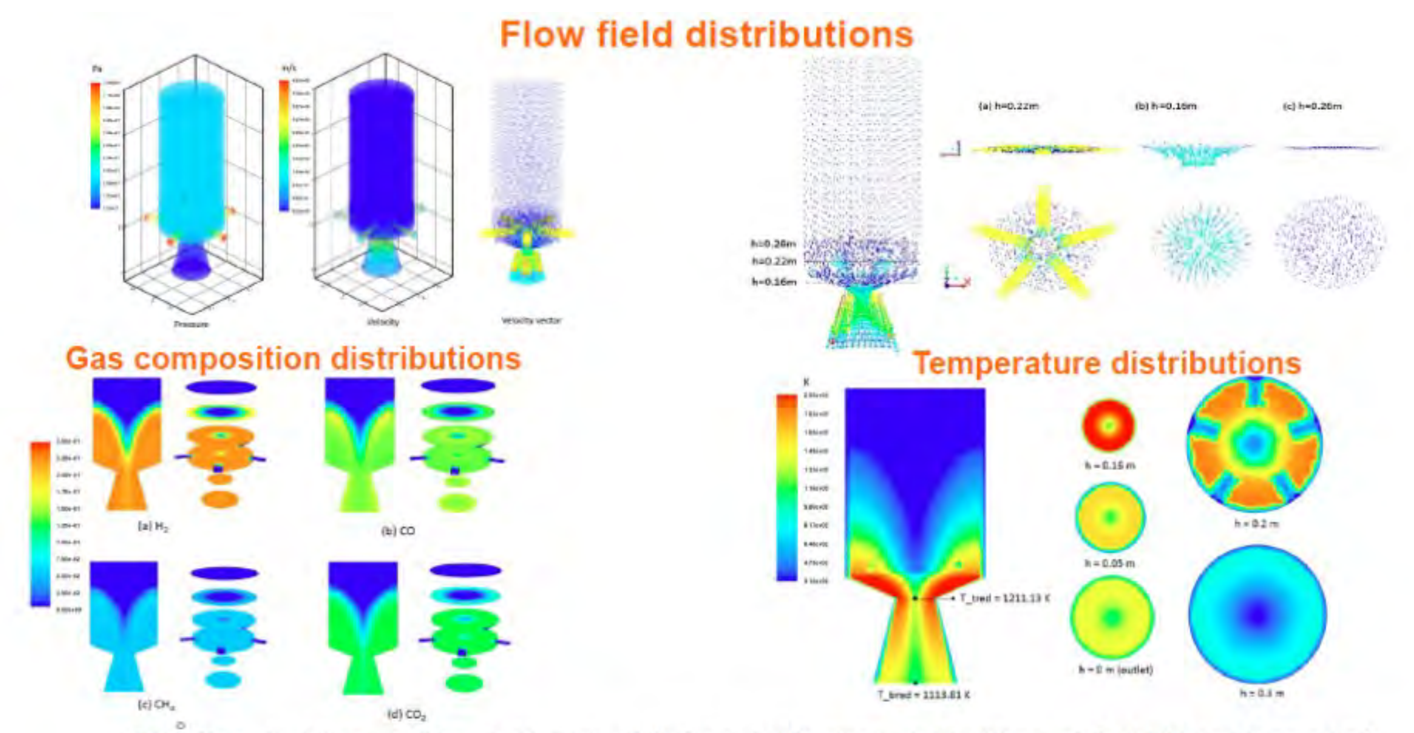
Figure 2. Biomedical and Pharmaceutical and Applications of Particle Technology. This diagram illustrates the overall design of the "Advanced Drug Delivery System".

Applying the flow instabilities concept, the study comprises of different phases such as the design and optimization of core-and-shell micro- and nano- particles and fibers for the delivery of bioactive therapeutic agents including anti-cancer drugs, antibiotics, growth factor, *in vitro* and *in vivo* characterizations. His team has also examined the transport of drugs in solid tumors and have made use of CFD simulations to optimize drug delivery to malignant brain tumors for patient-specific therapies.

3. Energy and Environmental Applications of Particles

The Chi-Hwa Wang research group has developed new projects based on the translational research of particle technology particularly for renewable energy applications. Since 2012, his research group has focused on the co-gasification based clean energy production from carbonaceous solid waste using advanced particle simulation models and renewable energy technology (e.g. solar energy). Chi-Hwa Wang's work has led to new projects, which include the development of modular gasifier integration packages for processing the mixed feedstock of biomass, sewage sludge, food waste, and others to produce energy.

Co-gasification of Coal and Biomass for Clean Energy Applications: Chi-Hwa Wang's research has also sought to probe and develop energy applications involving the use of particle technology. His team has applied past knowledge and has successfully completed the following studies related to coal gasification: hydrodynamics, mixing, and heat transfer of the triple-bed combined circulating fluidized bed [*Chem. Eng. Sci*., 75, 435-444 (2012)], and pyrolysis and gasification in the downer reactors [*Ind. Eng. Chem. Res.*, 53, 6624-6635 (2014)]. Chi-Hwa Wang is working on new pyrolysis/ gasification technology for waste-to-energy applications. His recent work has led to the birth of new projects which include the development of modular gasifier integration packages for the processing of the mixed feedstock of coal, biomass, sewage sludge, food waste, and others to produce energy [*Powder Technology*, 296, 87-101 (2016)]. All of this research work is done with the specific aim to achieve fine control in the production of particulates/aerosols, and the reduction of hazardous materials in the emission gas and bottom ash streams by converting the waste stream into valuable products [*Bioresource Technology*, 200, 350–359 (2016)]. These studies integrate CFD simulation for the gasification system and measurement of downstream chemical, biological [*Waste Management,* 50, 93-104 (2016)], and size characteristics of particulate materials produced from the gasifier, permitting design optimization that considers both the emission gas and bottom ash streams and the performance of the reactor in the gasification system to optimize the design. His team has also developed a three-phase flow model together with a thermal-equilibrium model to study the operation of downdraft biomass gasifiers. The thermal-equilibrium model was applied to study the effects of air to biomass ratio on gas composition, low heating value (LHV), and temperature. This model was then applied to investigate the gasification performance considering gasifier geometry, equivalence ratio and composition of biomass particles. Effects of reducing bell dimension and operation conditions on the temperature distribution and syngas production were also investigated by the 3D CFD model, which has shed light on the improvement of the design and operation of reactor. [*J. Cleaner Production, 178, 476-493 (2018)*].



W.C. Yan, Y. Shen, S. You, S.H. Sim, Z.H. Luo, Y.W. Tong, C.H. Wang, "Model-Based Downdraft Biomass Gasifier Operation and Design for Synthetic Gas Production", J. Cleaner Production, 178, 476-493 (2018).

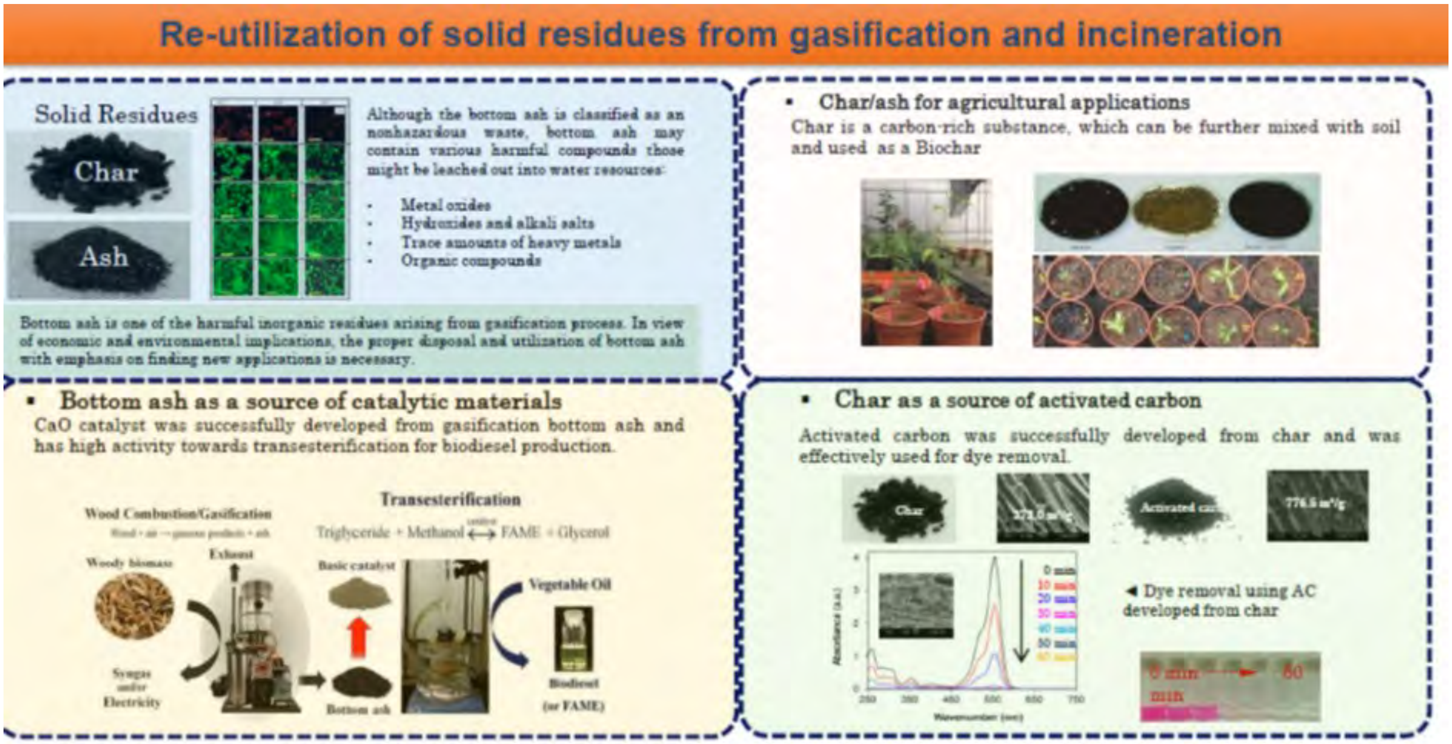
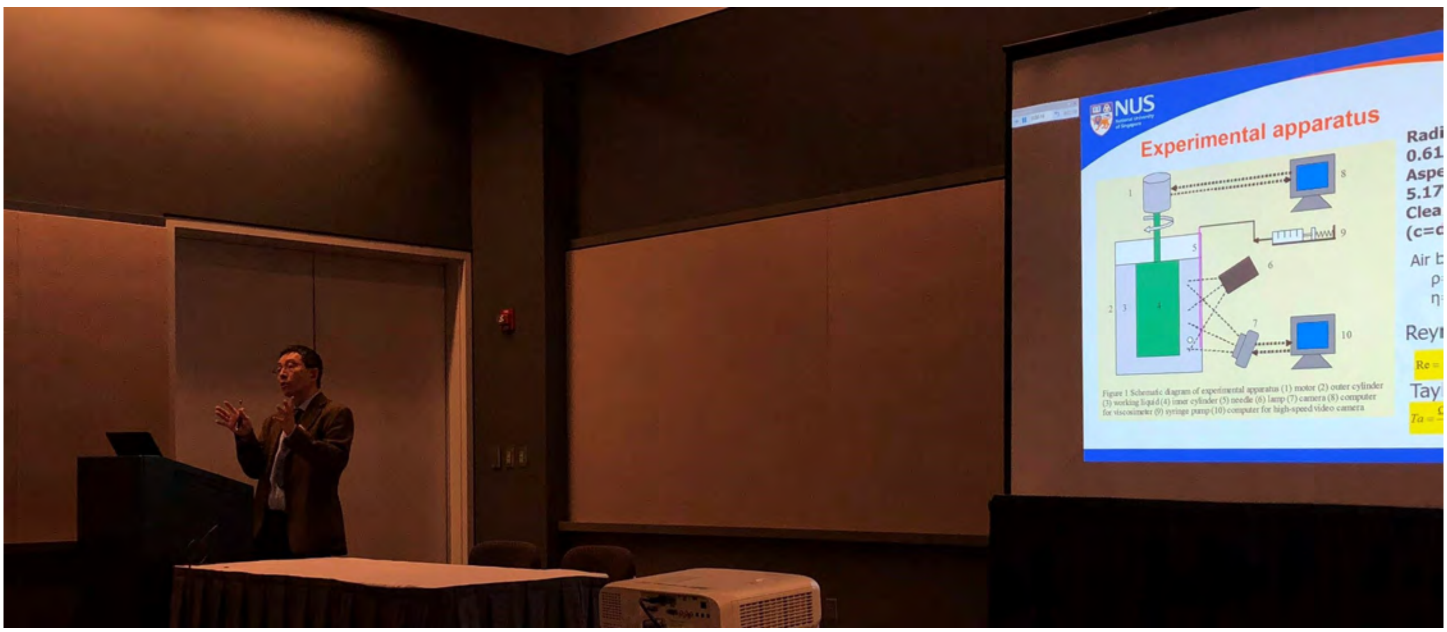


Figure 3. Energy and Environmental Applications of Particle Technology to Realize the Concept of Circular Economy. Through the co-gasification of various types and streams of waste feedstock (food waste, woody biomass, sewage sludge), synthetic gas and bio-char can be produced under different reactor conditions, which can be modeled and optimized through CFD simulations. The solid residue produced (such as char and ash) can be converted into various types of resource in the forms of "biochar" [Journal of Environmental Management, 172, 40-48 (2016)], "catalyst for biodiesels" [Energy Management and Conversion, 123, 487-497 (2016)], and "activated carbon" [Bioresource Technology, 200, 350–359 (2016)]. The processing of such solid residues through the design of reactors, and the control of production rate, pore and size distribution is a good example for the translational research of particle technology.

PTF Award Lecture



2018 PSRI Lectureship in Fluidization Award Lecture

Novel MOF-based Hybrid Sorbents for CO_2 Capture

A.-H. Alissa Park

Columbia University

Fossil fuels, which significantly contribute to anthropogenic CO_2 emissions, are likely to remain the main source of energy in the foreseeable future. Thus, the development of efficient carbon capture and storage (CCS) technologies is one of the great challenges faced by humanity.[1] A new advancement in the area of CCS includes the development of novel CO_2 capture solvents with high CO_2 capture capacity and selectivity. Unfortunately, amine-based solvent systems are often challenged by solvent loss, high parasitic loads and high operation cost.[2,3] Hence, solid sorbents have also been developed for CO_2 capture.

One of the most interesting and promising solid sorbents are the Metal-Organic Frameworks (MOFs), whose properties can be controlled by tuning the chemical blocks of their crystalline unit.[4] There have been rapid advances by researchers, including the PIs of this project, in the area of MOF synthesis and characterization as well as modeling of MOFs so as to identify the optimum MOF design for specific functions such as CO_2 capture with minimum theoretical parasitic energy consumption. Given that we have a wide range of MOFs[5] – such as the MOF-74 family, HKUST, and UIO-66 – that can be tested for CO_2 capture, the question becomes how to best deploy them for gas-solid contact. The direct use of MOF nanocrystals or micron particles in a large gas stream or a multi-phase CO_2 capture unit is not desired due to the difficulty of subsequent particle collection. A fixed bed reactor with nanoparticles is not possible due to a high pressure drop. Thus, some have investigated unique systems including loading MOFs on the permselective layer of advanced membranes.[6] Most MOF delivery systems, however, are in early stages of the development and it is not clear how they could effectively support CO_2 capture.

In this study, we have designed and investigated a novel class of MOF-based hybrid sorbent systems where CO_2 capturing MOFs are incorporated into polymer beads that are either porous solid or hollow by design. The polymer bead or the polymer shell in the encapsulated system (Figure 1) will not only provide the ease of MOFs handling during CO_2 capture but also protect MOFs from other components in flue gas, for example by selectively blocking water from entering the beads and capsules.

Microcapsule design and fabrication

The double-capillary microfluidic device shown in Fig. 2 is similar to many reported droplet-based microfluidics including the one reported by Vericella et al.[7] It consists of nested capillary tubes with three inlets fed by different fluids. The control of wetting behaviors within the device is one of the important keys for producing controlled double droplets. Our custom-made chip system is designed with an innovative 3D design so that the difficult internal surface coating step has been eliminated (patent application pending). The inner fluid (MOF precursor solutions), the shell fluid (photopolymerized silicone) and the outer fluid (carrier media consisting of aqueous glycerol and surfactant solution) are pumped into the device at controlled flow rates tuning the thickness of the shell. Once double emulsion droplets are produced and they are subsequently cured by UV light generating microcapsules with the clear MOF precursor solution inside. The microcapsules are then collected and heated up to 90 ^{o}C for 0~15 minutes to promote the nucleation and growth of MOF crystals. Before testing them for CO_2 capture, the MOF-bearing capsules are activated at

180 ^oC to remove the solvent. As shown in Fig. 1, produced capsules are highly uniform in geometry and size (500 μm with 35 μm thickness shell).

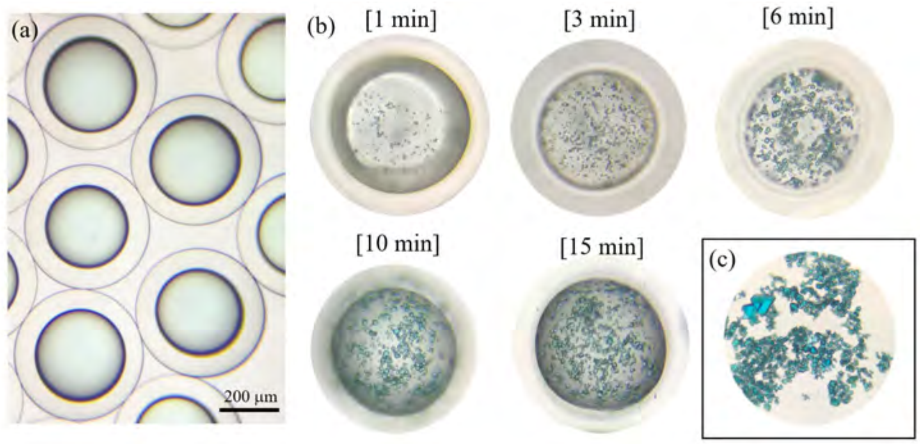


Fig. 1. First ever encapsulated synthesis of HKUST-1 MOF *that exhibited an accelerated nucleation and growth rates and provided inherent packaging of produced MOF crystals (Park group, unpublished work) - Microscopic images (a) Microencapsulated HKUST-1 before heating; (b) The formation of MOF crystals after 1~15 mins of heating; (c) image of HKUST-1 synthesized via conventional solvothermal method for comparison.*

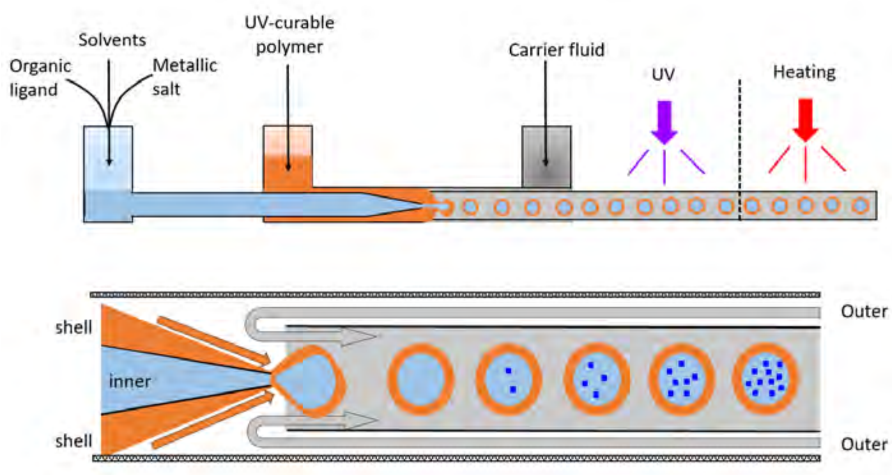


Fig. 2. *Microfluidic experimental set-up for microencapsulation*

In-situ synthesis of MOFs within the encapsulated system and their visualization

We have selected HKUST-1 as the model MOF because it has been well-studied CO_2 capture.[8-10] Further, its mild synthesis conditions (90 ^oC) and slow crystallization kinetics make it easier for visual observation of MOFs formation inside of the shell. The HKUST-1 precursor solution is prepared by dissolving $Cu(NO_3)_2 \cdot H_2O$ and H3BTC to a homogeneous solution of N,Ndimethylformamide (DMF). It has been reported that conventional solvothermal synthesis of HKUST-1 usually requires thermal treatment at 85 °C for 20 hrs.[11] As shown in Fig. 1, our synthesis only took less than 10 mins and the MOF crystals are identical to those produced via the conventional solvothermal method (Fig. 1(c)). The high surface area to volume ratio of the confined environment enhances heat and mass transfer, leading to faster crystallization of MOFs in the droplets.

One of the questions was where these MOF crystals are located within capsules, and whether there are agglomerates. Thus, microtomographic images of encapsulated MOF sorbents were taken at Argonne National Laboratory. Two types of capsules, flat and spherical, were observed in Fig. 3. The majority of MOF crystals (bright color) are densely packed near the inner surface of the capsules. No agglomerates were observed and MOF crystals were narrow in their size distribution.

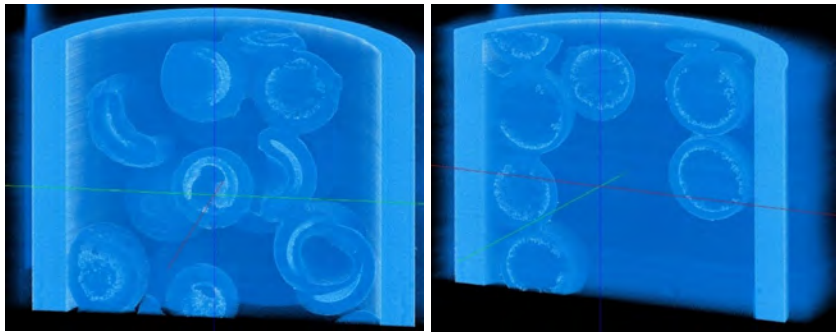


Fig. 3. *MicroTomography of encapsulated HKUST-1*

CO_2 Capture using Encapsulated MOFs

The CO_2 capture performance of encapsulated HKUST-1 was conducted using a TGA set-up with alternating gases. First, encapsulated MOFs were first heated up to 180 ^oC for 12 hrs to remove any residual solvents. Ten cycles of CO_2 adsorption and desorption were carried out at 40 ^oC via CO_2 and N_2 swing. As shown in Fig. 4, the encapsulated HKUST-1 demonstrated rapid CO_2 absorption and desorption rates, which reached equilibrium right after switching gases. The CO_2 capture capacity of the encapsulated HKUST-1 was 4.0 mmol/g-MOFs, which is slightly lower than the reported value (7.3 mmol/g-MOFs). This may be due to the interaction of MOFs with the shell material, which needs to be confirmed in the future. The great finding was that even after 10 cycles, capsules remained mechanically robust and the capture capacity of HKUST-1 kept at the same level suggesting great long-term stability.

Our collaborators at EPFL also produced MOF beads using three sets of polymers, PES, PVDF and PEI, with 65 wt% loading of ZIF-8. Our initial tests were performed for CO_2 capture in biogas containing CH_4. A series of breakthrough curves were collected and it was observed that ZIF-8 effectively captures CO_2 from CO_2/CH_4 mixture. The important finding was that the overall performance was also influenced by the chemistry of polymer itself. ZIF-8/PEI beads resulted in the best CO_2 capture capacity and selectivity, while the use of PVDF as the polymer base led to lower performance. These selectivity results would change for CO_2 capture from coal-fired power plant since CH_4 and N_2 interactions with polymers are quite different.

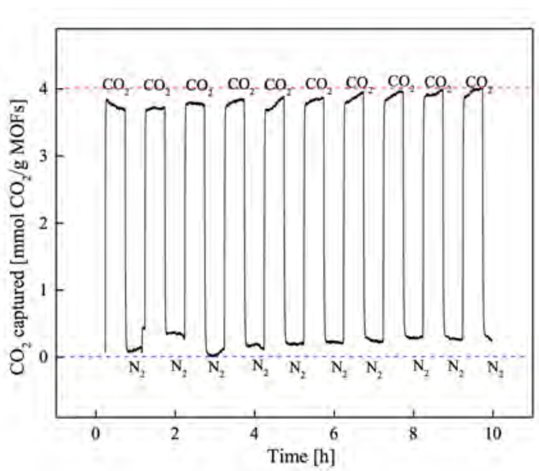


Fig. 4. *Cyclic study of CO_2 capture by encapsulated HKUST-1*

Summary

A novel class of MOF-based hybrid sorbent systems where newly developed CO_2 capturing MOFs are incorporated into polymer beads that are either porous solid or hollow by design has been developed. The polymer bead or the polymer shell in the encapsulated system not only provide the ease of MOFs handling during CO_2 capture but also protect MOFs from other components in flue gas, for example by selectively blocking water from entering the beads and capsules. The results have shown that the chemistry of the polymer matrix is as important as MOFs themselves. This study illustrates how different hybrid particle designs can be used to improve particle handling and provide flexible reactor designs during gas separations.

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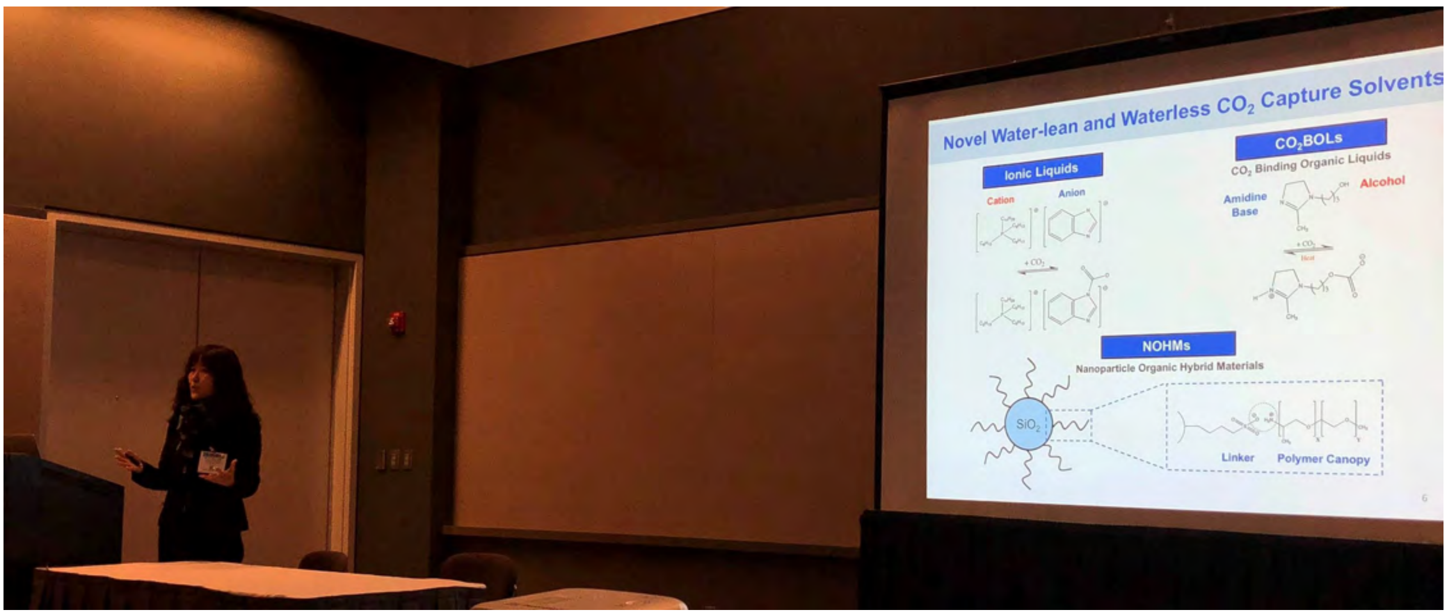

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PTF Awards Nominations - Now Open!

Dear PTF Members:

We are announcing the 2019 PTF awards. The nomination information, award criteria, and previous winners for each of these awards are found in the links below:

Elsevier Particle Technology Forum Award for Lifetime Achievements

George Klinzing Best PhD Award

PSRI Lectureship Award in Fluidization

Sabic Young Professional Award

Shell Thomas Baron Award in Fluid-Particle Systems

Dow Particle Processing Recognition Award (only awarded in odd-numbered years, open this year)

The Executive Committee strongly encourages nominations from all qualified applicants for each award, especially nominees who are women and/or otherwise underrepresented backgrounds in our Forum, the Institute, and in STEM fields.

Key information for this year is below.

- **The Nomination process is a single step.** The full package is due by **Sunday, May 19th, 2019**, containing items specific to each award.
- If the nominee has previously received any award from PTF, an explicit statement of new accomplishments or work over and above those cited for the earlier award(s) must be included (maximum of 1 double spaced page).
- Selected bibliography (including major papers published, books, and patents)
- **It is required that the nominators are current PTF members**
- For the PTF Lifetime Achievement Award, one of the support letters must be from a former PTF Lifetime Achievement Award winner.
- **Nominees are not required to be PTF members**
- Except for the PTF Service Award, the Executive Committee has released the nominee PTF membership requirement. PTF membership is still expected for the PTF Service Award.
- In a given year, the same person cannot win more than one PTF award
- Those making nominations must be members of AIChE-PTF at the time of the nomination.
- Wait period for nomination after previous award
- A former PTF award winner cannot be nominated for another award for at least three years after receiving any previous PTF award

All questions and concerns should be addressed to me by email to gilchrist@lehigh.edu with the subject line including the name of the award. The Executive Committee is actively developing processes to ensure equity, diversity, and inclusion in the forum and its awards.

James Gilchrist

PTF Vice Chair 2018-2020

Job Posting

Software Engineer - Advanced - HPC/DEM/Physics

Division: Digital Factory
Business Unit: Product Lifecycle Management-PLM
Requisition Number: 233440
Primary Location: United States-New Hampshire-Lebanon
Assignment Category: Full-time regular

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- New physics models
- State-of-the-art algorithms and parallelization techniques
- Performance optimizations
- Coupling the DEM physics with the multi-physics environment ofSTAR-CCM+

More details and application link at https://jobs.siemens-info.com/jobs/233440?lang=en-us&previousLocale=en-US

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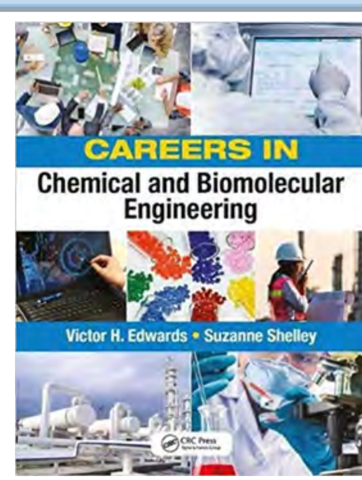
Book Review

Careers in Chemical and Biomolecular Engineering

Victor Edwards and Suzanne Shelley



- Written for high school and college students, teachers, and guidance counsellors
- Outlines many of the key principles of these two engineering disciplines
- Describes historical contributions. and highlights a few future achievements
- Tells where chemical and biomolecular engineers work and how much they are paid

The book also includes in-depth profiles of 25 outstanding chemical and biomolecular engineers, in a diverse array of industries and professional roles

Reference – 188 Pages – 86 Color & 4 B/W Illustrations, Published August 2018

ISBN 9781138099913

This book provides an excellent introduction to chemical engineering that will be highly valuable to high school students considering future careers and to college majors, and for those who have selected chemical engineering as a course of study but seek to understand what types of jobs are available in industry and academia, both undergraduate and through graduate school. The book highlights the significant contributions and achievements of the profession and grand challenges for the future, which is inspiring for both future and current chemical engineers. As such, it will be a welcome addition to the libraries of both. I would have loved to have seen a book such as this earlier in my career, as the perspectives and breadth of opportunities presented can be quite helpful in making career choices! Certainly, the book fills a need in describing careers and career opportunities for the chemical engineering profession.

Joseph B. Powell, Ph.D. (Shell Chief Scientist, Chemical Engineering)

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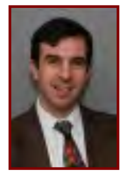

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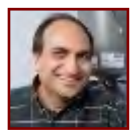

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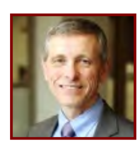

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