THE PARTICLE TECHNOLOGY FORUM (PTF) NEWSLETTER

An American Institute of Chemical Engineers (AIChE) Forum

A Glance at the Newsletter

Message from the Chair

I hope that your summer months have included a chance for relaxation and recharging your batteries. I know that for myself this has been a very busy summer with lots of unanticipated activities and opportunities. That said, the wheels of progress appear to march on relatively smoothly as we have an excellent slate of PTF awardees picked out for the Annual Meeting this fall. Thank you to Jim Gilchrist and his award committee participants for their good work in making those selections. I encourage each of you to consider for next year, who you think is deserving of one of our PTF awards.

In addition to our diversity initiative, AIChE is also working on defining its value proposition for each division and forum. So the PTF Executive Committee will be looking for your input on what makes PTF valuable to you.

Finally, registration is now open for the 2019 Annual meeting in Orlando this November. What an exciting venue to have our meeting and a chance to enjoy all of the opportunities that Orlando provides for entertainment (on the weekend and evenings, of course).

I look forward to seeing each of you at the Annual Meeting.

Regards,

Bruce D. Hook, The Dow Chemical Co.

Chair, Particle Technology Forum

Peaceful Transfer of Power

As you may recall from the Spring 2019 newsletter, Dr. Shrikant Dhodapkar has passed the baton for the position of PTF Newsletter to me after serving in this role for four years.

Shrikant has done a fantastic job in bringing the newsletter to its current form. While I will do my best to fill in some big shoes, I request for your voluntary contributions to the newsletter through PTF related material.

I will be working closely with my Editorial Advisory Committee to incorporate some of the new ideas that I bring to the table as well as their recommendations. An online survey is coming shortly your way to gather information on your thoughts on the PTF newsletter. After all, this newsletter is *"of the people, by the people, for the people"*. I hope that by participating in the survey, you all will use the *democratic process* to provide your valuable input to further improve the newsletter.

I look forward to bringing newsletters to you that would meet your expectations through your help throughout my term as the Editor!!

Mayank Kashyap, SABIC

Editor,

PTF Newsletter

Recap: Fluidization XVI Conference

Fluidization XVI – A Review

May 26-31, 2019, Guilin, China

Junwu Wang[1], Raymond Lau[2], Chi-Hwa Wang[3]

1 Institute of Process Engineering, Chinese Academy of Sciences

2 Nanyang Technological University

3 National University of Singapore

The Fluidization XVI conference aims to bridge fundamental research on fluidization and emerging applications of fluidization and novel fluidization technologies. As the 16th iteration of this conference, the conference brought together world renowned experts in the field. With a long established tradition, this series of conferences has been held all over the world tackling challenges and successes with the design and operation of fluidized beds and similar fluid-particle systems. This newest session, held in Guilin Shangri-La Hotel Guilin, China (26-31 May 2019), continues to play this role and stimulate the interplay between the academic, engineering and industrial communities to address the challenges for the future of fluidization technology. Over the course of four days, the key themes were explored by oral and poster presentations and through ensuing discussions, in which the delegates took active part in 221 papers from 27 countries. The plenary speakers set the stage for the overarching themes of the conference, which the keynote speakers and presenters in the technical sessions that followed and explored in depth. Regular networking breaks facilitated discussions between the speakers and audience. Fluidization XVI featured eleven Plenary Talks in four Plenary Sessions and one Panel Discussion Session.

In the two Plenary Sessions on the first day of Fluidization XVI, Professor Hans Kuipers (Technische Universiteit Eindhoven) shared the recent advances in the multi-scale simulation of mass, momentum and heat transfer in dense gas-particle flows. Professor Qingshan Zhu (Institute of Process Engineering, Chinese Academy of Sciences) gave a practical overview of applying fundamental research in industrial applications of fluidized bed mineral roasting. Professor Stefan Heinrich (Technische Universität Hamburg) communicated the opportunities and recent advancements in tailor-made particles by fluidized and spouted bed spray granulation. Professor Hamid Arastoopour (Illinois Institute of Technology) discussed the relevance and contribution of fluidization and fluid-particle systems research in creating a pathway to sustainable society. Professor Marc-Olivier Coppens (University College London) demonstrated several examples on how nature can inspire innovations in fluidization. At the closing of the conference Gala banquet, Professor Liang-Shih Fan provided an excellent overview for this series of conferences by sharing with the audience many interesting photos taken throughout the past fifteen conferences!

The Panel Discussion Session on the second day of Fluidization XVI started with Professor Jesse Zhu (Western University) sharing his view on Fluidization in 100 Years and future perspectives. The panel, consisted of Professors Xiaotao Bi (University of British Columbia), Liang-Shih Fan (Ohio State University), Masayuki Horio (Tokyo University of Agriculture and Technology), Olivier Simonin (INP Toulouse), Joachim Werther (Hamburg University of Technology), Aibing Yu (Monash University) and Jesse Zhu. The Panel Discussion Session was chaired by Professors Clive Davies (Massey University) and Atsushi Tsutsumi (The University of Tokyo). Emerging topics on fluidization in the Twenty-first century and the classical topics of verification and validation of numerical simulations were discussed.

The last day of Fluidization XVI concluded with two Plenary Sessions. Professor Fei Wei (Tsinghua University) showed several examples on the research of multistage fluidized bed reactor related to stability analysis, suppression of back-mixing and its application in heterogeneous catalysis. Professor Jamal Chaouki (Polytechnique de Montréal) presented his findings of hydrodynamics of high temperature gas-solid fluidized beds. Professor Benjamin Glasser (Rutgers University) showed the application of hydrodynamics, mixing, heat and mass transfer and scale-up of fluidized bed drying in pharmaceutical research. Professor Christine Hrenya (University of Colorado at Boulder) discussed the use of toolboxes to tackle practical issues in particle technology. The last plenary talk was given by Professor Clive Davies (Massey University) on behalf of Professor Gert Lube on the relevance of pyroclastic flows to fluidization and how pyroclastic flows outsmart granular friction during volcanic eruptions.

This conference would not be possible without the dedication and contributions from many of our colleagues. We acknowledge the efforts of our Technical Co-chairs and Organizing Committee, input from the International Advisory Board, the leadership of the Session Chairs. We extend additional thanks to all of our invited and selected presenters, corporate sponsors, and academic and government supporters, without whom the conference would not be possible.

Fluidization XVI Photo Gallery

Conference Co-Chairs and Opening Session

Panel Discussion

Gala Banquet Speaker/ Plenary Speakers


Prof. Liang-Shih Fan


Prof. Benjamin Glaser


Prof. Clive Davies

Prof. Christine Hrenya


Prof. Fei Wei


Prof. Hamid Arastoopour


Prof. Hans Kuipers


Prof. Jamal Chaouki

Plenary Speakers/ Panel Discussion Speakers


Prof. Marc-Olivier Coppens


Prof. Stefan Heinrich

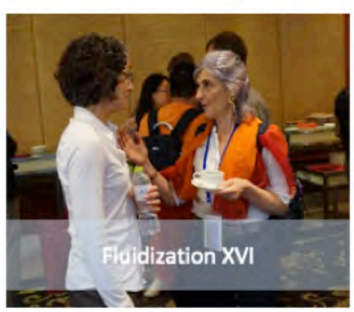

Prof. Qingshan Zhu

Prof. Jesse Zhu


Prof. Liang-Shih Fan


Prof. Masayuki Horio

Poster Session and Technical Tour



Gala Banquet

Group Photo

Fluidization XVI Plenary Lecture

Tailor-made particles by fluidized and spouted bed spray granulation: Opportunities and recent advancements

Stefan Heinrich

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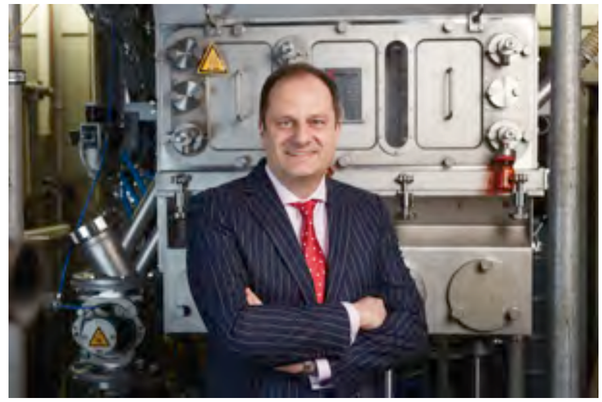

Fertilizers, detergents, animal feed or food ingredients – many products of our daily life are solids produced in fluidized or spouted beds via spray granulation. Depending on the product demand and the specifications, fluidized bed processes are conducted in batch (often in pharmaceutical industry) or in continuous operation. Continuously operated apparatuses often have a horizontal geometry, which can be separated into different chambers with separately adjustable process conditions allowing the combination of different process steps (granulation, coating, drying) in one apparatus. The core particles are continuously fed into the apparatus on one side and leave the apparatus on the other side. The outflowing particles are classified into the product, undersize and oversize fraction depending on their size. By the installation of a sieve-milling circuit, the oversize fraction is milled and fed back into the apparatus with the undersize fraction. Independent on the type of operation, the main quality criteria of the products are a homogeneous composition and constant product quality. For example, in pharmaceutical industry, a common main quality criterium is an even distribution of the active substance among all particles to ensure a constant dose. Even though the fluidized bed spray granulation has been applied for more than 60 years [1], it is still a challenge to control the outgoing product properties. Often, instabilities, dead zones or lump formations occur, which result in excess undersize or oversize particles or even bed defluidization. Frequently, the process does not assume a steady state at all and the properties and mass of outflowing product greatly fluctuates. For a better understanding of the processes, simulation methods have become more and more popular in particle technology during the last years as they give access to process information that are not detectable by experiments. For a detailed understanding the process must be described on different scales from micro to macro scales.

Our main research approach is the combination of experimental and numerical methods to get a deeper understanding of the process, which allows the process adjustment and the development of processing methods resulting in tailor-made particles during fluidized or spouted bed spray granulation. Exemplarily, some of the research projects are shortly introduced here. For further information, the reader is referred to the given references.

Coating in a 3D spouted bed - experimental and numerical investigations of coating homogeneity

The coating process in a three-dimensional prismatic spouted bed (ProCell 5, Glatt GmbH, Germany) was investigated experimentally and numerically. It was found that the range of stable spouting, quantified by a Fourier Transform of the pressure drop fluctuations, can be increased by the insertion of two parallel draft plates [2]. The coating homogeneity of Cellets 500 particles (Harke Pharma GmbH, Germany) was experimentally determined via a digital image analysis approach [3]. A coating suspension with blue dye (methylene blue) was injected and the process was tracked with a high-speed camera. From these images, the blue value of each single pixel was analyzed allowing the measurement of the coating fraction and uniformity. Nevertheless, as the blue values were not correlated with a certain layer thickness, this approach only led to qualitative information. A quantitative measurement of the coating layer thickness was possible by applying the optical coherence tomography (OCT) method to the spouted bed process. The measurement principle is based on different refractive indices of the core particles and the applied coating solution [4].

Coarse-grained CFD-DEM simulations identified the stable spouting regime to be disadvantageous in terms of coating homogeneity as the mixing in the depth of the apparatus is suppressed [5]. As the simulations could only cover some seconds of the process, it was additionally investigated by means of the recurrence CFD (rCFD) approach [6]. This approach allows the calculation of simulations for short periods of time to capture fast dynamics of the systems. Based on the assumption of chaotic, but recurrent behavior, recurrence plots are used to extrapolate dynamics patterns to longer times. As recurrent flow patterns emerge in fluidized and spouted beds, they constitute an ideal application case. rCFD simulations are based on a data base of resolved CFD-DEM simulations. In a first step, statistical analysis of a CFD-DEM simulation is performed to check for reappearing patterns of the investigated system over different time scales. The similarity of states is quantified within the recurrence matrix/plot. In the next step, system states are loaded either contiguously or continuing with the state with the highest similarity to the current state. Using this algorithm, real process times (hours) can be simulated which is not possible with pure CFD-DEM simulations (seconds). For spray coating in a spouted bed, a speed up of 2100x by applying the rCFD approach was reached and the whole coating process was simulated confirming the advantages of the instable spouting regime for the coating homogeneity (Figure 1) [7].

Strategy for coating of aerogels in spouted bed

Previous investigations were performed with model particles. In another project, the coating of aerogel particles in a spouted bed is investigated. Aerogels are very light particles with a mesoporous structure. They are physiologically harmless and represent an ideal carrier material in food and pharmaceutical industry. For protection of the porous structure and retarded release of applied active substances, the particles need to be coated. We have successfully applied the spouted bed coating process to the aerogels. Whey protein isolate aerogels were coated with shellac solution, whereby the high initial specific surface area could be decreased from 243 g/m² to 19 g/m² by the shellac coating (Figure 2). The layer thickness was quantified by focus ion beam method (FIB FEI Helios G3, Dual Beam) to about 1 mm [8].

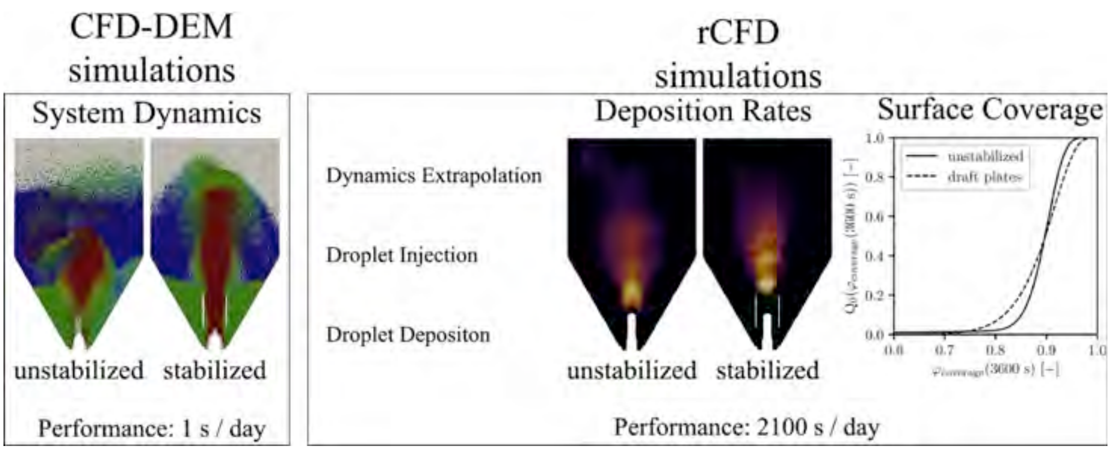

Figure 1: Results of rCFD simulation of spray coating in a 3D spouted bed in comparison to CFD-DEM results. The surface coverage of particles and thus the coating homogeneity is more homogeneous in the unstabilized system.

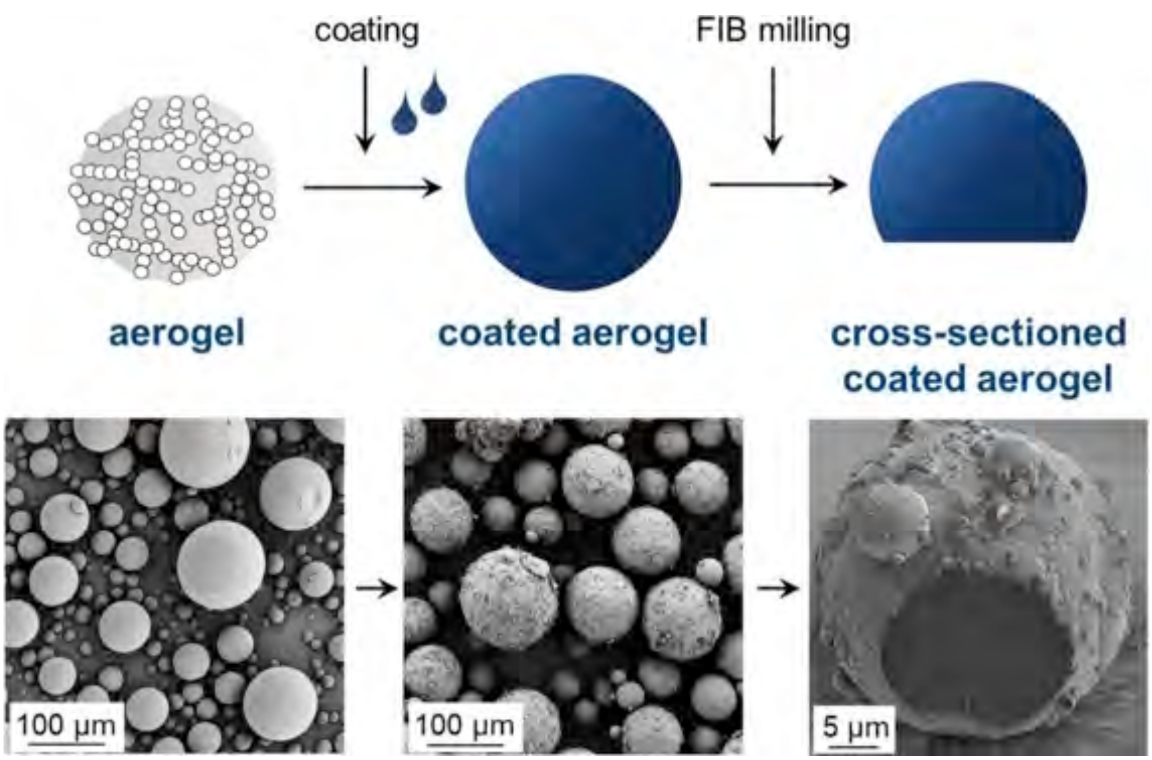

Figure 2: Decrease of specific surface area of aerogels by coating in a spouted bed. The layer thickness can be quantified by focused ion beam (FIB) method.

Fabrication of ceramic-polymer composites using the spouted bed spray granulation

In another project focused on the production of tailor-made particles, the spouted bed process is applied to produce ceramic-polymer composites. Based on composite materials found in nature (e.g. nacre), we aim to produce hierarchically structured composite material that combines the positive properties of the different components to achieve customized products, which are for instance both strong and elastic and at the same time having a high permittivity. By applying the polymer using a spouted bed apparatus with high expansion zone specially designed for fine particles [9] and subsequent hot pressing, copper–polymer composites with a high filling degree of copper and high relative permittivity were obtained [10]. Currently, different polymers are evaluated regarding their final product properties to produce tailor-made particles for a broad range of applications.

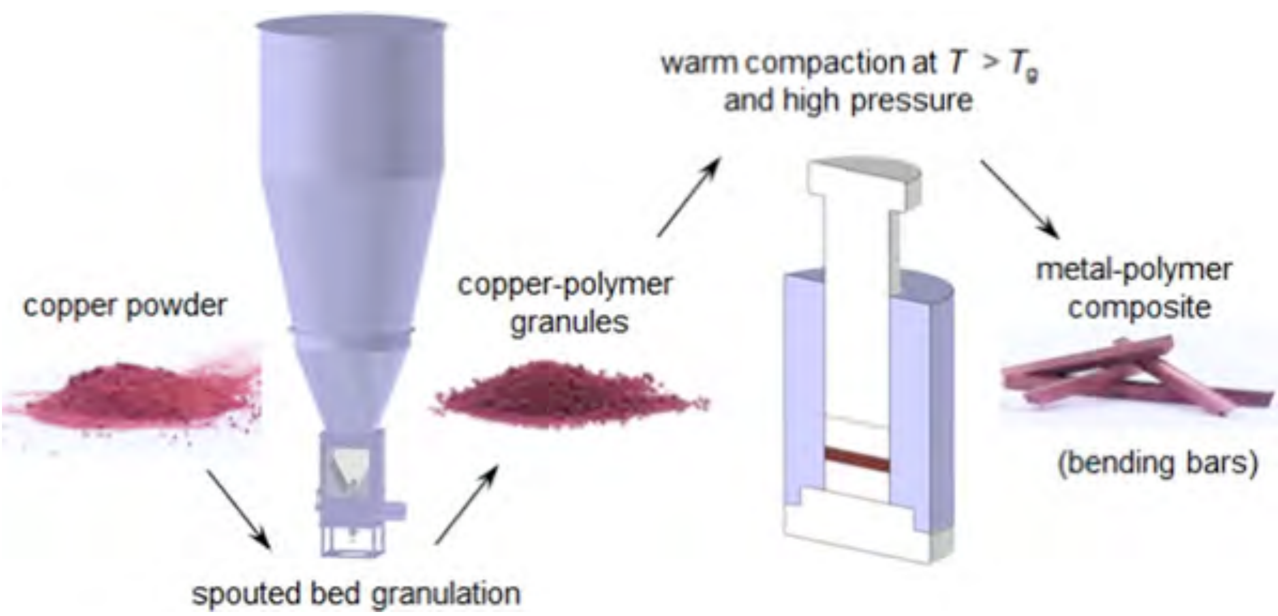

Figure 3: Production of metal-polymer composites by granulation in a specially designed spouted bed apparatus and following warm compaction.

Investigation of the dynamic behavior of spray granulation in a multi-staged continuous fluidized bed

As mentioned above, industrial fluidized bed spray granulation processes are often performed in continuous operation. In one project of the DFG priority program SPP 1679, headed by Prof. Heinrich, the dynamic behavior of a continuously operated fluidized bed with mill-sieving circuit (GF25, Glatt GmbH, Germany; Figure 1) is investigated experimentally and by CFD-DEM simulations. It was found that the drying potential has a major influence on the particle morphology during spray granulation of sodium benzoate particles. Both the drying temperature and the spray rate define the product morphology and result in very different product porosities [11]. The weirs installed between the four different chambers of the process chamber were found to have a significant influence on the dynamic behavior of the whole process. In a simplified apparatus geometry consisting of two chambers, the underflow and sideflow weir designs favored the directional transport along the horizontal fluidized bed, while the installation of the overflow weir and no weir lead to higher recirculation rates of the particles and, thus, stronger back-mixing [12]. Recently, a novel control concept for bed mass and particle size distribution was integrated resulting in an improved process stability [13].

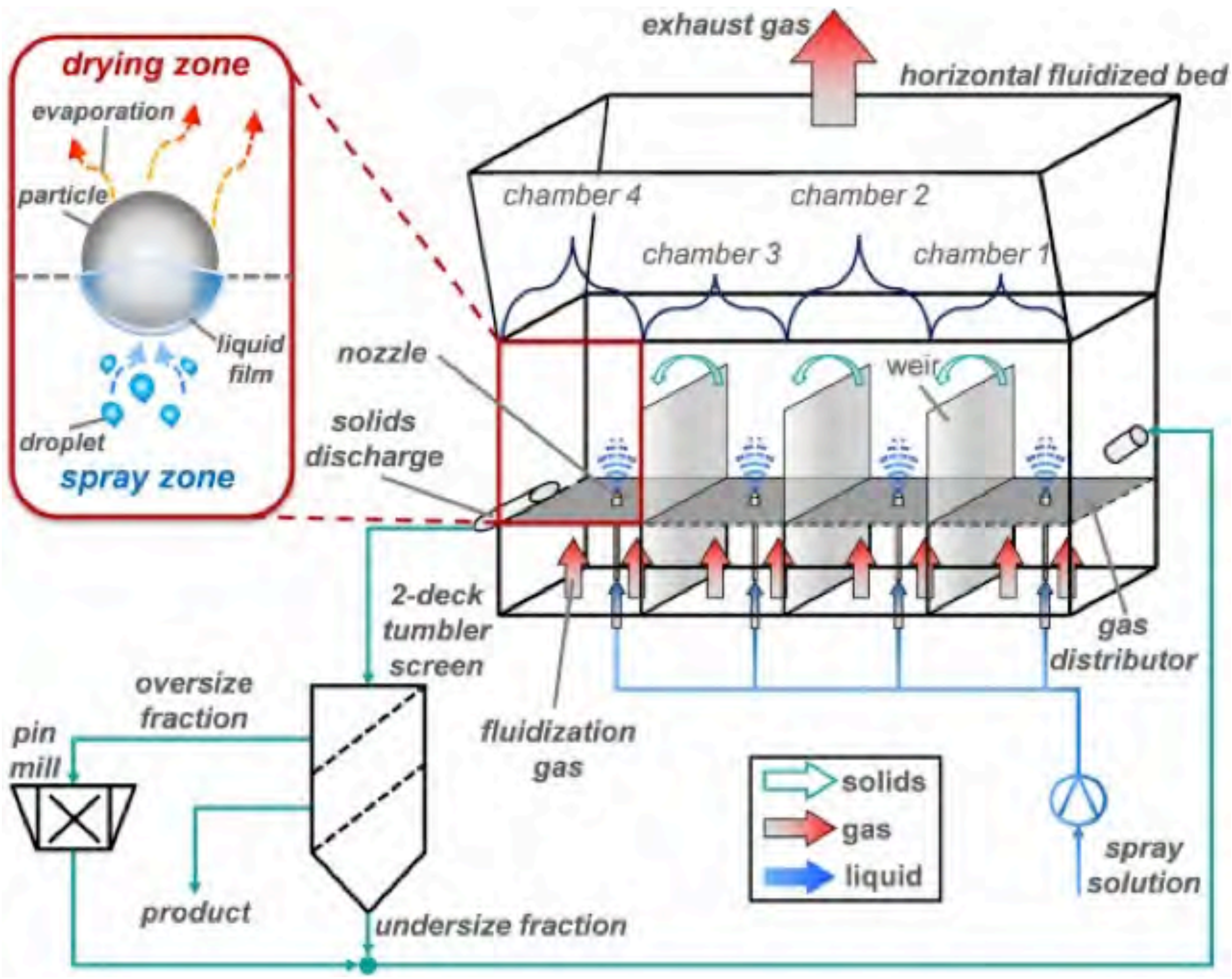

Figure 4: Scheme of a multi-staged horizontal fluidized bed apparatus with external product classification and internal zone formation.

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Special Recognition

Professor Raffaella Ocone of Heriot-Watt University, Scotland, was recently appointed Officer of the Order of the British Empire (OBE) for services to engineering in The Queen's 2019 New Year Honours.

Raffaella has about 30 years' experience in modelling complex systems and her area of experience includes hydrodynamics of granular materials, kinetics and thermodynamics of multi-component mixtures, and developing a model for chemical looping combustion for carbon capture and production of clean energy.

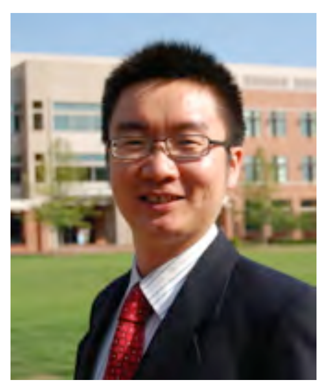
Raffaella is also the chair of the IChemE Research Committee and the chair of the Royal Academy of Engineering award committee. In 2018, she played a key role for the Research Excellence Framework (REF), the body that assesses the quality of research and studies in UK higher education institutions.

Raffaella said: "I am both humbled and honoured to have been awarded an OBE.

"I would like to take this opportunity to celebrate the international nature of engineering; the basis of my engineering skills come from Europe and the US, but I could have not reached what I did if the UK had not offered me huge opportunities to practise and enhance my skills."

"I have been lucky to live in countries without frontiers, free to move, to exchange ideas without any barrier. My hope is that the future generations can enjoy the same opportunities I had and be able to freely move and be enriched by diversity."

Molten Salt "Promoted" Mixed-Oxide Particles for Intensified Light Alkane Conversion



Fanxing Li

Associate Professor, Department of Chemical and Biomolecular Engineering

North Carolina State University

Molten salts have been used in glass manufacturing and metal extraction for centuries. In the modern days, they find applications in nuclear reactors, fuels cells, electrolysis, etc. A number of molten salts, with excellent solubility for oxides and/or unique redox properties, have been commercially used as catalysts for the production of SO_3, chlorine, and vinyl chloride.[1-2] While these liquid phase catalyzed reactions are not directly related to particle technology at a first glance, supported liquid phase catalysis, i.e. supporting an active molten phase on porous particles for catalytic applications, has been extensively investigated and commercially applied.

Given their applications in catalytic oxidations, it is not surprising that molten salts were investigated for selective oxidation of light alkanes, e.g. oxidative coupling of methane (OCM), in a number of studies since the 1980s by bubbling the gas through the liquid phase[3-5], on a porous support wetted by the molten salt[6], or through a molten salt modified mixed-conductive membrane.[7] In a recent study, molten salts on an oxide particle support were investigated in detail for oxidative dehydrogenation (ODH) of ethane.[8] In this case, the oxide substrate, i.e. Dy_2O_3 doped MgO (physical mixture), was covered with a layer of Li/KCl molten salt for ethane conversion into ethylene in the presence of gaseous oxygen. It was determined that the molten salt layer blocks the non-selective sites on the oxide while facilitates the activation of oxygen at the molten salt/MgO interface. Compared to the molten salt catalysts on porous supports, this Li/KCl on MgO/Dy_2O_3 catalyst takes the advantage of the surface catalytic activity of the oxide substrate, in addition to the benefits of ease in solids handling (v.s. molten liquid) and improved mass transfer.

Besides the intentionally designed, supported molten salt catalyst mentioned above, recent advances in *in-situ* and *operando* characterization techniques have revealed that some "classical" oxide catalysts, which were long considered as solid heterogeneous catalyst particles, consist of a molten active phase on the surface as well. For instance, the NaW-MnO_x-SiO_2 catalyst for OCM was revealed, by ambient pressure XPS (AP-XPS), *in-situ* XRD and *in-situ* TEM, to contain a molten Na_2WO_4 phase under working conditions in a paper published in 2017.[9] The active species was reported to be Na_2O_2 which is responsible for the formation of OH radicals. The latter is important for the gas phase OCM reactions.

Our group has been working on intensified olefin production from light alkanes (e.g. ethylene) via oxidative dehydrogenation[10-11] or oxidative cracking[12] approaches using redox catalyst particles, i.e. a redox-active (mixed) oxide that acts both as a catalyst and an oxygen carrier. When applied for ethane ODH reactions, the redox catalyst particles first converts ethane into ethylene and water using its active lattice oxygen. After completing this ODH step, the oxygen depleted redox catalyst is exposed to air (and/or steam), to replenish the lattice oxygen. This chemical looping – oxidative dehydrogenation (CL-ODH) process can be carried out either in circulating fluidized beds similar to a CFB combustor or parallel packed beds operated similar to the Houdry process. The advantages of the redox catalysts and CL-ODH compared to conventional, heterogeneous catalysts include: (i) integration of catalytic reaction with air separation (a simpler and safer process); (ii) potential to achieve high selectivity (absence of gaseous oxygen inhibits side reactions); (iii) potential to tailor heat of reactions in the redox steps for improved heat management.[13-14] Our recent studies indicated that up to 84% energy savings and emission reductions can be realized by CL-ODH.[13] From a particle technology and catalysis standpoint, it is particularly interesting that a number of redox active oxides supported molten salts performed rather well for ethane ODH, methane OCM, and oxidative cracking of naphtha. In most cases, a core-shell structure with the mixed oxide being the core and the molten salt being the shell, is formed.[10, 15] While the salt and mixed oxides could react at elevated temperatures to form additional phases, such phases can be largely avoided by carefully selecting the mixed oxide and salt species to arrive at a relatively simple core-shell particle with a well-defined molten shell. This article intends to share with the PTF community a number of interesting findings related to the design of these unique redox catalysts for ethane ODH, based on our recent published and unpublished results.

In terms of overall design considerations, we identified two methods to tailor redox catalysts for ethane CL-ODH. Type I catalyst can be simply an oxide that is selective for hydrogen combustion (SHC).[16] The SHC concept can work well by simply coupling gas phase ethane cracking reaction with a redox catalyst that only selectively oxidizes the H_2 formed in the gas phase into water. Type II catalyst, on the other hand, should be catalytically active for hydrogen abstraction from ethane with limited activity for re-adsorption and subsequent combustion of ethylene products.[17]

With respect to type I redox catalyst, we found that a Na_2WO_4 salt coated Mn oxides, e.g. Mg_6MnO_8, and $CaMnO_3$, being pretty effective.[12, 18-19] Without Na_2WO_4, the Mn oxides are nearly 100% selective towards CO_2. The presence of Na_2WO_4 layer, which becomes a molten phase between 600 and 700 °C according to differential scanning calorimetry (DSC) and *in-situ* XRD, largely inhibits the formation of CO_2. We further determined that the Na_2WO_4 layer is electronically conductive. In addition, it can transport lattice oxygen from the mixed-oxide substrate via redox reactions between WO_4^{2-} and WO_3^-. The coverage of the mixed oxide with the molten Na_2WO_4 shell limits the accessibility of C_2H_6/C_2H_4 to the non-selective mixed oxide surface. Meanwhile, the lattice oxygen shuttled by the molten salt facilitate selective hydrogen combustion at the gas/liquid interface. Figure 1 shows the low energy ion scattering results confirming the surface coverage of W and Na. Figure 2 illustrates the general reaction pathway for a Na_2WO_4(melt)@Mg_6MnO_8 in ethane ODH reactions.

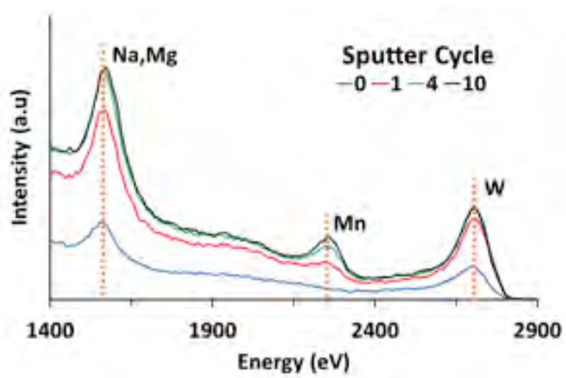


Figure 1. Low energy ion scattering results confirming the surface coverage

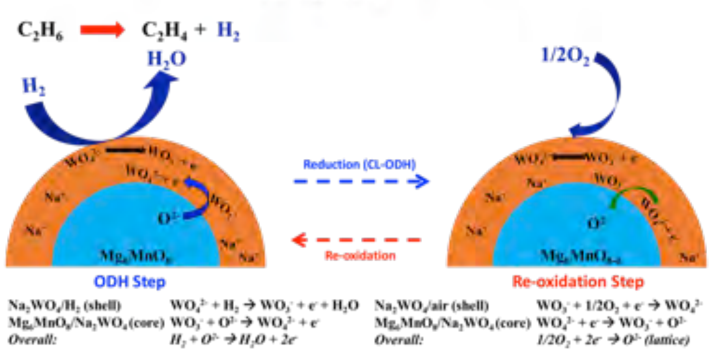


Figure 2. Proposed reaction mechanism of the CL-ODH reactions in the presence of a Na_2WO_4(melt)@Mg_6MnO_8 redox catalyst[10]

In terms of type II redox catalyst, we also discovered a number mixed oxides (e.g. perovskites) and molten salts being particularly effective. Our recent investigations indicate that peroxide species are likely to be responsible from hydrogen abstraction from the very stable C-H bond. Such peroxide species can be generated at on the oxide surface and transported by the molten salt to the gas-liquid interface. While Type I and Type II redox catalysts appear to operate under different reaction pathways, one can certainly envision a redox catalyst that combines the functions of both catalysts, i.e. a type I redox catalyst with high SHC selectivity could further benefit from an active surface which is effective for H abstraction and radical initiation.

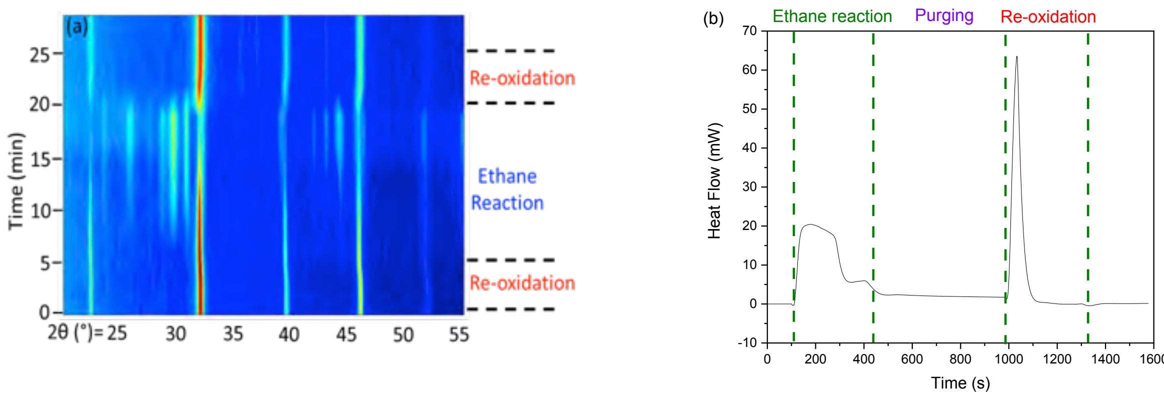


Figure 3. (a) in-situ XRD of a perovskite@molten salt catalyst particle showing reversible phase transition under redox conditions; (b) DSC results during the ethane CL-ODH reactions, both steps are mildly exothermic.

Another potentially interesting aspect of this redox catalyst design strategy is the ability to independently tune the properties of the oxide substrate and the molten salt. As Figure 3 illustrated, the heat of reactions of ethane CL-ODH can be tuned to be mildly exothermic in both the ethane ODH and the re-oxidation steps for a type II redox catalyst, allowing more efficient heat management. A type II redox catalyst was tested for over 400 hours in a large packed bed at our lab, showing excellent performance and durability (Figure 4).

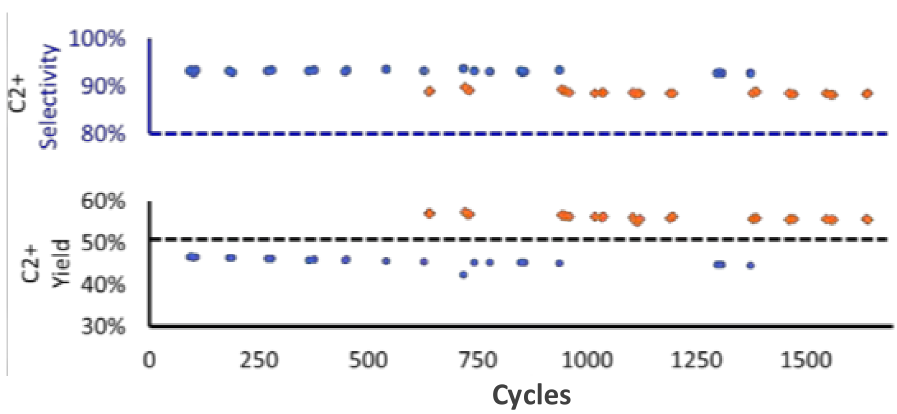


Figure 4. 1600 cycle results of a molten salt promoted redox catalyst for ethane ODH. The two sets of dots show operations at two different space velocities.

Again, this short article is intended to share our most recent findings with the community and to receive feedbacks. Although we cannot cover the concept extensively due to page limitations, our recent results do indicate the applicability of this general approach to convert a number of light alkanes to value-added olefins. The high tunability of the catalysts' redox and surface properties and their ability to integrate separation with chemical reactions, allow significant potential to design improved processes for chemical production with reduced energy/CO_2 footprints. Moreover, the potential applications of these liquid coated particles can go far beyond light alkane activation.

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MFiX-Exa: A CFD-DEM Code for Exascale Computers

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A much-anticipated milestone in high performance computing (HPC) will be reached in the next few years, the milestone of exascale computing or HPC systems capable of at least one exaflops, which is 10^{18} (a quintillion) floating point operations per second. Such computational power will enable gas-solids flow computations at resolutions hitherto impossible. A computational fluid dynamics–discrete element model (CFD-DEM) code called MFiX-Exa is being developed to conduct gas-solids flow computations efficiently on current and exascale computers [1].

Exascale Computing Project

In the United States, the U.S. Department of Energy (DOE) is spearheading the development of exascale computers. DOE has announced the delivery of two exascale computers. The first, named *Aurora*, will be delivered to Argonne National Laboratory in 2021 by Intel and sub-contractor Cray. A second computer, named *Frontier*, with a performance of greater than 1.5 exaflops, will be delivered to Oak Ridge National Laboratory in 2021 by Cray and AMD.

To achieve useful exascale computing power, these computers must meet several technical milestones such as billion-way concurrency, high resiliency, and low power consumption, which lead to computer architectures that are different from the current generation of HPC systems. Existing application codes may not run efficiently on the new architectures. DOE's goal is not just to increase the theoretical peak performance, but rather to achieve demonstrable 50X capability improvement in application codes against existing 20 petaflops machines. To that end, two DOE organizations– the Office of Science and the National Nuclear Security Administration—launched a collaborative effort in 2016 called the Exascale Computing Project (ECP) with the mission to [2]

•Deliver exascale-ready DOE applications and solutions that address currently intractable problems of strategic importance and national interest.

•Create and deploy an expanded and vertically integrated software stack on DOE HPC exascale and pre-exascale systems, defining the enduring U.S. exascale ecosystem.

•Leverage U.S. HPC vendor R&D activities and products for use in DOE HPC exascale systems.

The ECP comprises over a hundred subprojects, each executed by small teams of five-to-twenty domain scientists, computer and computational scientists, applied mathematicians, graduate students, and postdoctoral associates and led by a Principal Investigator (PI) within a tightly defined scope, schedule, and budget. The ECP is led by a management team drawn from six DOE national laboratories. Its PIs and scientists are drawn from over 50 laboratories, universities, and vendors. The ECP is organized into three technical focus areas: Application Development, Software Technology, and Hardware and Integration. Application Development is responsible for delivering science-based applications that can exploit exascale for high-confidence insights into and answers to critical problems in national security, energy assurance, economic competitiveness, and health care. The Co-Design Centers within Application Development target crosscutting algorithmic methods that capture the most common patterns of computation and communication, known as motifs. Software Technology concentrates on developing a comprehensive and coherent software stack that will enable application developers to productively write highly parallel applications that can portably target diverse exascale architectures. Hardware and Integration supports vendor and lab hardware R&D activities required to develop node and system designs for at least two capable exascale systems with diverse architectural features.

MFiX-Exa Subproject

MFiX-Exa is one of around 25 application subprojects under ECP. It is led by Dr. Madhava Syamlal of the National Energy Technology Laboratory (NETL) with co-PIs Dr. Jordan Musser (NETL), Dr. Ann Almgren of Lawrence Berkeley National Laboratory (LBNL), Dr. John Bell (LBNL), Dr. Christine Hrenya of University of Colorado, Boulder (CU), and Dr. Thomas Hauser (CU). NETL and CU represent more than six decades of experience in multiphase modeling and the MFIX code, while LBNL brings the same level of expertise in large-scale, multiscale multiphysics applications. Altogether, the MFiX-Exa leadership team is characterized by more than 90 years of relevant experience.

MFiX-Exa Challenge Problem

MFiX-Exa subproject is focused on solving a challenge problem aligned with DOE's goal of developing advanced carbon dioxide (CO_2) capture technologies for fossil fuel power plants, which must employ cost-effective carbon capture and storage technologies to ensure that the United States will continue to have sustainable, reliable, and affordable low-carbon energy. A method that could reduce the CO_2 capture costs is combusting fuels in chemical looping reactors (CLRs). Chemical looping combustion occurs in two reactors that avoid the direct mixing of fuel and air. A fuel reactor utilizes oxygen from oxygen carrier particles—such as metal oxides instead of air—to combust fossil fuels such as methane. An air reactor then regenerates the spent oxygen carrier particles with oxygen from air. The air reactor produces a hot air stream that is used to raise steam to drive a turbine for power generation; the fuel reactor produces gases from which CO_2 can be easily captured.

NETL's 50 kW chemical looping reactor. In the fuel reactor (left), a fuel such as methane reacts with an oxygen-carrier material. The reduced oxygen carrier is sent to the air reactor (right) where it is regenerated to its oxidized state. Then the oxygen carrier is returned to the fuel reactor. Courtesy: NETL

The challenge problem involves a CFD-DEM simulation of a 50 kW CLR at NETL [3]. The simulation will track 5 billion DEM particles for a sufficiently long period so that exit gas compositions reach a pseudo-stationary state, enabling the evaluation of reactor performance. It will represent the full-loop geometry, covering various gas-solids flow regimes occurring in the CLR (bubbling bed, riser, cyclone, standpipe, and L-valve) and include chemical reactions and interphase mass, momentum, and energy transfer. Without the capabilities of MFiX-Exa at exascale, it is not possible to resolve the distribution in particle-scale properties (size, density, chemical conversion) in simulations of gas-solids reactors at this scale.

Algorithmic Advances

The fundamental approach used to solve the MFiX-Exa challenge problem is CFD-DEM. This methodology tracks individual particles using DEM while the gas flow is calculated with CFD [4]. This method provides greater fidelity than the two-fluid model (TFM) and multiphase particle-in-cell (MP-PIC) methods currently popular in industry. By resolving the particles individually, the model does not need to use the approximations that reduce the fidelity of TFM and MP-PIC methods.

Although MFiX-Exa builds on the multiphase modeling expertise embodied in NETL's MFiX-DEM code, the core methodology has been both re-designed and re-implemented. The foundation for MFiX-Exa is the AMReX software framework supported by the ECP Block-Structured Adaptive Mesh Refinement (AMR) Co-Design Center [5].

MFiX-Exa uses more efficient algorithms than MFIX for reducing the computational time. A new CFD algorithm has been implemented in MFiX-Exa that leverages discretizations and linear solvers already available through the AMReX framework. Tests have shown that the new algorithm reduces the computational time for the CFD calculations by 4X. The new algorithm is expected to perform even better in the challenge problem simulation, which will use many more cores on an exascale machine.

In the DEM, tracking the collisions between the particles and the reactor walls requires considerable computational time. A new algorithm that calculates the distance to the nearest wall once, stores that value, and reuses it for millions of repeated calculations was implemented in MFiX-Exa, which has considerably reduced the time required for the DEM calculations.

The finer the mesh, the greater the accuracy with which geometry and flow features can be simulated, but the computational time is also greater. A recent success of the subproject was in enabling localized mesh refinement to more accurately resolve the shape of the CLR while not over-refining the interior of the reactor to considerably reduce the computational time without the loss of accuracy. Also, the ability to eliminate unneeded mesh in regions outside the CLR itself—i.e., the empty space between the fuel and air reactors—was implemented. For the challenge problem geometry, this will reduce the mesh size by 10X.

Next Steps

The most important next step for the MFiX-Exa team is to ensure that MFiX-Exa code can run effectively on hybrid CPU/GPU architectures expected in exascale machines. The first stage of development has focused on running MFiX-Exa on multicore architectures such as National Energy Research Scientific Computing Center's *Cori* machine. The next stage will focus on running MFiX-Exa effectively on machines like the Oak Ridge Leadership Computing Facility's *Summit*. Currently, the particle-particle collisions can be offloaded to the GPUs; work to migrate more of the algorithm to the GPUs to reap the benefit of the GPUs' compute power is in progress.

The capability being developed in MFiX-Exa will enable several other applications such as the design and optimization of gas-solids reactors required for process intensification and modularization. The 1000X increase in the number of particles enabled by MFiX-Exa will unlock the ability to simulate a host of industrially-relevant problems, based on a 2016 consortium survey of >30 companies (chemicals, energy, petrochemicals, pharmaceuticals, specialty chemicals) [6].

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In Memorium - Frederick A Zenz (1922-2018)

Dr. Frederick Zenz, 95, died Wednesday, February 28th at Vassar Hospital.

Born on August 1, 1922 in New York City, Dr. Zenz began his illustrious career in 1942 with the M.W. Kellogg Co. as a process development engineer. Two years later, he began working for the Kellex Corporation on the MANHATTAN PROJECT during World War II. From 1946 to 1962, he worked for HRI, M.W. Kellogg and Stone & Webster Engineering. In 1962, he became an independent consultant.

During his career, he also taught at Manhattan College, during which time he became the Technical Director of Particulate Solid Research, Inc. (PSRI), an industrial research consortium, from 1971 to 1989. He also founded and served as Technical Director of A.I.M.S. from 1989 and 2007. He authored at least 90 published papers, 18 book chapters, countless research papers for PSRI and A.I.M.S. and held 20 patents. In 1960, he co-authored one of the most influential books in engineering: Fluidization and Fluid-Particle Systems. His third and last book was published in 2015. He was named one of "30 Authors of Groundbreaking Chemical Engineering Books" and as one of the "100 Chemical Engineers of the Modern Era." He had a great passion for his field in engineering coupled with a strong work ethic, working until the last weeks of his life.

He is survived by his wife of 69 years, Elizabeth; 3 children, Dennis, Jonathon and his wife Donna, and Terese and her husband Jim; 9 grandchildren; and 2 great-grandchildren.

292 - Special Session: Celebrating Career Accomplishments of Fred Zenz

Tuesday, November 12, 2019 - 8:00 AM - 10:30 AM at *Hyatt Regency Orlando - Bayhill 19*

Description

As the author of at least 90 published papers, 18 book chapters, and co-author of the influential "Fluidization and Fluid-Particle Systems", Dr. Frederick A. Zenz can be regarded as one of the pioneers in modern fluidization practice. In this session, Dr. Zenz and his significant contributions will be remembered and celebrated.

Research Burgeons When Particle Technology Come across Mesoscience

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As witnessed in the international conference, *Fluidization XVI*, held recently in Guilin, China, particle technology continues to expand not only in traditional industries but also in fledgling fields such as catalysts, bio-materials, and nano-technologies, etc. On the other hand, the wide spreading application of particle technology also inspires contemplation about the common challenges and possible directions in its future development. To this end, it is meaningful to look for some clues between particle technology and the germinating *mesoscience*[1-2] which can find one of its roots in the energy-minimization multi-scale (EMMS) model for gas-solid systems[3-5].

Mesoscience is defined as a transdisciplinary science to cope with multiple levels of complexity at mesoscales or in mesoregimes[6]. Apart from the multi-phase systems in chemical engineering, the mesoscale convection systems (MCS) in meteorology and oceanology, the interfacial phenomena of nano-materials, and the protein folding in bio-chemistry all carry such complexity. Recent developments have shown that such complexity can be characterized by the *compromising in competition* of different dominant mechanisms in these systems[7]. Interestingly, when a single mechanism dominates, relatively simple behavior is found and quantitatively it defines the boundaries of the variable space of behavior. As demonstrated by Du et al.[8] for gas-solid system, the steady-state voidage of different fluidization regimes predicted by the EMMS model is actually enclosed by an upper limit of minimum energy dissipation rate and a lower limit of maximum energy dissipation rate, while other extrema of energy consumption terms lead to intermediate curves locating within the two boundaries. A similar study on gas-liquid bubbly flow reveals the same behavior for the gas holdup[9], indicating the generality of such behavior.

Beyond multi-phase flow, mesoscale models have been established for heterogeneous catalysis also[12], where the relevant processes are reaction, diffusion, adsorption and desorption. It was found that, while reaction may lead to the clustering of the products, the other factors may contribute to their homogenization[13]. A stability condition was thus proposed to close the models, which can capture the main features of the corresponding simulation results obtained under various conditions using the kinetic Monte Carlo (KMC) method.

Mesoscale structures were also studied in the synthesis of materials[14, 15]. Three growth modes, reaction-limited, diffusion-limited, and reaction-diffusion balance, were achieved for silver particles, which were well defined the shape evolution of particles, and it was found to be applicable to copper and gold, as well as calcium carbonate particles. In the surrounding region of the growth front, the consumption of monomers outpaces the rate of replenishment, creating concentration gradient regions, which induces a kind of instability of the growing front. The concentration gradient drives a preferential growth perpendicular to the gradient, generating anisotropic structures. The secondary nucleation on the side of the primary structure leads to the formation of complex structures such as dendritic structures[16]. The regulation on the reaction and diffusion for shaping particle provides a powerful technique for the rational synthesis of materials.

Another example is the mesoscale research on bio-particles which is still being conducted. Bio-particles assembled by many bio-molecules such as proteins, have attracted accumulating attention in bio-engineering in recent years. Among them, virus-like-particles (VLP) composed by one or more types of protein subunits to form the native viral conformation whilst containing no genetic material and therefore incapable of spreading infection, is one of the hot topics in the field of biopharmaceutical engineering[17]. For the widely existed icosahedron VLP, the protein subunits first assemble into pentamers or hexamers, which are referred as the mesoscale structures of the VLP, and then these ordered pentamers or hexamers further assemble into the complete icosahedron structure of VLP. Manipulation of the mesoscale structure through modification of the protein structure or the solvent formulation so as to obtain stable VLP with highly efficient antigens is one of the most challenging problems in bio-engineering.

Mesoscience and its application[18-21] in multiphase flow and other systems have invoked widespread attentions[22-24]. To foster the networking and collaboration of researches worldwide on mesoscience, a preparatory meeting of the International Panel of Mesoscience (IPM) was held during 27–29 May, 2018 in Beijing[25]. Over 30 scientists from 8 countries, though working in different disciplines, gathered to discuss the status and forward pathways for mesoscience, as summarized by the consensus announcement, *A Call for Work on Mesoscience*. The development of mesoscience attracts continued supporting from the Chinese Association of Science and Technology (CAST), National Natural Science Foundation of China (NSFC), and Chinese Academy of Sciences (CAS). An upcoming website which can be accessed through "http://www.mesoscience.org/" will provide more information and latest progress. In particular, the major research plan on mesoscience initiated by NSFC, "Mechanism and manipulation of meso-scales in multi-phase reaction processes", has been leading Chinese scientists in chemical engineering to focus on mesoscale problems at various levels. The plan deployed 117 projects which were assigned to more than 36 research institutes. These projects stimulate substantive cooperation among disciplines of chemical engineering, mathematics, physics, biology, and scientific computing, etc. Thousands of researchers and students are thus attracted to the study of the mesoscience with wide-ranging topics on multiphase reactors, material design, catalysis, energy storage, separation, and on various methods to model and simulate the complex systems involved. This is certainly a piece of good news for both the relevant engineering fields such as particle technology and mesoscience as a whole.

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Scaling Up Granular Fluid Reactors

PSRI

Ray Cocco,

S.B. Reddy Karri

As far as chemical reactors are concerned, fluidized bed and circulating fluidized bed (CFB) reactors tend to be on the top of the list in terms of difficulty. They are difficult. Gas and solids motion can lead to erosion and attrition, gas distribution is critical, solids collection impacts downstream contamination, environmental issues, and additional catalyst costs. However, all these difficulties can be mitigated or managed effectively such that a fluidized bed reactor could be the right choice for an economically profitable process.

However, the practice of putting a fluidized bed reactor in the ground comes with a flood of challenges, not technical challenges but management challenges. For most chemical engineers, fluidized beds and CFB reactors are a complete unknown. In the US, an undergraduate in chemical engineering may see only a one or two hours on fluidized bed concepts, at best. These undergraduates grow up to be managers, and now you are proposing to build a $0.5 to $2 billion US dollar petrochemical or chemical plant based on the mysterious fluidized bed which is known for scale-up problems.

However, scaling up a fluidized bed poses no more challenges than any other reactor. The issue is that most engineers use the scale-up concepts from these other reactors for the scale-up of a fluidized bed reactors. Challenges are not any more complicated or numerous than with a plug flow reactor, they are just different.

This is where Particulate Solid Research, Inc. or PSRI comes in. We have been providing scaling up procedures for almost 50 years that results in on-time start-up to full capacity with better than expected reliability and lower operationing costs. Our success comes from the marriage of experiments done on the correct scale, with applicable modeling, and having world renowned experts. Our work process has resulted in successful scale-up for fluidized catalytic cracking, coal and biomass gasifiers, coal and biomass pyrolysis, chemical looping, catalytic oxidation, oxychlorination, titanium dioxide production, acrylonitrile production, methane to olefin process, ethane and propane dehdrogenation process, polycrystalline silicon production, polyolefin production, sulfur capture, CO_2 capture, etc [1].

The PSRI Scale-up Process

PSRI has the capability of providing the large-scale experiments, the modeling, and the expertise needed for successful scale-up of commercial fluidized bed and CFB reactors. PSRI has the experimental capabilities to further explore and validate fluidization design concepts including 3-ft (0.9-m) diameter x 90-ft (27-m) tall CFB riser, an 18-in (0.5-m) diameter x 90-ft (27-m) tall CFB riser, several 12-inch (0.3-m) x 72-ft (21-m) tall risers, a 7-ft (2.1-m), 5-ft (1.5-m), and several 3-ft (0.9-m) diameter fluidized beds, cyclones, conveying lines, etc. Wall effects are typically significant on the hydrodynamics of small-scale units, in contrast to the larger commercial units. The small-scale units may exhibit different flow regimes, including slugging, than those in large-scale units (bubbling and turbulent beds). Thus, experiments need to be done on a large-scale to fully capture the parameters that are important for the design and operation of a commercial fluidized bed or CFB unit. PSRI has shown that cold-flow simulations of a stripper operation less than 3-ft (0.9-m) in diameter are affected by wall effects. In a fluidized bed (without internals) of Geldart Group A powder, the vessel diameter needs to be at least 12-inches (0.3-m) in diameter. For Geldart Group B powder, the vessel diameter needs to be even larger (i.e., slugging, etc.). With risers, the diameter also need to be at least 12 inches (0.3-m) and over 60-feet tall to ensure a fully developed flow regime.

PSRI has a wide range of modeling capabilities including population balance models (PBM), reduced-order models (ROM), computational fluid dynamics (CFD), and discrete element method (DEM) models via Barracuda VR and Star CCM+. Many projects involve using a combination of models to assist with scale-up. A CFD model may help with solids injection location but cannot help with attrition modeling. Thus, a PBM is needed as well. Kinetics are often better with ROMs than when fully integrated into a CFD model. Furthermore, CFD models are not ideally designed for larger number of simulations that is often needed model parameter estimation (i.e., empirical fits). Although this is often needed to capture detailed hydrodynamics in a fluidized bed or CFB (i..e, drag model). Yet, a ROMs may not be able to provide the global 3D hydrodynamics in a fluidized bed.

Finally, PSRI has a wide range of world-renowned experts such as Greg Mehos, Manuk Colakyan, Ulrich Muschelknautz and C.J. Farley along with Ted Knowlton and S.B. Reddy Karri to provide expertise in all aspects of granular fluid flow problems involving fluidized beds and CFBs, cyclones, diplegs, hoppers, conveying lines, purge bins, slurry columns, risers, heating coils, gas distributors, feeders, injectors, etc. [2].

Figure 1 provides an example of how these capabilities are integrated into one work process. The Problem is scaling up a new process. It starts with experts developing a conceptional design in which unknowns are defined, preliminary math models such as a PBM or a ROM are recommended, and a process risk analysis is applied. Then there is the Process Risk Analysis wherefrom the conceptual design, operating strategy and just about every other aspect of the unit are examined from a systems integration point of view. In other words, if something does not meet design specifications, how does that affect everything upstream and downstream of it. Such an exercise may only take a day or so, but it reveals what the key parameters needed for a successful scale-up and saves a lot of time and headaches later.

The next step would be to design the cold-flow experiments needed to address the perceived unknowns and measure some of the key scale-up parameters that were determined earlier. Cold-flow studies are also crucial in validating any preliminary models that were developed as well as providing further validation data for more advanced models to be developed. Without validation, models will be perceived by the management as useless, at best. At worst, the unvalidated model(s) are used to address key scale parameters which predict completely erroneous results.

Also, mathematical models in any form are limited in providing reliable predictions for entrainment, solids mixing, mass transfer, and bubble size without additional fitting parameters (tuning) for the drag and collisional stress models. These math models can be limited by the same deficiency. Models that have not been validated and tuned can only capture global effects at best. Local effects, such as bubbles, clustering, and micro-mixing are missed. Since most fluidized bed reactor applications are geared towards fast kinetics, local effects are controlling in most fluidized beds. CFD and DEM models often are the biggest offenders in this case. Some assume they are fundamental and need no tuning or even validation. However, many CFD and DEM models only capture bulk drag and particles stresses Interparticle forces, particle size distribution effects, and nearest-neighbor effects are not considered; yet, they can have a significant impact on fluidized bed and riser hydrodynamics [3-5].

There have been several incidents where CFD models were used to estimate the transport disengagement height and entrainment rate for a fluidized bed of Geldart Group A particles. The model over predicted the entrainment rate by more than 1000 times as clustering was not captured. The results were an oversized freeboard and oversized primary cyclone diplegs. The latter resulted in insufficient solids flux to keep the solids in the dipleg fluidized. As a result, plugging of the dipleg became a persistent problem. Fortunately, the aeration of the dipleg provided a relatively inexpensive solution to the plugging problem. The higher than required freeboard resulted in waisted capital, but did not compromise productivity or reliability.

In another case, a CFD model did not capture the correct bed expansions at higher pressures. This was most-likely due to a drag model limitation that could have been identified and fixed with cold-flow experimentation. Either a new drag model should have been applied, or the parameters in the drag model should have been fitted to the experimental data (i.e., tuning) or both.

However, the unvalidated model underpredicted the bed expansion, and when the unit was built, the freeboard region and cyclones became flooded during operations. At this point, the solution was to lower the bed, increase the freeboard region, run at lower feed rates, or run at a lower pressure; none of which were desirable.

In each case, providing appropriate cold-flow experiments to help validate and develop the models needed to do the simulations could have alleviated these problems. For fluidized bed scale-ups, the model needs to capture, at the very least, the measured bed density, gas tracer RTD and solids mixing as defined by a Peclet number. Only then would we consider such a model to be

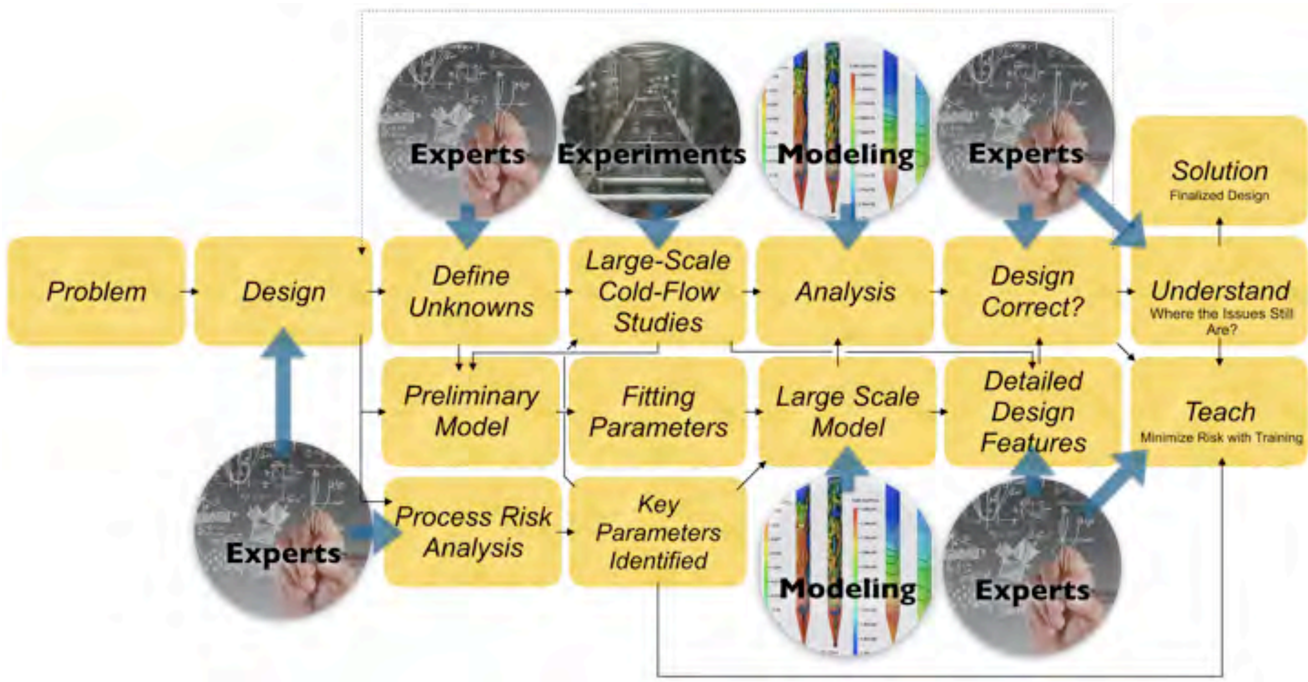

Figure 1: PSRI's work process for scaling up fluidized bed and CFB reactors.

Figure 2: PSRI's work process for retrofitting existing units with new technologies.

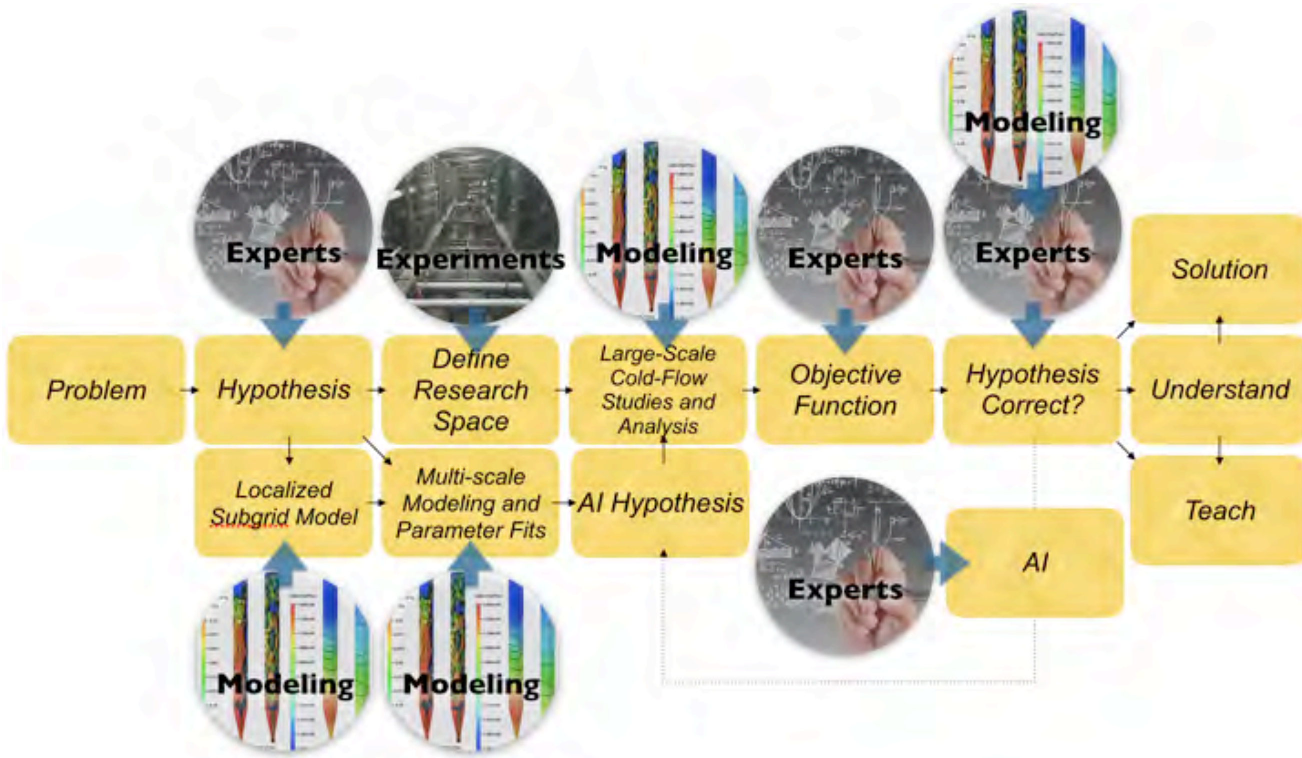

Figure 3: How a work process such as that used by PSRI for scale up might change with the incorporation of AL.

useful aid for scale-up. For a riser, the model needs to capture the core-annulus profile in all regions (developing flow, fully developed flow and termination) along with the level of backmixing.

Cold-flow experiments provide more than the data needed for model validation. If done correctly, cold-flow experiments can provide data on segregation, gas hold-up, and mass and heat transfer, particle collection efficiencies with cyclones, particle attrition, and the key source(s) of particle attrition. Particle losses can be significant if the fluidized bed unit is not designed correctly. In one situation, a fluidized bed reactor was losing $30MM per year in catalyst losses. However, with the right design, those losses were reduced to less than $150M per year. It was a great success story except it took years to implement the new designs.

A good cold-flow study uses a battery of analytics to get the data needed for successful scale-up. A typical run for a fluidized bed experiment should measure the bed density, entrainment, cyclone collection efficiency, fluidization quality, bubble hydrodynamics, and gas and solids tracers. Such information not only provides the data needed for scale-up but can highlights start-up and operational issues.

Gas bypassing can be one of these issues. Gas compression at the bottom of the bed results in less permeability of the gas into the emulsion phase [6]. The lower permeability provides an instability issue that can spark most of the gas to flow in a transient but stable stream of fastmoving bubbles, leaving a significant part of the bed defluidized. Often, gas bypassing is missed in pilot plants as they tend to have smaller beds and shorter bed heights and thus have less gas compression at the bottom of the bed. Cold-flow experiments, done at the right bed height, will capture this issue.

With cold-flow data in hand, a more detailed model may be value-added. From cold-flow experiments, validated preliminary models and the resulting parameter estimations, a full-scale model of the commercial unit may be warranted. Fortunately, today's CFD codes can handle such large problems and deliver results in a few weeks or less. With a large-scale CFD model, detailed design features such as riser termination design, baffle locations, sparger, feed locations, standpipe locations, and aeration ring location can be explored. Caution should be exercised if fast kinetics are incorporated into the CFD model as, noted above, micro-mixing is not captured well.

With the combination of cold-flow experiments, the resulting analysis, and the large-scale model, the design concept can be further scrutinized. Design corrections may be proposed by the experts which can tested with the large-scale model. In addition, more novel concepts can be tested as well, although such changes can add a host of non-technical challenges in an organization. Such concepts may be tabled for the next scheduled shut down or turn-around.

In the final stage, the experimental data, analysis, and models are in place to clearly define what is now understood and what is still not clearly understood. This is an excellent time to go back to the process risk analysis and make sure what is not understood does not result in a significant impact on start-up and profitability. It is also a good time to bring the process engineers onboard if you have not done so already. Many times a perfectly good design has been changed, for the worst, by process engineers who were not brought in early enough in the work process. The finalized design needs to be a team decision between the experts, project managers, research engineers, development engineers, stake-holders, and process engineers.

Yet, the work process is not done. The experts need to impart all learnings to those who will be involved with the engineering designs, fabrication, construction, start-up, and operation of the commercial unit. Many of which have had little exposure to granular-fluid flow. The team needs to be taught the fundamentals, design criteria, and operational criteria for building and running these units. The focus point needs to include the key parameters highlighted by the process risk analysis. This alone will have a significant impact on reducing design and fabrication errors as well as start-up delays. A Rand study [7] showed that processes with granular-fluid hydrodynamics have only a 50% probability of meeting start-up goals compared to the industrial standard of 90%. A significant contributor of this is due to neglecting the necessary training needed for commercializing fluidized bed and CFB reactors.

Beyond the Scale-up

The scale-up is done, and your start-up was a big success. It five to seven years from start-up and the unit is scheduled for a shutdown or turn-around in a year. The last few years provided additional learnings, and some modifications are likely to be needed. Perhaps a better catalyst is being applied, or the feedstock or product mix needs to be changed. Regardless, there is a likelihood of an equipment change with the scheduled shut down. Fortunately, a similar process can be applied, as shown in Figure 2.

The previous large-scale model or even a better one is available. Experts will be needed to define the research space. Is modeling enough or should some additional cold-flow experiments be needed? For novel retrofit designs, both are usually required. What is different though is the timeline. Retrofits tend to have a more compressed timeline. Model development or even usage as well as the number of experiments needed for validation of the new concept will have to be selected. Again, this is were we depend on the experts to help limit what is a must to do or a nice to do. There have been many success stories with retrofits that use both modeling and experimental tools to understand what is changing. There has been even more stories of unsuccessful retrofits because those tools were not used. New processes are expected to have problems; retrofits are not. One should use all the tools at their disposal (Experiments, Modeling, and Experts) to reduce unexpectedly extended downtimes.

West World

In the future and maybe the not to distance future, this work process will change. As computers get faster, the understanding of particle physics is better, and artificial intelligence (AI) becomes mainstream, both the experimental and mathematical modeling resource loads should significantly reduce. AI will provide a better design of experiments while using an earlier formulated large-scale, multi-scale model supported by a predetermined subgrid model for localized effects. Cold-flow studies will still be needed as there will always be unknowns, at least in our lifetimes. Thus, the tools remain the same: Experiments, Modeling, and Experts. Figure 3 gives a good example of this modified work process.

The role of the expert, however, does change. Experts will be needed to not only generate hypotheses but to develop the objective function and validate the final results. However, Experts will be doing less process risk analysis and detailed design features. Here, AI will be able supplement these task by exploring all options in a systematic but optimized fashion with respect to the objective function. For example, AI will test all the scenarios and not the likely scenarios with the process risk analysis. The detailed design would be treated in a similar fashion where, for instance, all the possible locations for the feed injects can be explored and not just the obvious locations. Of course, the Experts will have to make sure that the path AI has taken make sense.

The final steps will be more critical than with today's work process. Knowing what we understand and don't understand will be harder as AI will be taking away some valuable experiences. Teaching will also be more critical here as well for the same reason. AI will reduce cost and reduce the time for delivery, but understanding and learning are path-dependent, and a short path reduces them. This is not to say AI is going to be bad, quite the opposite actually, but we may need to change our emphasis and order in Figures 1 and 3.

Summary

Successful scale-up, and retrofits, do not need to be expensive and time-consuming provided that the tools of Experiments, Modeling AND Experts are used appropriately in a systematic and organized fashion [8]. Communication is key between all these tools. Also, in the end, don't forget to review what still needs to be understood and to teach all those now on the team.

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PTF Dinner at 2020 AIChE Annual Meeting

Dinner Description

PTF Awards Banquet - B.B. King's Orlando

Date: November 13th, 2019 (Wednesday)

Time: Drinks and hors d'oeuvres 6pm-7:30pm, Dinner 7:30-9:30pm

Location: 9101 International Dr. # 2230, Orlando, FL 32819

(Only 0.6 miles from Hyatt Regency Orlando!)

Featuring live music by throughout the event.

Travel Grant

CPFD Sponsorship

PTF has extended the deadline for applications for the CPFD travel grant awards. It aims to support early registration to the Annual Meeting and one ticket to the PTF Awards Dinner. In addition, this award is intended to encourage the winners for future engagement in the PTF community. The awards are contingent on a candidate meeting the criteria and all four awards may not be granted every year. Interested graduate students whose advisor is a member of the Particle Technology Forum and who are planning on presenting a paper at the meeting (regardless of receipt of the award) should contact Professor James Gilchrist at gilchrist@lehigh.edu.

Upcoming Conferences

2020 Frontiers in Particle Science and Technology (FPST)

Frontiers in Particle Science & Technology
FPST

2020 Frontiers in Particle Science & Technology

Designer Particles: Product Engineering in Particle Technology

March 2020 in Houston, TX, co-located with the AIChE Spring Meeting

The 2020 Frontiers in Particle Science and Technology (FPST), hosted by the AIChE Particle Technology Forum (PTF) is proud to announce a conference focused on particle design in product engineering. The 2020 FPST will bring together practitioners and researchers in the field of particle science and technology.

This innovative 2.5 day program will provide plenty of opportunity for attendees to learn about the latest in particle technology research as well as network with other professionals in the field.

Program Highlights Include:

- **Keynote Presentations** from academic and industrial experts
- **Invited Technical Sessions** focused on particle design
- **Poster Session** featuring research of junior scientists from academe
- **Networking** receptions, coffee breaks, lunches, and more!

Learn more at www.aiche.org/fpst

Circulating Fluidized Bed 13 (CFB13)

http://cfb13.org

13th International Conference on Fluidized Bed Technology (CFB-13)

The 13th Conference in a Series

Following the successful CFB-12 Conference in Krakow, Poland, we are pleased to welcome you to the 13th International Conference on Fluidized Bed Technology, CFB-13, to be held on the campus of the University of British Columbia, Vancouver, Canada between May 11-15, 2020.

The CFB-13 conference seeks to bring together prominent and young researchers, educators and practitioners of circulating fluidized bed technology to share their impactful research discoveries, achievements and practicing experiences. Since CFB-11, the conference scope has also been extended to other fields of fluidization and fluidized bed technologies such as bubbling fluidized bed, turbulent fluidized bed and spouted bed.

Conference Themes

The CFB-13 Conference will continue in the tradition of this conference series dating from 1985, with its focus on the fundamental research and applications of fluidized bed technology. It will incorporate novel fluidized bed reactor technologies, especially those related to green processes, clean and renewable energy such as hydrogen and bio-fuels, and carbon capture and utilization such as chemical looping combustion and gasification. In addition to studies on fundamental and applied aspects of fluidized beds and fluidization systems, CFB-13 will also place an emphasis on fluidized bed technologies aimed at solving energy and environmental issues our society is facing. In addition, short courses taught by prominent experts will be offered on May 11.

Conference Topics

- Hydrodynamics of gas-solid flow
- Modeling and simulation
- Heat and mass transfer
- Scaling and scale-up
- Measurements and instrumentation
- Fluid catalytic cracking and other catalytic processes
- Combustion, pyrolysis and gasification
- Novel reactor design and assisted-fluidization
- Micro-reactor and nano-particle systems

Conference Accommodation

CFB-13 has negotiated a discount for conference delegates to stay at UBC Ponderosa buildings. Minutes away from the conference venue, Ponderosa offers single rooms and shared apartments, which you can book at a later date from the link at the conference website: www.cfb13.org. One can also choose to stay at various hotels across Vancouver. Hotels in downtown are only 12km from UBC.

Conference Organization

Local Organizing Committee

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Junnan Chao – University of British Columbia
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Conference Venue

CFB-13 will be hosted on the campus of the University of British Columbia in Vancouver, a city known around the world as both a popular tourist attraction and one of the best places to live, with significant tourist attraction sites such as Stanley Park, Capilano Suspension Bridge and Cypress Mountain Resort. Whistler, the world-renowned premium ski and outdoor destination is only two hours away.

Sponsorship and Contact Information

CFB-13 will offer opportunities for organizations to sponsor a wide range of events (Special/regular sessions, posters, banquet), as well as create dedicated Sponsor and Exhibition areas for you to showcase your products and services and to interact with all conference attendees over three full days of the conference. We encourage you to contact the Organizing Committee cfb13@chbe.ubc.ca to discuss your package.

CFB-13 Organizing Committee

2360 East Mall, Vancouver, BC V6T 1Z3, Canada

Website: http://cfb13.org

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THE UNIVERSITY OF BRITISH COLUMBIA
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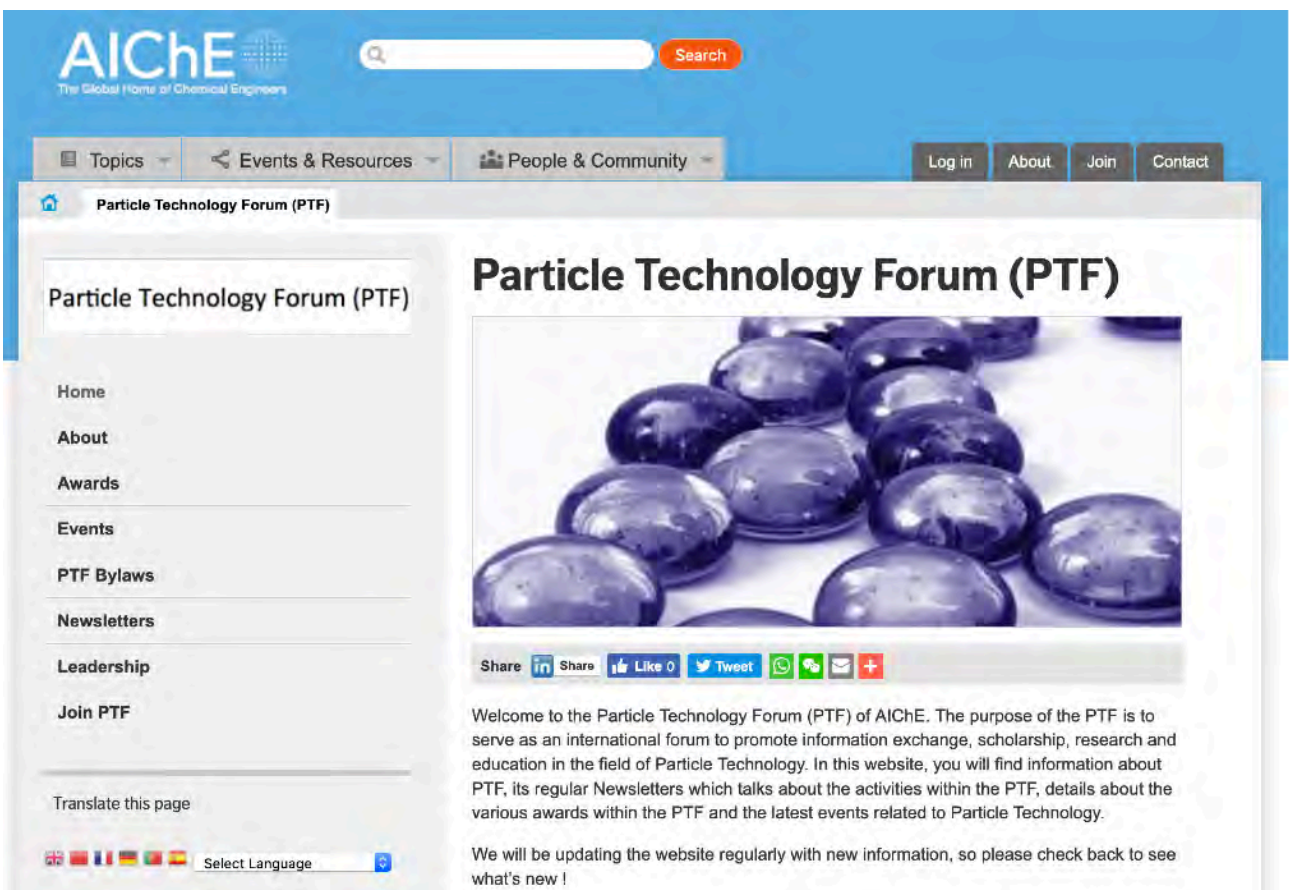
University of British Columbia, Vancouver, BC, Canada

Call for Nominations for Annual Meeting Programming Co-Chairs

Programming chairs are responsible for insuring the PTF sessions at the AIChE Annual Meeting are engaging, run smoothly, and represent the state of the art of particle technology. The candidates elected to the position of co-chair will serve a two year commitment (2020–2021) and then transition to area chair for another two years (2022–2023). Co-chairing offers the opportunity learn the programming system from the chair, and then step into the role to mentor a future co-chair. This position not only provides an excellent opportunity to contribute to the PTF leadership, those that serve have a direct impact on the quality of the Annual Meeting for all attendees. Please submit your nominations to the current (2018–2019) area chair (below), or directly to the PTF programming chair (Ben Freireich, ben.freireich@psri.org) before the Annual Meeting.

PTF Website

Check out the new and improved AIChE PTF website!!! The website now has all the historical PTF Newsletters (worth going back and reading them, if you want to learn more about the legacy of PTF), latest information on the PTF awards, the PTF leadership info, and the recent and upcoming events in the field of Particle Technology.



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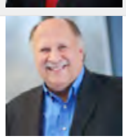
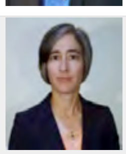
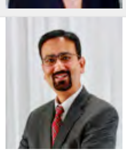
Willie Hendrickson whendrickson@aveka.com	
Dr. Brenda Remy Brenda.remy@bms.com	
Dr. Mayank Kashyap mkashyap@sabic.com	

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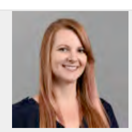
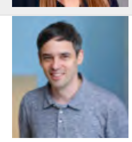
Dr. Heather Emady Heather.emady@asu.edu	
Dr. Aaron Moment ajm2293@columbia.edu	
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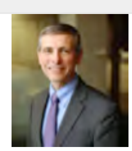
Dr. Richard Lueptow r-lueptow@northwestern.edu	

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