THE PARTICLE TECHNOLOGY FORUM (PTF) NEWSLETTER

An American Institute of Chemical Engineers (AIChE) Forum

A Glance at the Newsletter

Editorial

Dear Fellow PTF Members,

I hope you and your families are safe, healthy, and in good spirits amidst the ongoing global health crisis. When I edited and released the Spring newsletter towards the end of April

Message from the Chair

What a year we've had so far!! I hope that you and your families are safe and healthy and not impacted too much by the Covid Pandemic. I also hope that you benefited from the excellent article in the Spring Newsletter on working from home and COVID safety. Thanks very much to our editor Mayank Kashyap for writing this up.

One of the casualties of the Pandemic has been large conferences and live gatherings. We have seen the Spring AIChE meeting get delayed until later in August, along with our concurrent Frontiers in Particle Science & Technology Symposium. Both are now running virtually. Similarly, we have seen that most of our technical meetings for work have gone to a virtual mode to limit the potential for cross contamination of people. We have just received a final word that the Annual Meeting in the Fall, will be virtual, but we will still have our Awards ceremony, Awards Lectures and all of our sessions. Additionally, we will plan to recognize folks in person the following year when we are able. We will miss the interpersonal contact, I'm sure, but we will be able to enjoy the information sharing just the same.

In spite of the Pandemic, the business of the Particle Technology Forum continues. The sessions for the Fall

2020, I was hoping that the global COVID-19 situation would be much better at the time of the release of Summer edition. Unfortunately, this is not the case, not by a long shot. The ongoing pandemic has touched the lives of almost every human being on the planet, negatively affecting the physical, emotional and mental health of millions, if not hundreds of millions. In just 4 months, the global COVID-19 cases and deaths have increased by 8 and 4 times, respectively. In addition, the impact of pandemic on the global economy cannot be overstated.

You may recall the article I wrote in the last newsletter on the challenges and blessings of working from home, which included a few thoughts and recommendations on maintaining good physical, mental and emotional health during these unprecedented times. As the new school year begins, some of us return to our workplaces, and we enter the seasonal flu season, I believe that all of us have the responsibility of playing a role in slowing down the spread of COVID-19 by maintaining social distancing, wearing a face mask when around others, practicing good hygiene, monitoring our health daily, and following other public health guidelines

Annual meeting have been filled, the Awards for 2020 have been nominated and selected, and the Election of Officers for 2021-2022 and Liasons for 2021-2024 is in progress. There is more information later in this newsletter on some of these topics.

Finally you may have noticed our new PTF Logo selected by the EC and approved by the membership last fall. Likewise, The EC and our membership approved a "Statement on Diversity and Inclusion" at last fall's Annual meeting. This final version is reprinted later in the newsletter.

Please endeavor to remain healthy and maintain safe practices during this challenging time. We are all under strain of one sort or another. Some in not seeing loved ones, some in seeing too much of loved ones. Either way, patience and forgiveness of each other is a great "Best Practice" as we go forward.

Stay Safe, Stay Healthy, and we look forward to seeing most of you later this year, whether in person or virtually!

Regards,

Bruce D. Hook, The Dow Chemical Co.

Chair

Particle Technology Forum

from reputed health officials and sources.

"Alone, we can do so little; together we can do so much." – Helen Keller

In addition to taking a decision on organizing the 2020 AIChE Spring Meeting and 2020 Frontiers in Particle Science and Technology (FPST) Meeting virtually a few months back, AIChE has now decided to also make the 2020 AIChE Annual Meeting virtual. This newsletter includes information on some of those changes, AIChE PTF Statement on Diversity and Inclusion, contributions from two 2019 AIChE PTF award recipients, technical contributions from the industry and academia, Executive Committee (EC) election candidates at-a-glance, and more.

If you would like to contribute to the 2020 Fall newsletter, please contact me as soon as possible with your idea.

"If you are working on something exciting that you really care about, you don't have to be pushed. The vision pulls you." – Steve Jobs

Stay safe!! Stay healthy!! Stay strong!! Stay positive!!

Mayank Kashyap, SABIC

Editor

PTF Newsletter

AIChE Particle Technology Forum Statement on Diversity and Inclusion

Approved at 2019 AIChE Annual Meeting

The AIChE Particle Technology Forum is committed to maintaining a diverse and inclusive community of highly skilled chemical engineering professionals within the environment of the Institute and profession in which all members, regardless of characteristics such as gender identity and expression, race, religion, age, physical condition, disability, sexual orientation, educational level, socioeconomic class, nationality or ethnicity, are valued and respected."

As a global scientific and engineering society, we affirm the international principles that the responsible practice of science, free from discrimination in all of its forms, is fundamental to scientific advancement and human wellbeing, as outlined by the International Council for Science's (ICSU) Statute 51. We also affirm our commitment to an engineering and scientific environment that facilitates the planning, execution, review and communication of engineering and scientific work with integrity, fairness, and transparency at all organizational levels. This extends to our general scientific endeavors–including our professional interactions and engagement with other engineers, scientists, students, trainees, and the general public. We recognize that harm to our profession, our scientific credibility, individual wellbeing, and society at large is caused by not doing so.

To this end, the PTF will implement the principles of diversity, inclusivity, and equity within PTF leadership and membership to build a community across the chemical enterprise. We are committed to quantifying and monitoring our diversity at least annually at the Executive Committee and reported at the general business meeting.

2019 AIChE PTF Awards

Thomas Baron Award Sponsored by Shell

Small Particles, Big Science – An Overview of SIMPAS Work

Aibing Yu

Professor, Vice Chancellor's Professorial Fellow, Pro Vice-Chancellor and President - Suzhou

Department of Chemical Engineering

Monash University, Melbourne, Australia

Abstract

Particle science and technology is a rapidly developing interdisciplinary research area with its core being the understanding of the relationships between micro- and macro-scopic properties of particulate/granular matter – a state of matter that is widely encountered but poorly understood. The macroscopic behaviour of particulate matter is controlled by the interactions between individual particles as well as interactions with surrounding gas or liquid and wall. Understanding the microscopic mechanisms in terms of these interaction forces is therefore key to leading to truly interdisciplinary research into particulate matter and producing results that can be generally used. This aim can be effectively achieved via particle scale research based on detailed microdynamic information such as the forces acting on and trajectories of individual particles in a considered system. In recent years, such research has been rapidly developed worldwide, mainly as a result of the rapid development of discrete particle simulation technique and computer technology.

This talk presents a brief overview of the theoretical developments in discrete element modelling. It covers three important aspects: models for the calculation of particle-particle and particle-fluid interaction forces under different conditions, coupling of discrete element method with computational fluid dynamics to describe particle-fluid flow, heat and mass transfer, and the theories for linking discrete to continuum modelling. Focus is however given to those developed in my laboratory for Simulation and Modelling of Particulate Systems "SIMPAS", specifically answering the five questions given below. It is also demonstrated through examples that the study of small particles is well linked to many challenging problems in big science. The examples also demonstrate that particle scale approach has gradually emerged to be a powerful tool not only for fundamental research but also for engineering application.

What particles?

Particles can be found in nature and in industry in many forms (ore, coal, grains, sands, rice, beans, powder, nanoparticles, etc.). They can be either wet or dry, and normally range in size from

nanometres to centimetres. They are the second largest material – next to water – we human beings handle, and over 70% of industrial final and intermediate products are in particle forms. In simple words, a particle system is an assembly of particles, often involving other phases such as gas and/or liquid in industrial handling and processing.

Particles have properties that are characteristic of each of the three primary states of matter. For example, under certain conditions they can with stand deformation like solids, flow like a liquid and exhibit compressibility like a gas. These features give rise to another state of matter–particulate/granular matter–that is poorly understood, posing a challenge to the scientific and engineering community for years (Fig. 1). Because of the poor fundamental understanding of this matter, our current practice is very problematic. For example, on average we can only achieve about 50% of the design capacity of an industrial operation, compared to 90% for gas or liquid phase. Although widely used, many industrial processes are actually operated as 'black box' reactors (Fig. 2).

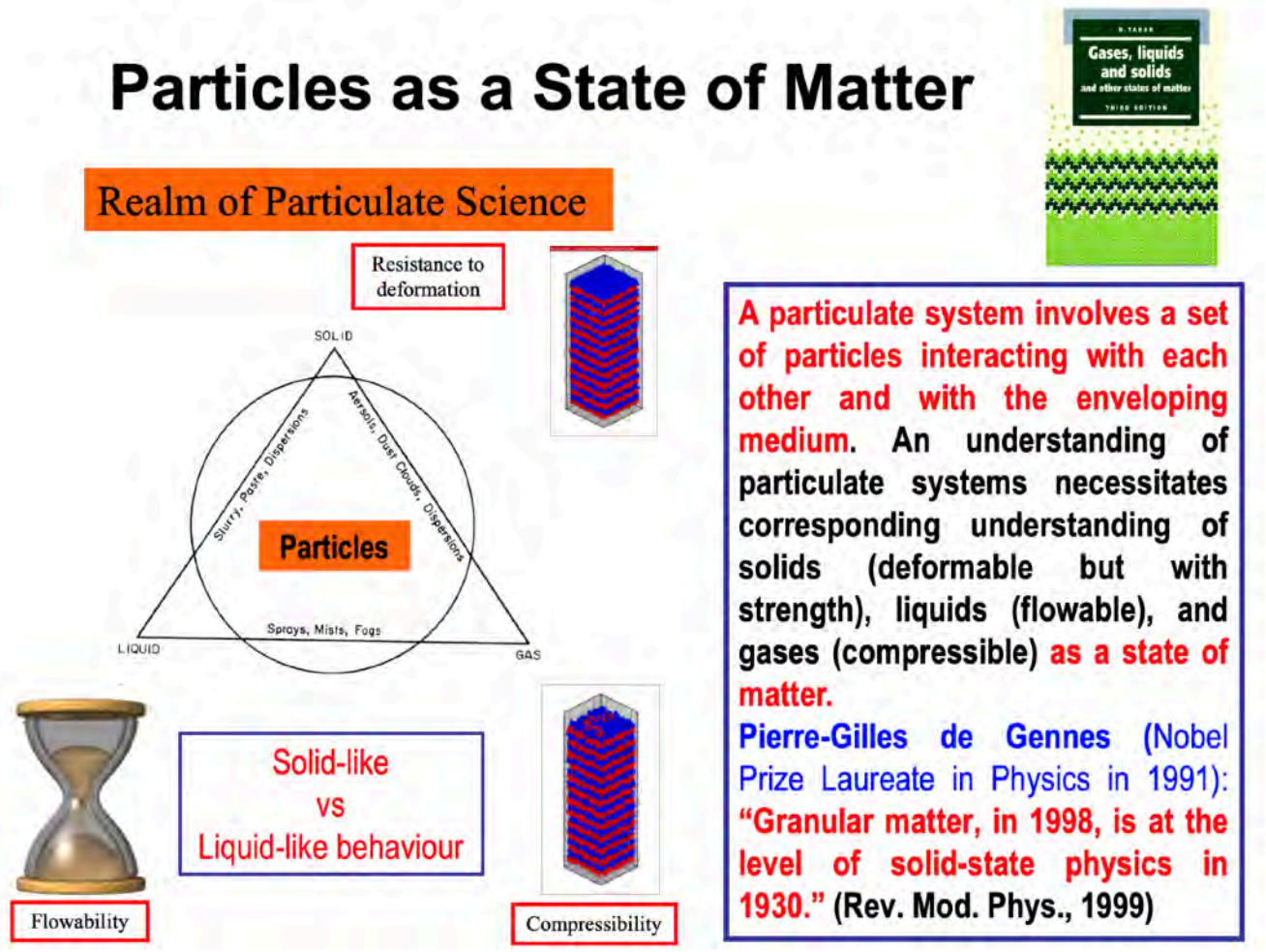


Fig. 1 Particles as a state of matter

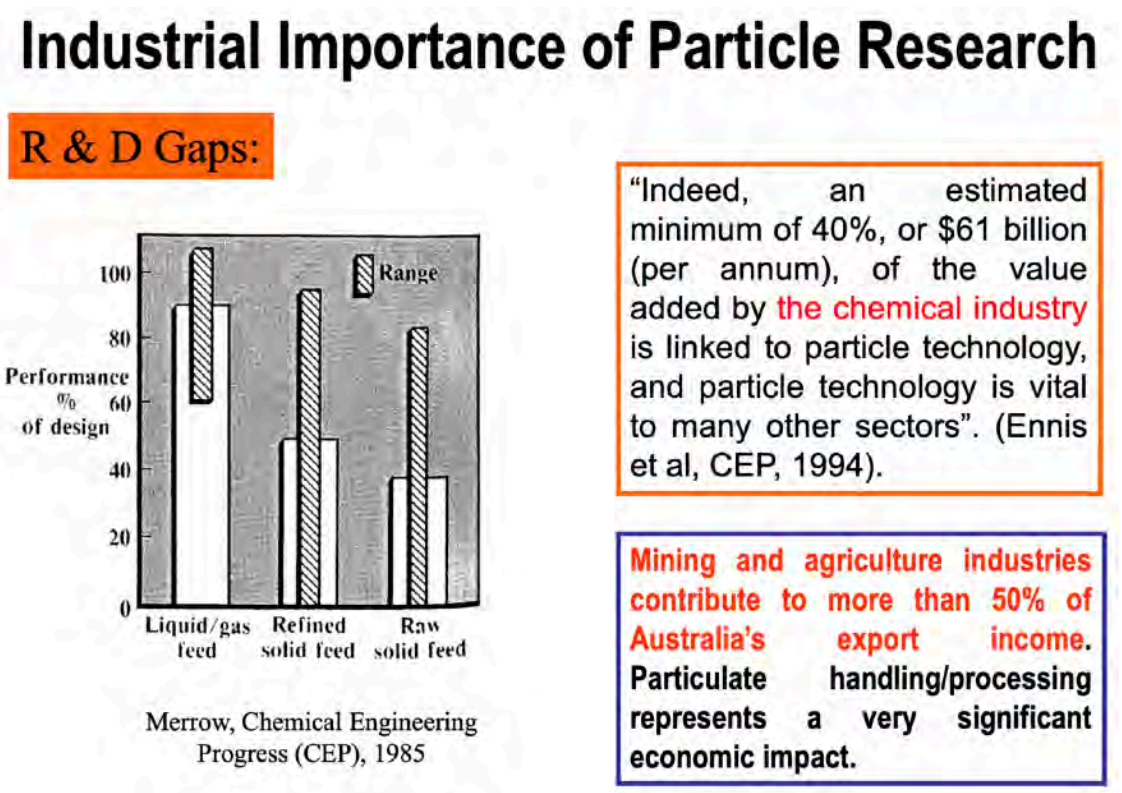


Fig. 2 Industrial importance of particle research

Because of the extremely large scale of particle systems, any improvement in operation will provide a very significant economic benefit. For example, an estimated minimum of 40%, or US$61 billion per annum, of value added by the chemical industry alone (in the USA) is linked to particle studies. Grinding is a common process in the mineral industry, which is, however, known as a low-efficiency (<10%, typically), energy-intensive process and may account for up to 40% of the direct operating cost of a mineral processing plant. Therefore, there is a strong need for research to generate an ultimate solution for better design, control and optimization of many industrial processes and/or products. Particle science and technology is an interdisciplinary research subject dedicated to this purpose.

Why computation?

Understanding the fundamentals governing particle behaviour is of paramount importance to the design, control and optimization of many industrial processes or operations. In the past, different measurement techniques have been developed, but there have been problems in probing the underlying physics and solving practical problems generally and reliably. This is evidenced by the study of the dynamics of a particle system that includes at least three factors: velocity, structure and force. Previous studies have been limited to velocity because of the difficulty in obtaining information about the other two.

A promising technique that can overcome this problem is computer modelling and simulation. This often involves a multiscale approach to understand phenomena at different length and time scales, including: (1) at the molecular/sub-particle scale to determine the interaction forces

between particles, fluid and wall, and the transport behaviour between particles and/or pores; (2) at the micro/particle scale to understand particle flow and force structures in relation to different flow conditions; (3) at the meso/macro scale to formulate governing equations, constitutive relations and boundary conditions for continuum based process modelling and simulation; and (4) at the process equipment scale to quantify flow and process performance for control and optimization. There is also a need to consider the presence of fluid(s) and the coupling between fluid flow, heat and mass transfer. The ultimate aim is to develop a generic theories and methods to solve problems of various types in different industries (Fig. 3).

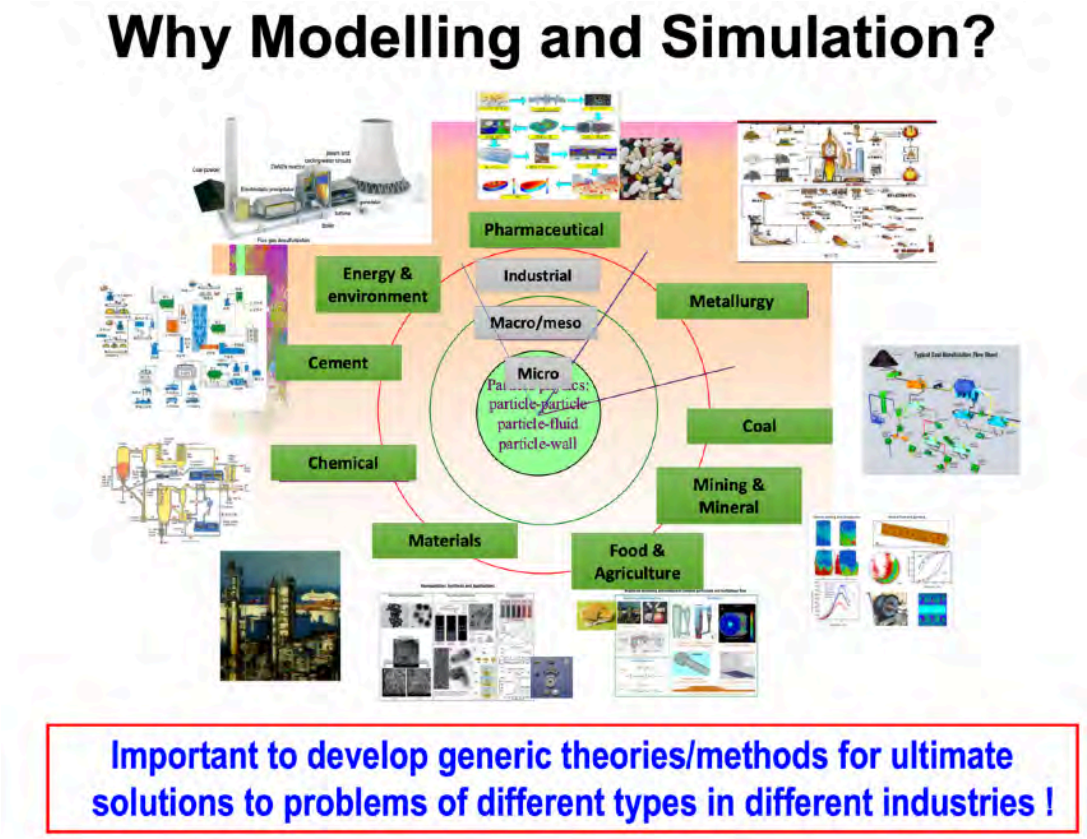


Fig. 3 Why modeling and simulation?

In the past two decades or so, with the rapid development of computer technology, many advanced computational technologies have been developed and applied to tackle problems of various types. Indeed, computation has gradually emerged to be a powerful tool not only for fundamental research but also for engineering application.

How to do computation?

The phenomena encountered in process engineering are often multiscale. Correspondingly, there is a need to develop a multiscale approach to describe them at different time and length scales. Generally speaking, there are two extreme approaches: continuum and discrete. In materials science, the finite element method (FEM) is often used for macroscopic, continuum modelling and molecular dynamics (MD) for microscopic, discrete simulation. Indeed, similar to material research,

the existing approaches to modelling granular matter can essentially be classified into two categories: the continuum approach at a macroscopic level and the discrete approach at a microscopic level. The continuum approach is often realized by use of computational fluid dynamics (CFD), and the discrete approach by use of the so-called discrete element method (DEM). They are equivalent to FEM and MD in material research, but the forces involved differ. Depending on the research needs, different numerical methods are used to assess behaviours at different time and length scales. For example, we can use MD or FEM to determine the forces between particles, DEM to simulate particle flow at the particle scale, and CFD or FEM to simulate particle flow at the process-equipment scale (Fig. 4).

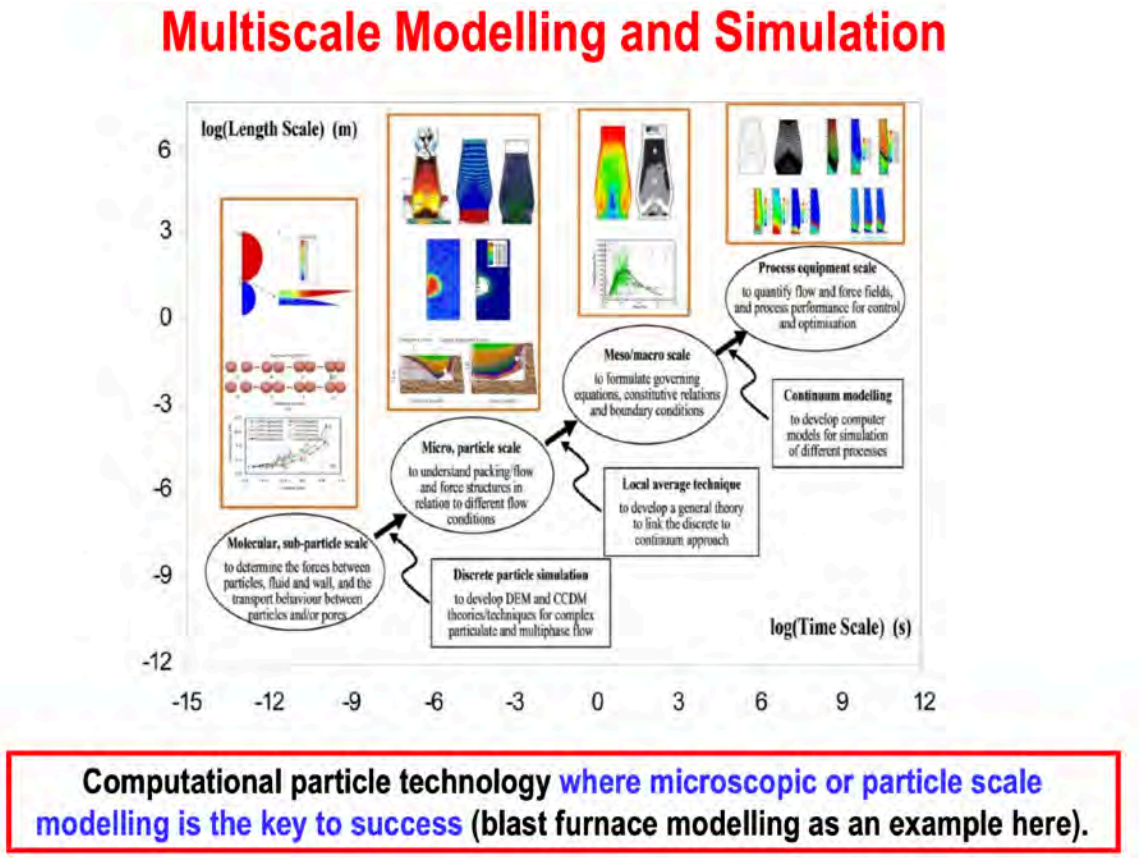


Fig. 4 Multiscale modelling and simulation

Moreover, as mentioned above, granular matter can compare with the other three primary states of matter: gas, liquid and solid. However, its basic elements are particles, not atoms, resulting in a significant difference in time and length scales. Consequently, the forces involved and the methods for physical experiments differ. On the other hand, mathematically the governing equations – if not all – are comparable. Consequently, the methods for numerical experiments are similar. For example, when we talk about the material and particles, the MD and DEM are very much related, so is the case for FEM and CFD. The so-called micro, meso and macro scales are just relative concepts, depending on which systems, atomic or particle, are considered. Hence the methodology in multiscale modelling can, in principle, be extended from one matter to another,

while recognizing the uniqueness of each of the matters. One of the aims is to understand why and how atoms and particles behave differently because of the different forces in time and length scales.

There is also a need to simulate coupled particle–fluid two-phase flows, as mentioned earlier. The time and length scales for fluid flow can be much smaller than particles (e.g., the lattice Boltzmann method (LBM) or direct numerical simulation (DNS)) or much larger than particles (e.g., the so-called two-fluid model (TFM)). Correspondingly, they produce different coupling methods such as LB-DEM, DNS-DEM and CFD-DEM.

All these modelling techniques are available now in the literature. However, their effective use will depend on the need for research, or the phenomena to be investigated, which may have a scale from sub-particle to particle, and to process equipment.

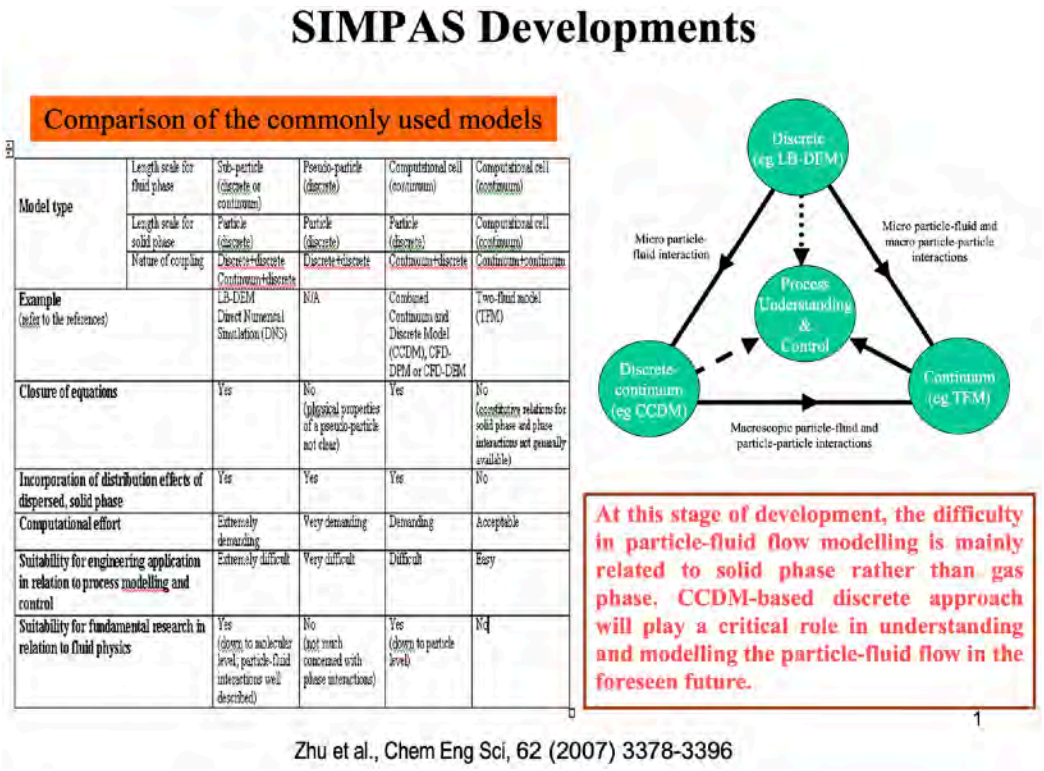


Fig. 5 SIMPAS developments

What results?

Modelling particle systems is very challenging because such a system is always made up of a large number of particles that interact in varying and complex ways. Particle systems demonstrate complex behaviour that is difficult to understand, predict and manage at a macroscopic scale. On the other hand, the bulk behaviour of granular matter depends on the collected outcomes of individual particles, indicating that the complex behaviour can be described as a deterministic process at a microscopic, particle scale. The implementation of this approach in practice, however, needs comprehensive knowledge and skills from a broad range of disciplines including mathematics, physics, engineering and computational technology.

A highly novel, systematic study of particulate/granular matter truly at various time and length scales ranging from atomic to process equipment is therefore necessary. It will certainly help establish comprehensive theories for micro- and macroscopic modelling and analysis. Therefore, as concluded in a few of my review articles, the major challenges in the modelling and simulation of particle systems lie in the following three related areas:

1) to develop a more comprehensive theory and experimental techniques to determine the interaction forces between particles, and between particle and fluid under various conditions, generating a more concrete basis for particle-scale simulation.
2) to generalize a theory to link the discrete and continuum approaches, so that the particle–particle, particle–wall and particle–fluid interactions can be quantified based on the particle-scale results in terms of constitutive relations and boundary conditions that can be implemented in continuum based process modelling.
3) to develop robust model(s) and efficient computer code(s) so that particle-scale simulation can be extended, say, from two-phase to multi-phase and from simple to complicated flow, and from flow to heat and mass transfer, which is important to transform the present phenomenon simulation to process simulation.

Our research, or the research in my team SIMPAS at the University of New South Wales and then at Monash University, in the past 30 years or so is largely developed in these three areas. Its theme is 'Simulation and modelling of particulate systems'. The aim is to understand the fundamentals governing particle packing and flow, with application oriented to the mineral/metallurgical/material industries Fig. 6. In the past, many processes have been studied, with some examples given in Fig. 7.

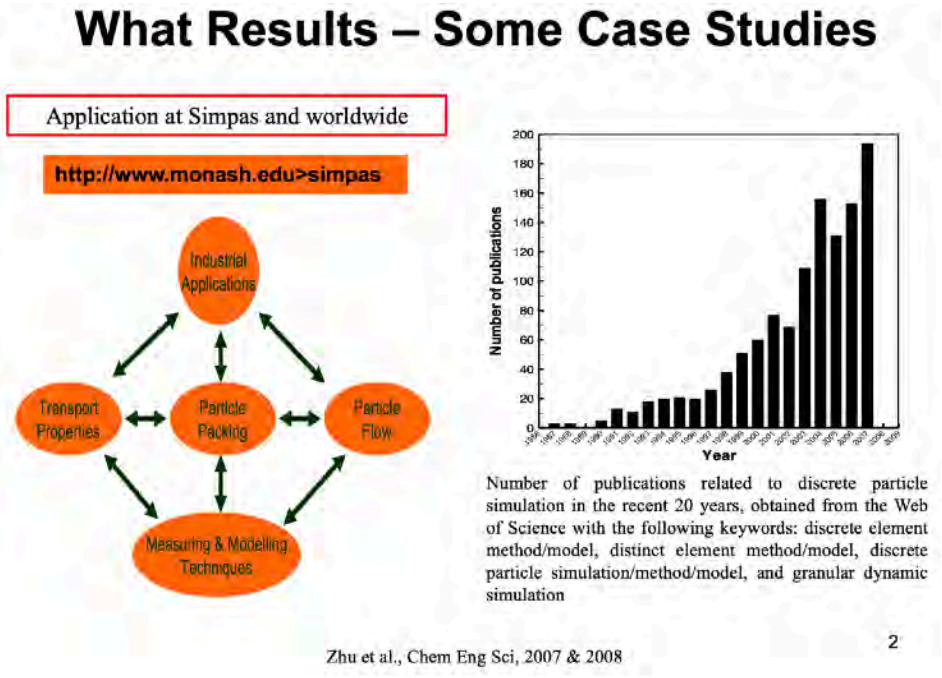


Fig. 6 Case studies

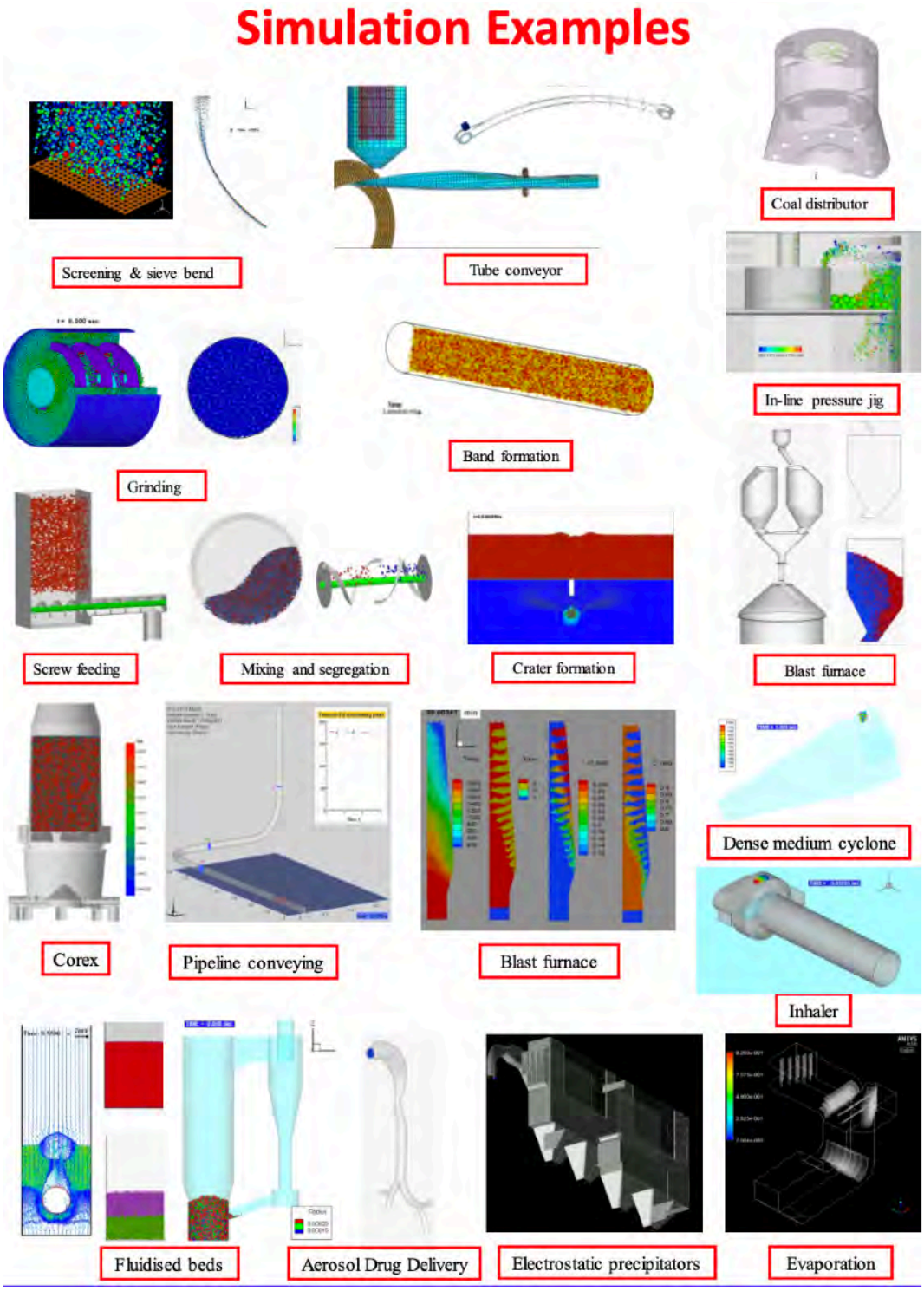


Fig. 7 Simulation examples

While the work is very extensive, our research achievements can be highlighted by two examples. Firstly, we have developed mathematical models to predict porosity (=1-packing density), the

most common macroscopic parameter to characterize a packing as a function of particle-size distribution for systems from spherical to non-spherical, coarse (cohesionless) to fine (cohesive), and dry to wet particles. The models can answer many questions, including 'what is the optimum particle-size distribution for maximum packing density under different conditions?' which has puzzled the research community for more than a century. Microscopic, particle scale simulation plays a very helpful role in supporting this macroscopic modelling, particularly in understanding the underlying mechanisms in terms of interparticle forces and packing structure. Secondly, we have made comprehensive instrumental contributions to the development of the so-called CFD-DEM approach to describe coupled particle–fluid flows. This involves the determination of particle–particle and particle–fluid interaction forces by MD, FEM and LBM, and the theory for coupling the CFD for fluid phase and the DEM for particles at different time and length scales. This modelling technique is now widely accepted as one of the most effective ways to study the fundamentals of the particle–fluid flows that are widely found in industries. The method has recently been further developed to include heat and mass transfer so that particle-scale modelling of complicated industrial multiphase processes such as blast furnace ironmaking is feasible.

With the rapid development of computational technology, computer-aided design of particle systems has become increasingly popular. The continuum approach is preferred in process modelling and applied research because of its computational convenience. But the discrete approach, although computationally much more demanding, becomes more and more attractive because it can generate more fundamental information and is more reliable. Supercomputers and advanced computational techniques such as GPU (graphics processing unit) make industrial-scale simulations feasible now.

There are many successful examples, even just from my research team. This can be highlighted by the fact that we have developed mathematical models, using both continuum (Fig. 8) and discrete (Fig. 9) approaches, to describe the complicated flow, heat and mass transfer in an ironmaking furnace, and the multiphase flow in a dense medium cyclone and other processes (Fig. 7). The models and outcomes are very useful to the design and control of such complicated industrial processes. Our research has led to significant financial benefits to various industries.

Where to?

Clearly, particle research is multiscaled and very challenging. According to Pierre-Gilles de Gennes, the 1991 Nobel Prize Laureate in Physics, 'Granular matter in 1998 is at the level of solid-state physics in 1930'. At present, solid-state physics is still one of the most active research areas, so granular or particle research is probably still in its infancy. There remains a lot to learn, so it is difficult to predict its future. The good thing is that the importance of particle research has been fully recognized, as highlighted by the fact that developing a theory to effectively describe the dynamics of granular matter is listed among the 125 grand challenges in *Science*.

There will be many new developments in theories, physically meaningful models and advanced research techniques in the coming years. Particle-scale studies will represent a major trend. Simulation and modelling offer an opportunity to study granular matter at various length and time scales, promising to generate a step change in process design, control and optimisation.

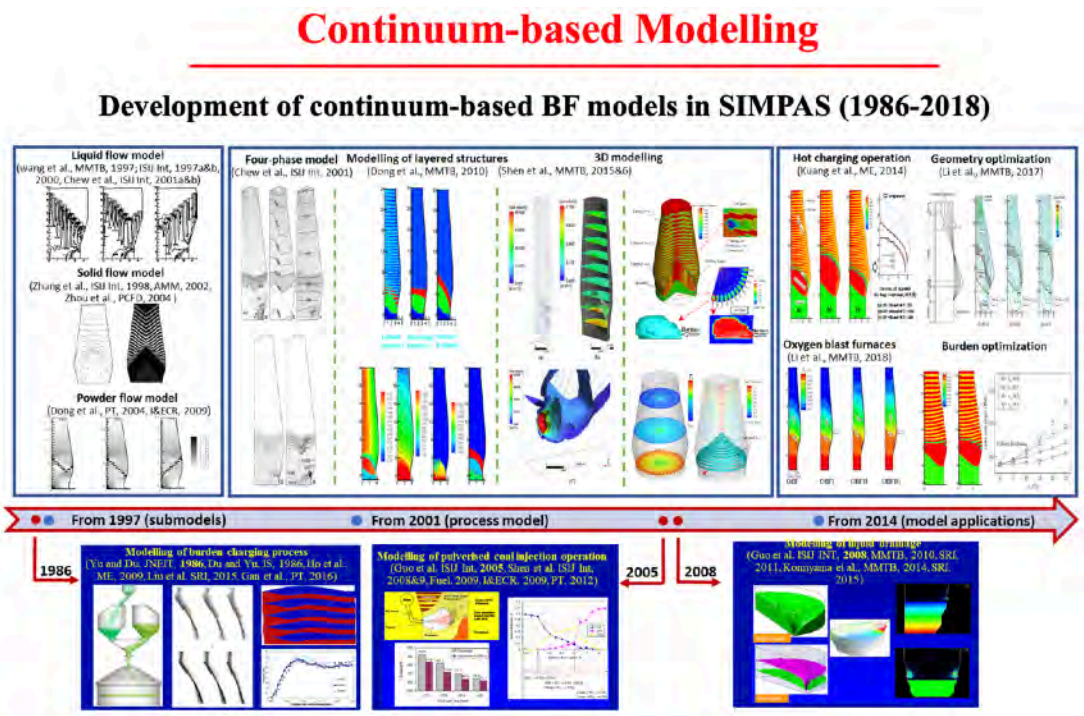


Fig. 8 Continuum-based modelling

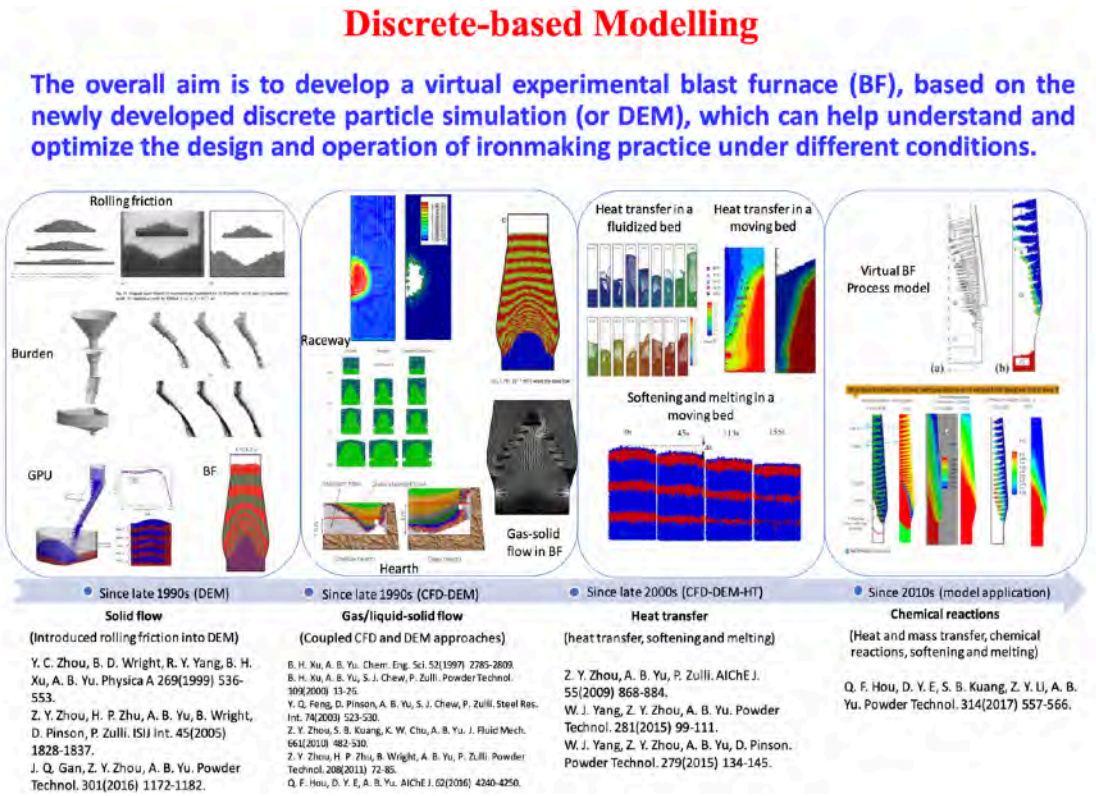


Fig. 9 Discrete-based modelling

Selected articles and reviews

1. B.H. Xu, A.B. Yu. Numerical simulation of the gas-solid flow in a fluidized bed by combining discrete particle method with computational fluid dynamics. *Chemical Engineering Science, 52* (1997) 2785-2809.
2. A.B. Yu and R.P. Zou, "Prediction of the porosity of particle mixtures: a review", KONA Powder and Particle, 16 (1998) 68-81.
3. Y.C. Zhou, B.D. Wright, R.Y. Yang, B.H. Xu, A.B. Yu. Rolling friction in the dynamic simulation of sandpile formation. *Physica A*, 269 (1999) 536-553.
4. R.Y. Yang, R.P. Zou, A.B. Yu. Computer simulation of the packing of fine particles. *Physical Review E*, 62 (2000) 3900-3908.
5. Y.C. Zhou, A.B. Yu, R. Stewart and J. Bridgwater, Microdynamic analysis of particle flow in a bladed mixer, Chemical Engineering Science, 59 (2004) 1343-1364.
6. A.B. Yu, X.Z. An, R.P. Zou, R.Y. Yang, K. Kendall. Self-assembly of particles for densest packing by mechanical vibration. *Physical Review Letters, 97* (2006) 265501.
7. H.P. Zhu, Z.Y. Zhou, R.Y. Yang, A.B. Yu. Discrete particle simulation of particulate systems. *Chemical Engineering Science* 62 (2007) 3378-3396 and 63 (2008) 5728-5770.
8. Q.H. Zeng, A.B. Yu, G.Q. Lu. Multiscale modeling and simulation of polymer nanocomposites. *Progress in Polymer Science*, 33 (2008) 191-269.
9. Z.Y. Zhou, A.B. Yu and P. Zulli, Particle scale study of heat transfer in packed and bubbling fluidized beds, AIChE Journal, 55 (2009) 868-884.
10. Z.Y. Zhou, S.B. Kuang, K.W. Chu, A.B. Yu. Discrete particle simulation of particle–fluid flow: model formulations and their applicability. *Journal of Fluid Mechanics*, 661 (2010) 482-510.
11. J. Chen, K.W. Chu, R.P. Zou, A.B. Yu and A. Vince, Prediction of the performance of dense medium cyclones in coal preparation, Minerals Engineering, 31 (2012) 59-70.
12. Q.F. Hou, Z.Y. Zhou and A.B. Yu, Micromechanical modeling and analysis of different flow regimes in gas fluidization, Chemical Engineering Science, 84 (2012) 449-468.
13. W.F. Sun, Q.H. Zeng, A.B. Yu and K. Kendall, Calculation of normal contact frces between silica nanospheres, Langmuir, 29 (2013) 7825-7837.
14. Q.J. Zheng, A.B. Yu. Why have continuum theories previously failed to describe sandpile formation? *Physical Review Letters,* 113 (2014) 068001.
15. Z.A. Tian, K.J. Dong and A.B. Yu, Structural evolution in the packing of uniform spheres, Physical Review E, 89 (2014) 032202.
16. L.W. Rong, K.J. Dong and A.B. Yu, Lattice-Boltzmann simulation of fluid flow through packed beds of spheres: Effect of particle size distribution, Chemical Engineering Science, 116 (2014) 508-523.
17. J.Q. Gan, Z.Y. Zhou and A.B. Yu, CFD–DEM modeling of gas fluidization of fine ellipsoidal particles. AIChE Journal, 62 (2016) 62-77.
18. S.B. Kuang, Z.Y. Li, A.B. Yu, Review on modelling and simulation of blast furnace, Steel Research International, 89 (2018) 1700071-1/25.
19. Q.J. Zheng, L. Bai, L.Y.M. Yang, A.B. Yu, Continuum modeling of granular mixing in a rotating drum, Industrial & Engineering Chemistry Research, 58 (2019) 19251-19262.
20. S.B. Kuang, M.M. Zhou, A.B. Yu, CFD-DEM modelling and simulation of pneumatic conveying – A review, Powder Technology, In print (2019).

Young Professional Award Sponsored by SABIC

"Gaseous Bubbles" and "Granular Bubbles" in Fluidized Particles

Christopher Boyce

Assistant Professor

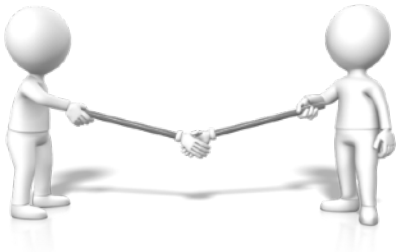
Department of Chemical Engineering

Columbia University, New York, USA

Granular particles are "fluidized" when upward gas flow is passed through them above a critical velocity, the minimum fluidization velocity, U_{mf}, such that the drag on the particles suspends them and they begin to behave like a liquid[1]. It is well known that when the gas velocity U is greater than U_{mf}, hydrodynamic instabilities set in[2], causing voids or "bubbles" to rise through the particles. In short, these bubbles form because once a small gas void is created, gas channels through it, since it provides a lower resistance for gas to flow than traversing between interstices between particles. This gas channeling toward the void causes the void to grow and the void rises due to buoyancy. These "bubbles" are different from those in conventional fluids, since gas passes freely between the bubble and the particulate phase and there is no surface tension between the bubble and the particulate phase.

Characterizing the motion of bubbles as well as the dynamics of gas and particles in fluidized beds has presented significant difficulties, since motion in 3D opaque systems prevents optical access. Recently, the use of magnetic resonance imaging (MRI) to study fluidized beds has enabled measurement of particle concentration and velocity in the interior of 3D fluidized beds[3,4]. Figure 1 shows the setup the author and co-workers[5] used to measure time-averaged particle concentration and velocity in a bubbling fluidized bed, showing that bubbles rose through the center of the system (marked with a dotted circle). Further, Figure 1 shows that MRI can further measure image gas velocity quantitatively, confirming that gas channels through bubbles, while rising more slowly through particles surrounding the bubbles[5].

Two main limitations of MRI have been a small system size (52 mm diameter) and limited temporal resolution. Recently, the author and co-workers[6] have developed techniques to use medical MRI scanners and multi-channel radiofrequency receivers to measure particle dynamics with a system size of 190 mm diameter, a temporal resolution of 7 ms and a spatial resolution of 3 mm (see Figure 2).



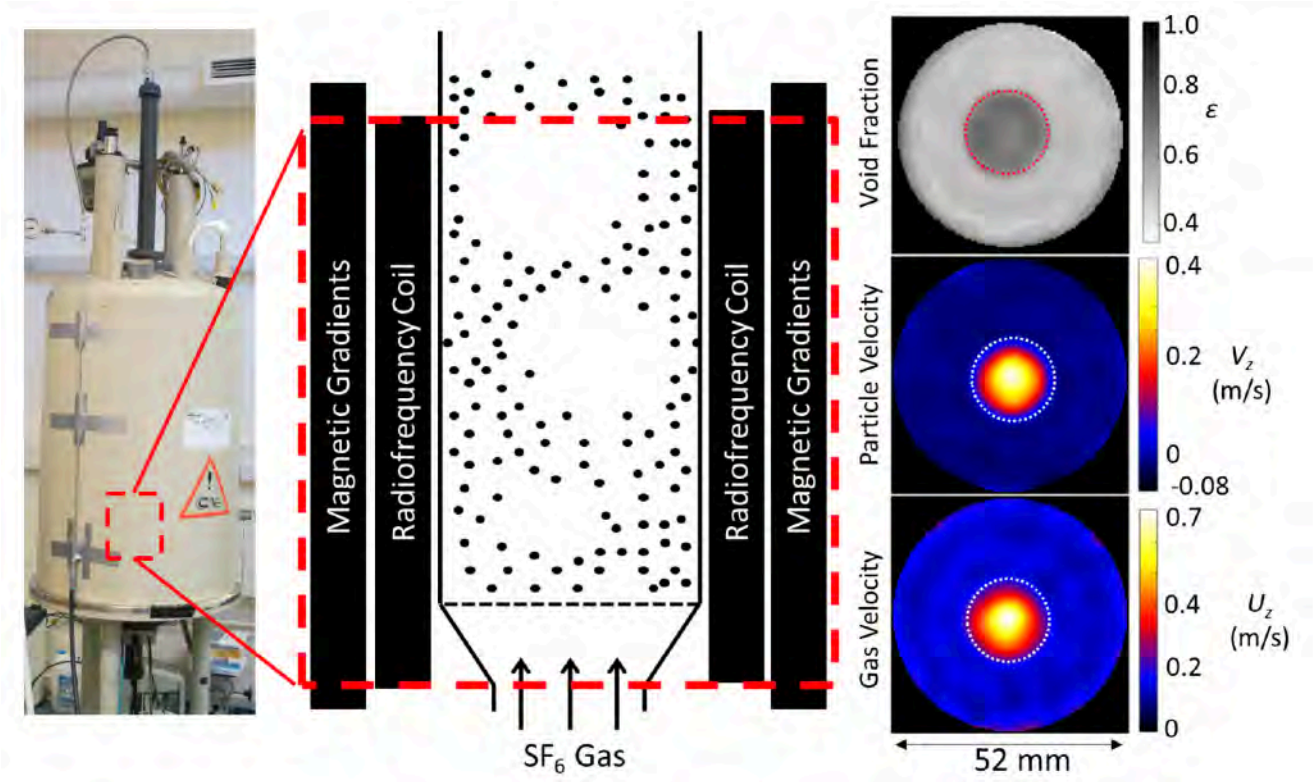


Fig. 1 Image of fluidized bed cylinder placed through a chemistry-style MRI magnet (left), schematic of the fluidized bed in the interior (center) and MRI measurements of void fraction, particle velocity and gas velocity in a horizontal cross-section through the fluidized bed[5].

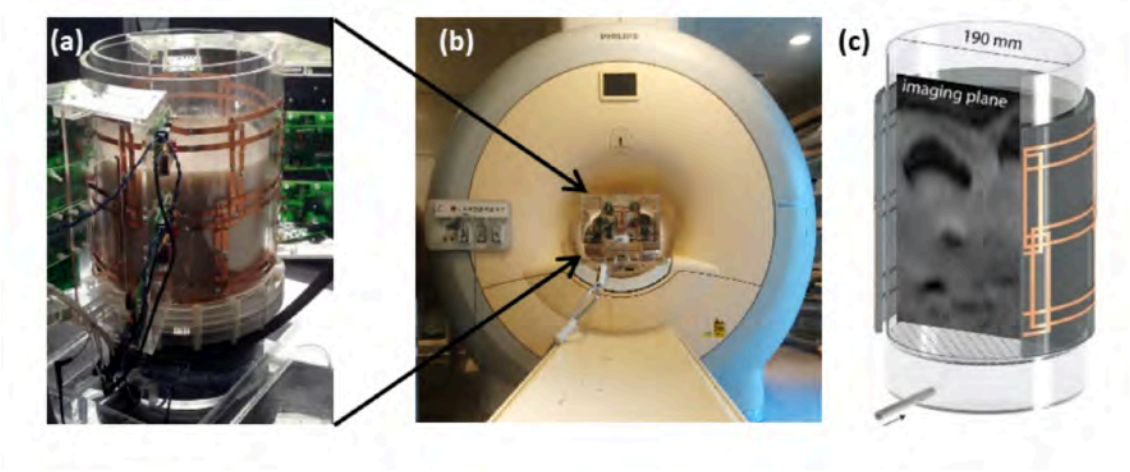


Fig. 2 A fluidized bed surrounded by a multi-channel radiofrequency recorder (a), the entire system placed in a medical MRI scanner (b) and a schematic showing rapid imaging of bubble dynamics in a cenral plane in the system (c)[6].

The author and co-workers have used these rapid, large-scale MRI capabilities to study a variety of phenomena[7–11], including two bubbles injected side-by-side into an incipiently fluidized bed. In this experimental study, one bubble would inevitably be slightly smaller than the other, and the smaller bubble would collapse, as seen in Figure 3[12]. Figure 3 also shows that "CFD-DEM" simulations[13] in which gas flow is modeled using Computational Fluid Dynamics and particle motion was modeled using the Discrete Element Method were able to recreate this phenomenon. Further, CFD-DEM simulations show that the bubble does in fact collapse, rather than move out of the central plane, and that gas channels toward both bubbles, with more gas channeling toward the larger bubble. These simulation predictions support the hypothesis of author and co-workers that gas channeling toward the larger bubble causes not enough gas to flow through the smaller bubble to support its roof, causing the smaller bubble to collapse (see Figure 4)[12].

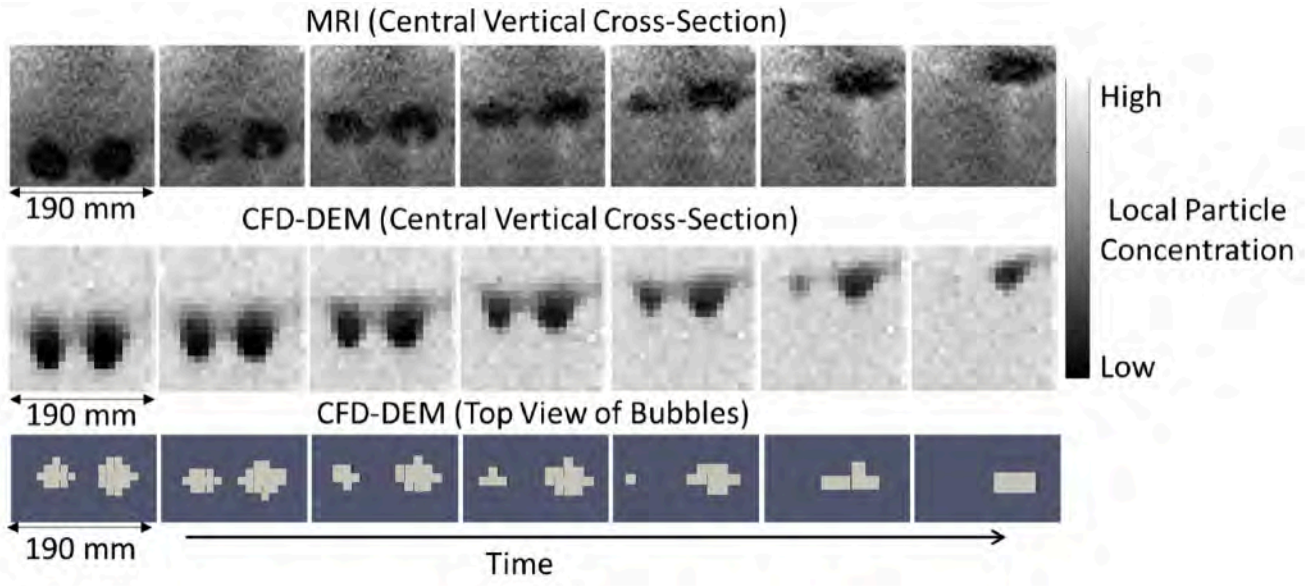


Fig. 3 Images of two bubbles injected side-by-side into an incipiently fluidized bed. (a) MRI images of a central vertical plane, (b) corresponding CFD-DEM images and (c) CFD-DEM images of the bubbles from a top view[12].

While gaseous "bubbles" in fluidized beds were first observed and studied decades ago[1,14], the author and co-workers have recently demonstrated the "granular bubbles" of lighter grains can rise through heavier grains in fluidized beds[15]. Figure 5 shows how lighter particles were placed below heavier particles in a pseudo-2D system, in a classic Rayleigh-Taylor setup[16]. This system was then subject to both gas flow and vibration, such that no gas bubbles rose through the system. In this setup, the heavier particles were larger than the lighter particles, such that both particles fluidized under the same gas flow conditions. Figure 5 shows that the system proceeded to undergo a Rayleigh-Taylor like instability, with lighter particles rising to the top in the form of "fingers" and "bubbles" commonly seen in lava lamps[15].

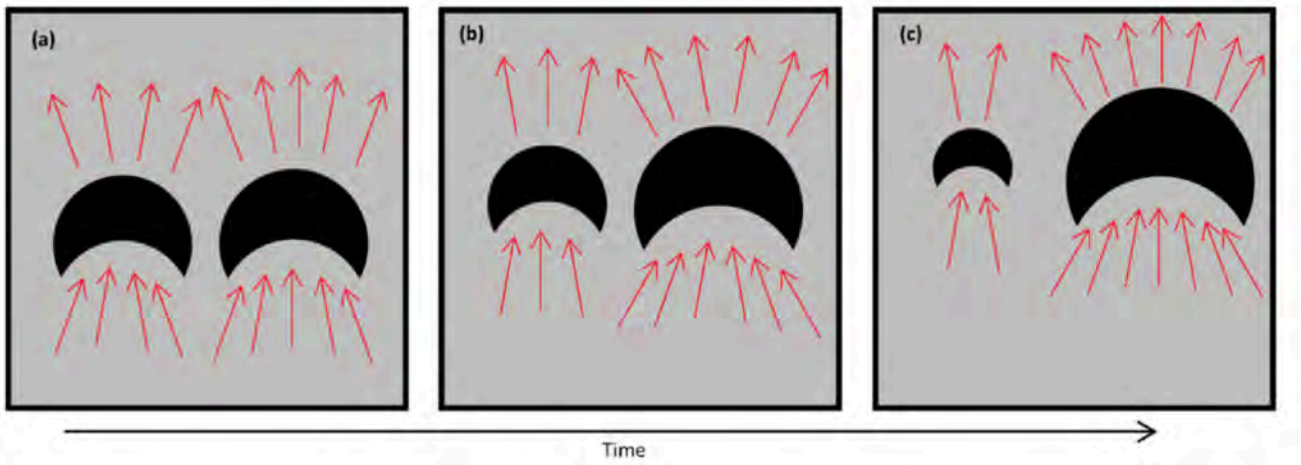


Fig. 4 Hypothesis of the author and co-workers that gas channeling through the bubbles, preferentially to the larger bubble leads, to the collapse of the smaller bubble[12].

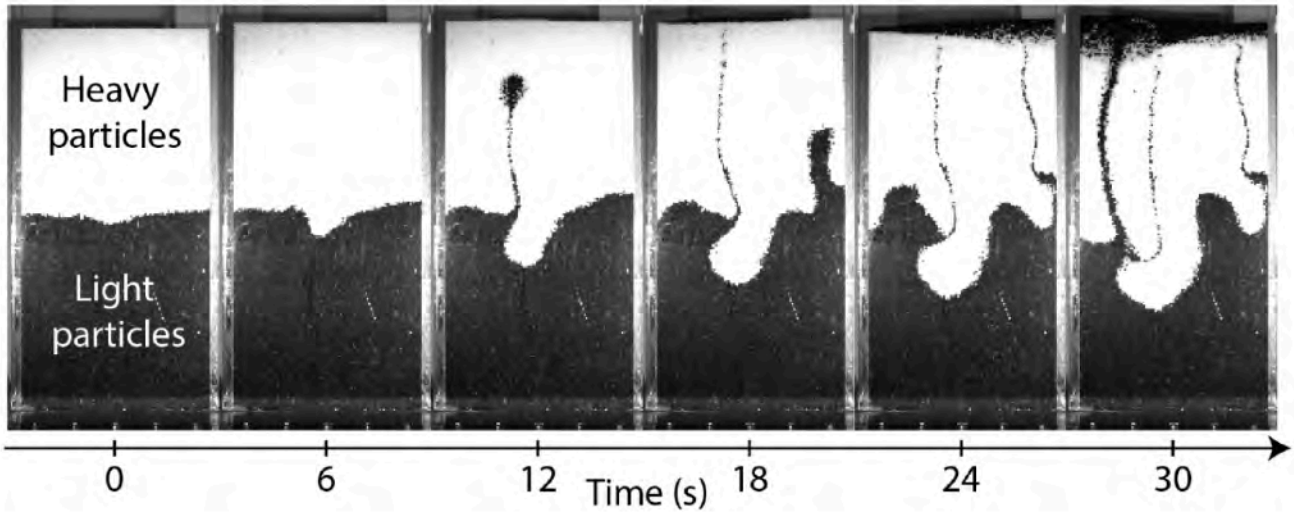


Fig. 5 Optical images of a vibrated pseudo-2D fluidized beds with larger, lighter particles (black) below larger heavier particle (white). "Fingers" and "bubbles" of lighter grains form and rise to the surface, similar to the "Rayleigh-Taylor" instability observed between fluids[15].

Figure 6 shows CFD-DEM simulations of the same system shown in Figure 5, zoomed in on the interface between the heavy and light particles, demonstrating the CFD-DEM simulations can recreate the "fingering" and "bubbling" phenomenon[15]. Figure 6 shows that gas channels through crests of light particles which form, causing the drag force on them to increase, overcoming downward contact forces, and causing the crests to grow into fingers and then break off into bubbles. This gas channeling occurs due to gas flowing more easily through larger interstices between larger particles rather than smaller interstices between smaller particles. Thus, the CFD-DEM simulations show that granular bubbles are formed due to gas-channeling[15], just as do gaseous bubbles in fluidized particles.

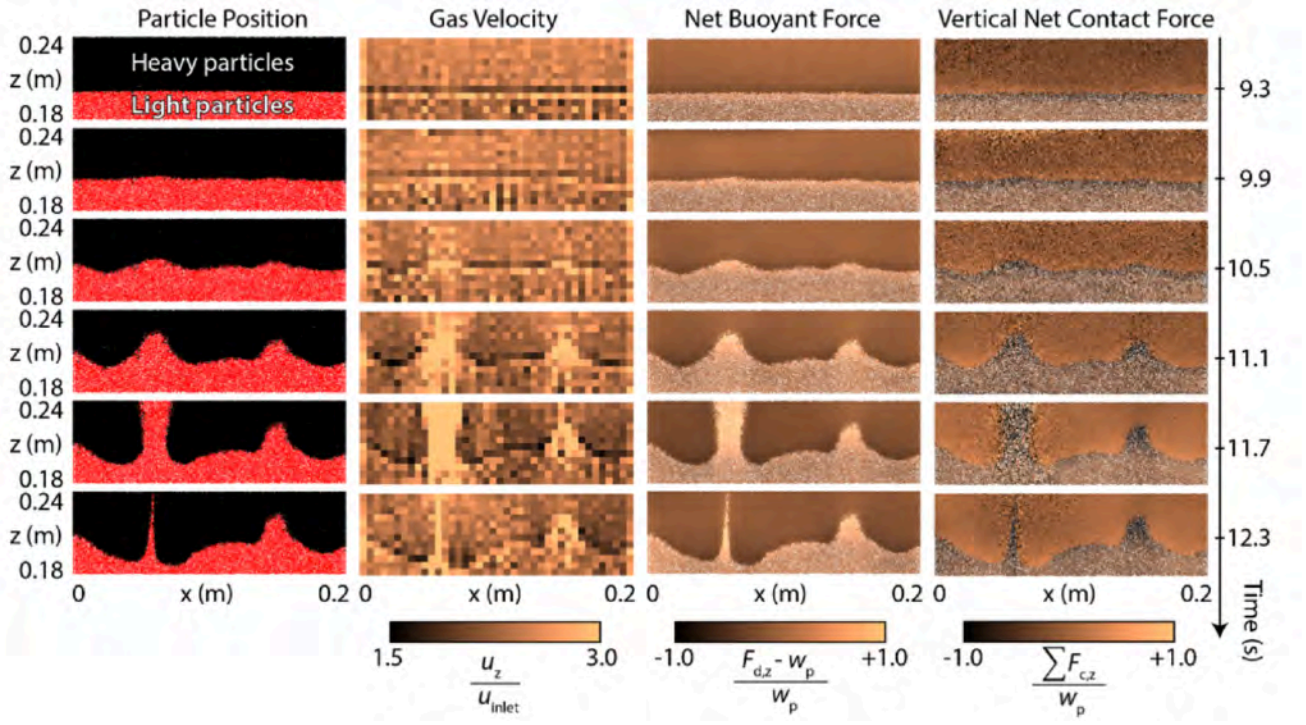


Fig. 6 CFD-DEM simulation results of the same system as in Figure 5, showing that the simulations can reproduce the results and showing the patterns of gas flow which lead to the drag and contact forces on the particles[15].

In summary, "bubbles" of gas and grains can form in fluidized beds, but MRI measurements and CFD-DEM simulations show that these bubbles form due to gas-channeling rather than surface tension, making them physically different from those in conventional fluids.

References

(1) Davidson, J. F.; Harrison, D. *Fluidised Particles*; Cambridge University Press: Cambridge, 1963.

(2) Sundaresan, S. Instabilities in Fluidized Beds. *Annu. Rev. Fluid Mech.* 2003, *35* (1), 63–88. https://doi.org/10.1146/annurev.fluid.35.101101.161151.

(3) Savelsberg, R.; Demco, D. E.; Blümich, B.; Stapf, S. Particle Motion in Gas-Fluidized Granular Systems by Pulsed-Field Gradient Nuclear Magnetic Resonance. *Phys. Rev. E* 2002, *65* (2), 020301. https://doi.org/10.1103/PhysRevE.65.020301.

(4) Müller, C. R.; Davidson, J. F.; Dennis, J. S.; Fennell, P. S.; Gladden, L. F.; Hayhurst, A. N.; Mantle, M. D.; Rees, A. C.; Sederman, A. J. Real-Time Measurement of Bubbling Phenomena in a Three-Dimensional Gas-Fluidized Bed Using Ultrafast Magnetic Resonance Imaging. *Phys. Rev. Lett.* 2006, *96* (15), 154504. https://doi.org/10.1103/PhysRevLett.96.154504.

(5) Boyce, C. M.; Rice, N. P.; Ozel, A.; Davidson, J. F.; Sederman, A. J.; Gladden, L. F.; Sundaresan, S.; Dennis, J. S.; Holland, D. J. Magnetic Resonance Characterization of Coupled Gas and Particle Dynamics in a Bubbling Fluidized Bed. *Phys. Rev. Fluids* 2016, *1* (7), 074201. https://doi.org/10.1103/PhysRevFluids.1.074201.

(6) Penn, A.; Tsuji, T.; Brunner, D. O.; Boyce, C. M.; Pruessmann, K. P.; Müller, C. R. Real-Time Probing of Granular Dynamics with Magnetic Resonance. *Sci. Adv.* 2017, *3* (9), e1701879. https://doi.org/10.1126/sciadv.1701879.

(7) Boyce, C. M.; Penn, A.; Pruessmann, K. P.; Müller, C. R. Magnetic Resonance Imaging of Gas–Solid Fluidization with Liquid Bridging. *AIChE J.* 2018, *64* (8), 2958–2971. https://doi.org/10.1002/aic.16036.

(8) Penn, A.; Boyce, C. M.; Kovar, T.; Tsuji, T.; Pruessmann, K. P.; Müller, C. R. Real-Time Magnetic Resonance Imaging of Bubble Behavior and Particle Velocity in Fluidized Beds. *Ind. Eng. Chem. Res.* 2018, *57* (29), 9674–9682. https://doi.org/10.1021/acs.iecr.8b00932.

(9) Penn, A.; Boyce, C. M.; Conzelmann, N.; Bezinge, G.; Pruessmann, K. P.; Müller, C. R. Real-Time Magnetic Resonance Imaging of Fluidized Beds with Internals. *Chem. Eng. Sci.* 2019, *198*, 117–123. https://doi.org/10.1016/j.ces.2018.12.041.

(10) Boyce, C. M.; Penn, A.; Lehnert, M.; Pruessmann, K. P.; Müller, C. R. Effect of Liquid Bridging on Bubbles Injected into a Fluidized Bed: A Magnetic Resonance Imaging Study. *Powder Technol.* 2019, *343*, 813–820. https://doi.org/10.1016/j.powtec.2018.11.091.

(11) Boyce, C. M.; Penn, A.; Lehnert, M.; Pruessmann, K. P.; Müller, C. R. Wake Volume of Injected Bubbles in Fluidized Beds: A Magnetic Resonance Imaging Velocimetry Study. *Powder Technol.* 2019. https://doi.org/10.1016/j.powtec.2019.02.021.

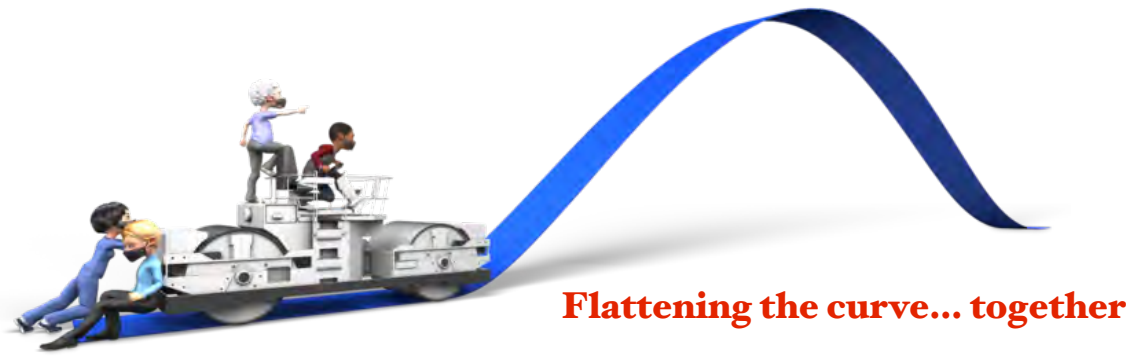
(12) Boyce, C. M.; Penn, A.; Padash, A.; Lehnert, M.; Pruessmann, K. P.; Müller, C. R. Anomalous Collapse of Interacting Bubbles in a Fluidized Bed: A Magnetic Resonance Imaging Study. *Phys. Rev. Fluids* 2019, *4* (3), 034303. https://doi.org/10.1103/PhysRevFluids.4.034303.

(13) Tsuji, Y.; Kawaguchi, T.; Tanaka, T. Discrete Particle Simulation of Two-Dimensional Fluidized Bed. *Powder Technol.* 1993, *77* (1), 79–87.

(14) Toomey, R. D.; Johnstone, H. F. Gaseous Fluidization of Solid Particles. *Chem. Eng. Prog.* 1952, *48* (5), 220–226.

(15) McLaren, C. P.; Kovar, T. M.; Penn, A.; Müller, C. R.; Boyce, C. M. Gravitational Instabilities in Binary Granular Materials. *Proc. Natl. Acad. Sci.* 2019, 201820820. https://doi.org/10.1073/pnas.1820820116.

(16) Sharp, D. H. An Overview of Rayleigh-Taylor Instability. *Phys. Nonlinear Phenom.* 1984, *12* (1), 3–18. https://doi.org/10.1016/0167-2789(84)90510-4.



2020 AIChE Annual Meeting, 100% Virtual, November 16-20, 2020

A Message from AIChE

2020 AIChE ANNUAL MEETING | ASC20 AIChE Annual Student Conference

Dear Colleagues,

In the wake of the current pandemic, AIChE's first concern is for the health and safety of our members, volunteers and staff. AIChE® has therefore made the decision to **hold its 2020 Annual Meeting virtually.** The meeting – which originally had been scheduled to take place in San Francisco, CA, November 15–20 will now be held virtually from **Monday, November 16 through Friday, November 20.** The **Annual Student Conference,** held in conjunction with the Annual meeting, **will take place online November 13–16**.

This new virtual experience, developed by our programming team, including meeting chairs, session organizers, presenters and exhibitors, will ensure that the new format provides you with the valuable experience you expect. As you know, AIChE's Annual Meeting is the **premier forum for chemical engineers interested in innovation and professional growth** as experts cover a wide range of topics relevant to cutting-edge research, new technologies and emerging growth areas. We are excited to bring AIChE's 2020 Annual Meeting to a larger global audience as a virtual event.

The Annual Meeting program will continue to provide virtual meeting attendees with compelling technical sessions, inspiring lectures, and valuable opportunities to network with speakers, exhibitors, and chemical engineering colleagues. Alternating program blocks, consisting of technical sessions and networking events will enable attendees to interact with presenters during Q&As, participate in workshops, attend panel discussions and committee meetings and engage with colleagues in the community.

Among the many benefits of the virtual platform, attendees will enjoy the flexibility of being able to **revisit recordings of the technical sessions** up to one month after the meeting. Full meeting registration will include permanent access to recordings of all available presentations as part of the conference proceedings. Ancillary events, university receptions, and all networking will be set up by AIChE using best practices for platforms and networking. Each event will proceed as listed with modifications for virtual (e.g., dinners will become networking events that will include several

options). Staff will contact the responsible person for each ancillary event (as listed in Confex) to make individualized arrangements with your group, beginning the week of September 1.

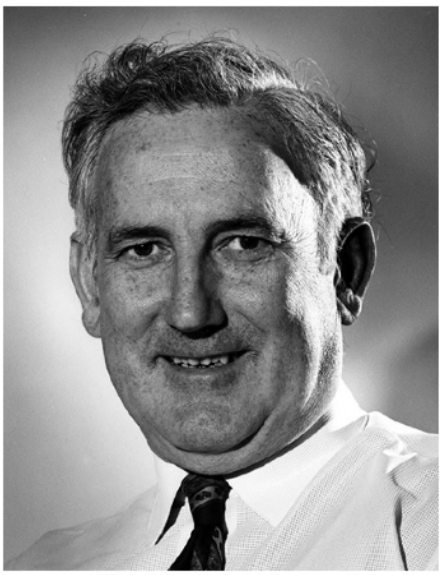
AIChE has adjusted our registration fees to reflect this new virtual format and the cancellation policy has been adjusted to provide flexibility. Please see the FAQs for more information and watch your email for updates.

Join us in November for our 2020 Annual meeting! AIChE looks forward to providing you with a unique, virtual experience that will enhance your career development and professional growth and to sharing quality time and great programming!

June C. Wispelwey

Executive Director and CEO, AIChE

In Memoriam - Owen E. Potter (1925-2020)



Professor Owen Potter passed away recently in his 95th year. Owen was Monash University's first professor of chemical engineering and led the chemical engineering department for 26 years from the university's establishment in the mid 1960s until his retirement.

Owen Potter held a Bachelor's degree from the University of Queensland, a master's degrees in applied science and a second master's degree in the history and philosophy of science from the University of London. Held academic positions at Manchester University, UK (where he completed a PhD), University of Melbourne, Royal Melbourne Institute of Technology (RMIT) and Monash University.

Owen's research was characterised by original ideas and a strong mathematical approach to experimentation. His interest in fluidisation began in the early 1960s. The University of Manchester awarded him a Doctorate of Science in 1974 for his outstanding contribution on the elucidation of the mechanism of gas and solid mixing in fluidised beds. Du Pont retained him as a consultant on the design of high-pressure gas-liquid reactors. His steam fluidised bed drying process, patented in 1981, allowed power stations using brown coal to achieve significant reductions in emissions and operating costs. After his retirement Owen pursued an interest in developing a novel high-efficiency gas-particle contacting device with applications for heat recovery, drying and reaction in a wide range of industries.

Owen was the recipient of many awards, including being appointed a Member of the Order of Australia for significant service to chemical engineering and the Catholic Church. Owen's death is a loss to the fluidization community.

Fluidization IX, Durango, Colorado

Fluidization VI, Banff, Canada

Fluidization V, Elsinore, Denmark

Fluidization III

Computational Modeling Solving Real-Time Industrial Problems

Raj Singh, Paul Marchant, Steve Shimoda

TechnipFMC Process Technology

Houston, Texas, USA

Abstract

Recent advances in computational fluid dynamic (CFD) techniques and computing power have opened opportunities to use this tool for design developments and troubleshooting operational problems. This article discusses a recent development to improve spent catalyst distribution in a Fluid Catalytic Cracking (FCC) regenerator. Uniform spent catalyst distribution is key to achieving even coke combustion and bed temperatures resulting in more complete coke burn and improved catalyst activity retention. This paper highlights how CFD tools were used in the development of TechnipFMC's latest "compound angle wye bathtub" distributor. Data from several commercial regenerators show uniform temperature profiles with the new spent catalyst distributor, validating the use of CFD to develop and design FCC equipment and resolve operational issues.

Keywords: Fluid catalytic cracking (FCC), FCC regenerator, spent catalyst regeneration, computational fl uid dynamics (CFD)

Introduction

The FCC process is well established with over 300 refineries using FCC units to upgrade low value feedstocks to valuable products such as gasoline and propylene. As the FCC environment evolves, refiners are often challenged to operate their FCC units to meet the optimum economic point. TechnipFMC's suite of FCC technologies are licensed in over 60 grassroot units and more than 250 revamps. To support this position TechnipFMC, along with its FCC Alliance partners, Axens, IFPen and Total, make considerable efforts to optimize existing designs and develop new designs to meet the operating objectives set by operators.

TechnipFMC's recent FCC technology improvements include a riser termination device to quickly separate FCC catalyst from the product vapors to avoid post riser cracking reactions, catalyst distributors to uniformly distribute spent catalyst in the regenerators, air distributors for uniform gas distribution and fluidization, high efficiency oil injectors, and many others. These developments have, to some extent, benefitted from the use of computational fluid dynamic (CFD) modeling. CFD provides unique insight into how existing designs perform and understanding of how design changes will perform in the real world. CFD is currently playing a major role in the FCC industry allowing innovative solutions to enter the market faster and more cost effectively. As CFD capabilities and computing power improve, the use of this tool will continue to increase.

For over a decade, TechnipFMC has actively used CFD for design optimization and to troubleshoot FCC operation. CFD provides information required to understand and determine how hardware modifications and operational changes will impact gas-particle flow behavior and

overall performance of the unit. TechnipFMC generally uses Barracuda VR® software, which is specifically designed to model gas-particle fluidized bed reactors. VR or Virtual Reactor® is able to model industrial-scale, thermal, chemically reacting, fluid-particle systems in a computationally efficient manner. It is parallelized using the latest graphics processing units and transient simulations of full-scale FCC regenerator systems, such as those presented in this paper, and can be run to completion quickly enough to allow for evaluation of multiple design alternatives. VR considers the full particle size distribution (PSD) of catalyst within the reactor, which is important for achieving a realistic representation of the particle-fluid dynamics within a fluidized bed. The software features and capabilities have been well validated with both large-scale experimental data and with commercial operating reactors across the broad industry. Additionally, Fluent and FEA simulations are used as necessary, to address specific problems.

This paper discusses development by TechnipFMC of the FCC Alliance's spent catalyst distributor from a simple "hockey stick" distributor to most recent "compound angle wye bathtub" distributor. The goal behind this development was to improve spent catalyst distribution in the regenerator bed to promote uniform coke combustion. CFD modeling was used to predict the catalyst distribution for various design options and guide the development of the mechanical design.

Catalyst regeneration

Regeneration of catalyst is a fundamental step of the FCC process. Catalyst is regenerated by burning coke deposited on the catalyst during the catalytic conversion of oil to regain its activity. During regeneration, the catalyst absorbs heat which it transfers to the riser in order to provide heat for oil vaporization and endothermic cracking reactions. Traditional FCC regenerators operate in either partial or full burn combustion mode. In the early 1980's Total developed a Resid FCC processing scheme, with two stages of regeneration, known as R2R™. This RFCC technology is exclusively licensed by TechnipFMC and Axens and is under continual improvement by the FCC Alliance partners.

A key differentiating design feature of R2R technology, illustrated in Figure 1, is that catalyst regeneration is achieved in two stages in series, where the first stage operates in partial combustion mode followed by complete combustion mode in the second stage. The first regenerator typically burns 60 to 80 percent of the coke on the catalyst and any hydrocarbons entrained from the stripper. The resulting low first stage regenerator temperature minimizes hydrothermal deactivation of the catalyst. Partially regenerated catalyst is then transferred to the second stage regenerator where it is completely regenerated. The configuration rejects a portion of the heat of combustion as carbon monoxide (CO) enriched flue gas from the first stage regenerator, resulting in low first and second stage regenerator temperatures. Lower regenerator temperature increases catalyst-to-oil ratio maximizing unit conversion. Additionally, it reduces catalyst deactivation, resulting in low catalyst make up rate.

Performance of a regenerator is generally determined by parameters such as uniform bed densities, stable and even combustion / temperature profile. These parameters depend on effective distribution and mixing of spent catalyst and combustion air. Maldistribution can lead to temperature variation in the bed, afterburn, catalyst losses and inadequate regeneration, which can impact catalyst circulation, activity and the product yields. Ensuring even distribution of

combustion air is relatively easy, however, the uniformity of the spent catalyst into the regenerator bed depends on the distributor design. The progression of FCC Alliance's spent catalyst distributor technology from a simple "hockey stick" with open slots at the bottom for catalyst outflow to a "compound angle wye bathtub" distributor is shown in Figure 2. The main driving force behind this development has been to improve the spent catalyst coverage in the regenerator, especially for large size regenerators.

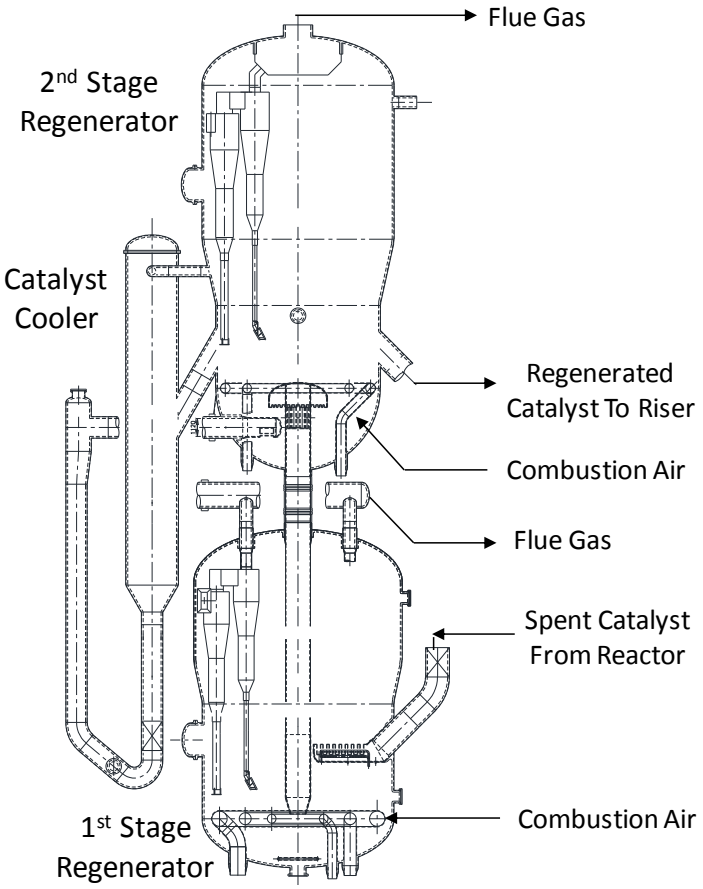


Fig. 1 RFCC technology with two stage regeneration, R2R™

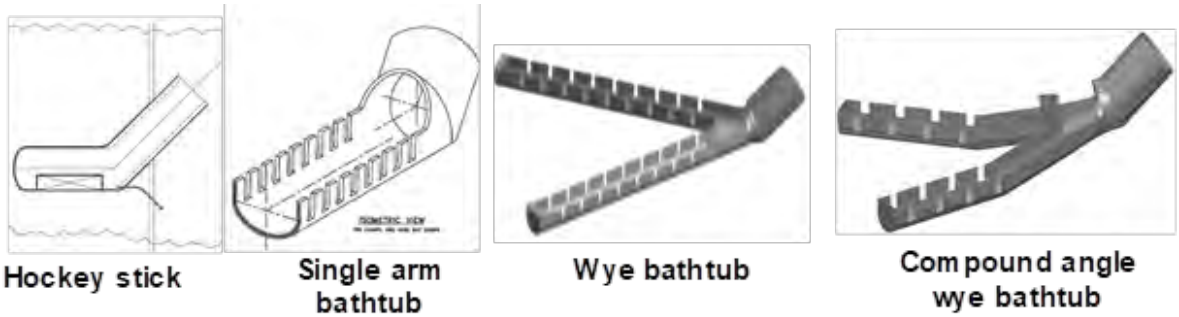


Fig. 2 Evolution of TechnipFMC spent catalyst distributors

FCC regenerator catalyst beds are essentially turbulent "back mixed" beds where the inherent mixing of gas and catalyst is reasonably good and strongly influenced by the bed geometry and in-flow/out-flow of catalyst. The vertical / axial mixing is generally better compared to radial, and radial mixing generally suffers with an increase in regenerator diameter. If spent catalyst is not well-distributed across the vessel, then variations in the catalyst bed temperatures are seen. Earlier, smaller regenerators had acceptable temperature variations, but as units increased in size, the dense bed temperature variation also increased as shown in Figure 3. These regenerators include either the "hockey stick" or short "single arm bathtub distributor", which are generally extended from the regenerator wall towards the vessel centerline, providing limited coverage and distribution of spent catalyst into the catalyst bed. The limited distribution of spent catalyst across the regenerator results in an uneven coke burn-off from the catalyst, impacting unit performance, such as reduced catalyst activity leading to increased catalyst addition, as well as potential for afterburn, even in partial burn units.

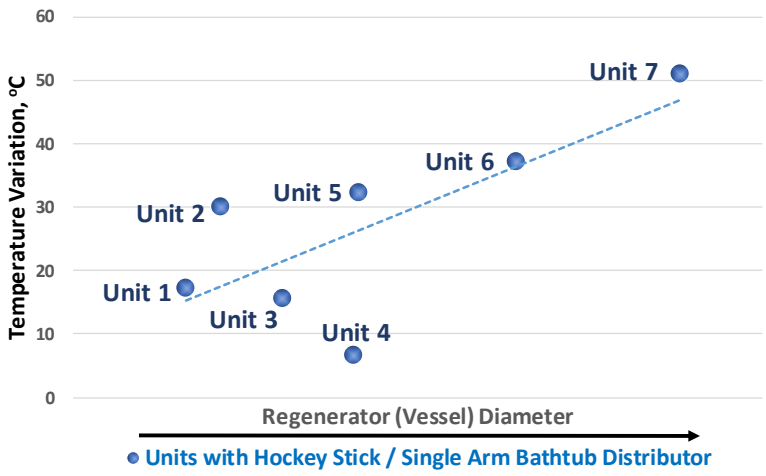


Fig. 3 Industrial data of Partial Burn 1st stage Regenerator – Dense bed temperature variation vs. regenerator size

The data in Figure 3 is from 1st stage regenerators of R2R units, which operate in partial burn, removing the majority of hydrogen from coke, and thereby reducing the potential for high temperature hydrothermal deactivation in the second stage. The impact of uneven coke burn-off in the first stage does not greatly influence catalyst activity in two-stage regeneration. However, it can result in localized afterburn in the first stage and can impact the performance of the second stage regenerator. In single-stage full burn regenerators, where the temperatures are higher, the impact on the catalyst is more severe. The uneven coke burn-off may result in excessively coked particles flowing to the riser and poor catalytic performance, poor yields and increased dry gas formation. Bed and dilute phase temperature variation and afterburn can impact the mechanical reliability of the internals and may often require a capacity reduction to control the dilute phase temperatures. These issues have driven the improvement of the spent catalyst distributors for use in all types of regenerator designs, especially for large regenerators.

Compound Angle Wye Bathtub Distributor Development

TechnipFMC's "compound angle wye bathtub" spent catalyst distributor has been developed to address catalyst maldistribution which is observed as non-uniform bed temperatures in the regenerator. The compound angle wye bathtub distributor design, which is an improvement to an original concept of slanted wye bathtub distributor design, was optimized using extensive CFD modeling and has been validated through commercial results. Multiple simulation cases were performed to understand the significance of parameters such as wall height, bathtub inclination angle, slot width by height ratio, wye angle, catalyst flux, aeration and many others. Several different configurations were modeled prior to finalizing the compound angle concept. CFD was instrumental in studying different configurations with a wide range of parameters, which would not be possible with physical testing and investing a significant amount of time and money.

The original slanted wye bathtub concept was based on having multiple arms extending into the regenerator so that incoming spent catalyst travels along the length of the arm and distributes through the slots. Compared to the original slanted wye bathtub, the optimized design is initially inclined at a steep angle to ensure catalyst flows into and down the arms, followed by a shallower angle to reduce the catalyst velocity and prevent it from overflowing at the end of the bathtub arms. Where catalyst flows into the distributor arms a baffle is positioned to prevent catalyst overflowing and direct it into the two branches. Open slots in the upper section of the arms are eliminated to prevent premature distribution.

A comparison of CFD modeling results from the original slanted wye and the optimized compound angle wye bathtub is shown in Figure 4. The catalyst flow in the bathtub is presented as density distribution in a plan view, as well as along the length of the arms. Modeling of the original design shows a large portion of catalyst from the standpipe accumulates and overflows at the split into the two bathtub sections with a relatively small amount of catalyst flowing down the arms and through the slots. A plan view of the density profile indicates that catalyst coverage is concentrated at the split section only. The catalyst density profile along the side view indicates the flow in the initial section of the wye arms is more active compared to the latter half.

In the optimized compound angle wye bathtub design, catalyst build-up and overflow at the split section is eliminated via increased angle of inclination and installation of a baffle. The initial angle of inclination ensures sufficient catalyst momentum to move it down the bathtub, represented by the active catalyst zone. In the latter half of the bathtub arms, the lower angle slows the catalyst down allowing it to flow uniformly through the slots. The improved catalyst discharge density along the bathtub length, resulting from the two-angle design, is shown in the plan view. It indicates that the design achieves uniform flow of catalyst along the span of the arms, which improves spent catalyst coverage across the regenerator.

A quantitative comparison of percent mass flow deviation from ideal uniform catalyst distribution along the bathtub length for original and optimized configuration is shown in Figure 5. The results indicate that the compound angle wye design is closer to the ideal "even" catalyst distribution than the original concept. This is achieved by incorporating features such as a raised baffle section at the split, compound angle of inclination and optimized slot distribution. The use of the CFD modeling technique was key in optimizing the wye bathtub design parameters. The CFD results

were promising enough that TechnipFMC adopted the "compound angle wye bathtub" for subsequent regenerator designs.

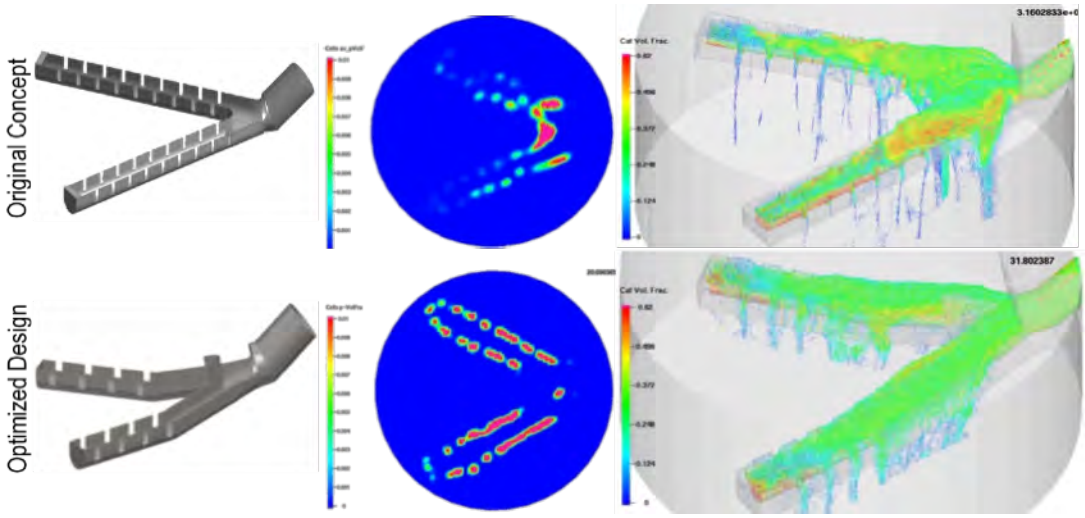


Fig. 4 Wye bathtub performance comparison (original vs. optimized design)

Industrial Example

The original and compound angle wye bathtub distributor designs have been applied to several commercial FCC regenerators and resulted in improved performance. Two commercial regenerators, one with original slanted wye bathtub (Unit A), and other with compound angle wye bathtub (Unit B), are shown in Figure 6. Both the regenerators are single stage and operate in complete combustion mode. They are large regenerators with reduced catalyst bed section diameters in the range of 35 to 40 feet. Unit A regenerator with original wye bathtub did use a baffle at the split to ensure catalyst flowing down the standpipe would not end up overflowing above the crotch area.

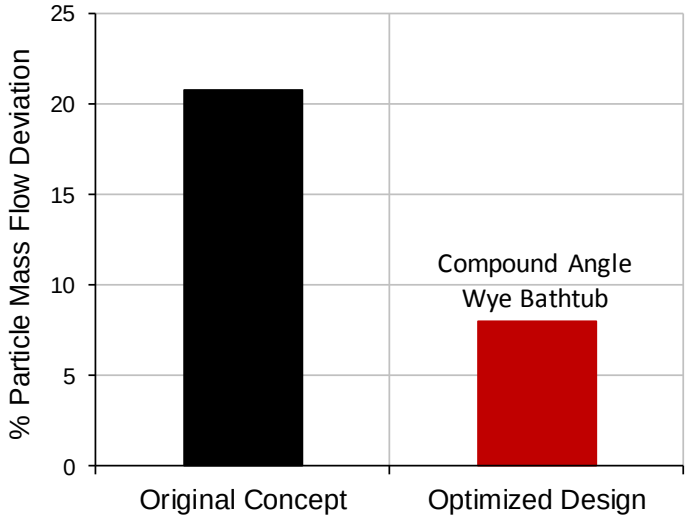


Fig. 5 CFD results Comparison - Max standard deviation from ideal uniform distribution

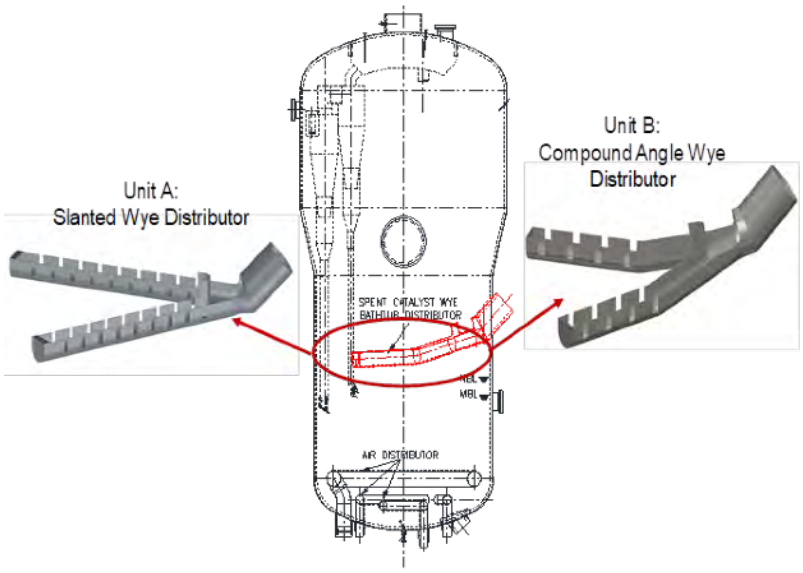


Fig. 6 Commercial regenerators with original and compound angle wye bathtub distributor

The performance of both regenerators is compared in Figure 7. Unit A has an average dense bed temperature variation of 7°C, whereas Unit B is experiencing an average of 2°C dense bed temperature variation across the bed. The dilute phase temperature variation for Unit A and B is 35°C and 12°C respectively. The Unit B regenerator is running with minimal temperature variation in both dense and dilute phase and low afterburn in the range of 15°C. The improved temperature profiles in Unit B with the compound angle wye bathtub present greater unit flexibility to operate at high throughputs or provide more flexibility on feed selection. The commercial results shown here and results of CFD analysis indicate that the compound angle concept is superior to the original wye design. This distributor is now offered as a standard design for the first stage regenerator in R2R technology as well as for single-stage regenerators. Even with the successful implementation of the compound angle wye bathtub design, we continue to explore ways to further improve the design.

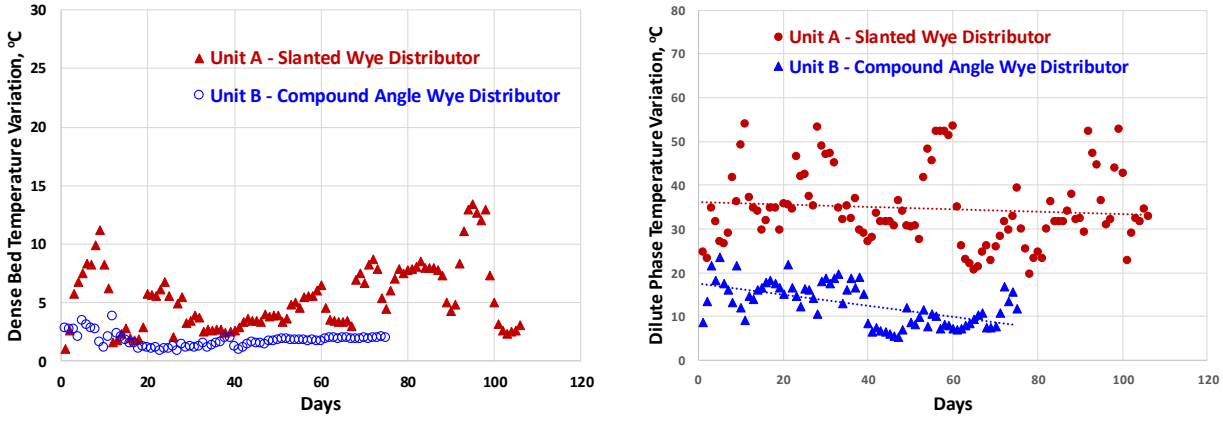


Fig. 7 Industrial data – Dense bed and dilute phase temperature variation (Slanted vs compound angle wye bathtub distributor)

TechnipFMC has recently introduced a "submerged compound angle wye" bathtub as an improved version of the compound angle wye design, where the major portion of the distributor arm(s) is submerged in the catalyst bed. The main driving force behind this modification is to enhance spent catalyst mixing in the catalyst bed, promote bed combustion and reduce afterburn. This concept was, again, extensively modeled to gain confidence prior to commercial application. The design has now been in operation for more than two years and has shown significant improvement in unit performance with respect to reduced afterburn and temperature variation in dense and dilute phase. The pre- and post-turn around operation along with some of the CFD results are published in PTQ 2019 Revamp Issue.

A survey of 12 commercial regenerators is presented in Figure 8 and it indicates how they are performing with respect to dense bed temperature variation with different distributors as a function of regenerator vessel diameter. The performance of the new compound angle design shows clear improvement over earlier designs. There is minimal temperature variation in the bed and bed temperatures are not sensitive to vessel diameter.

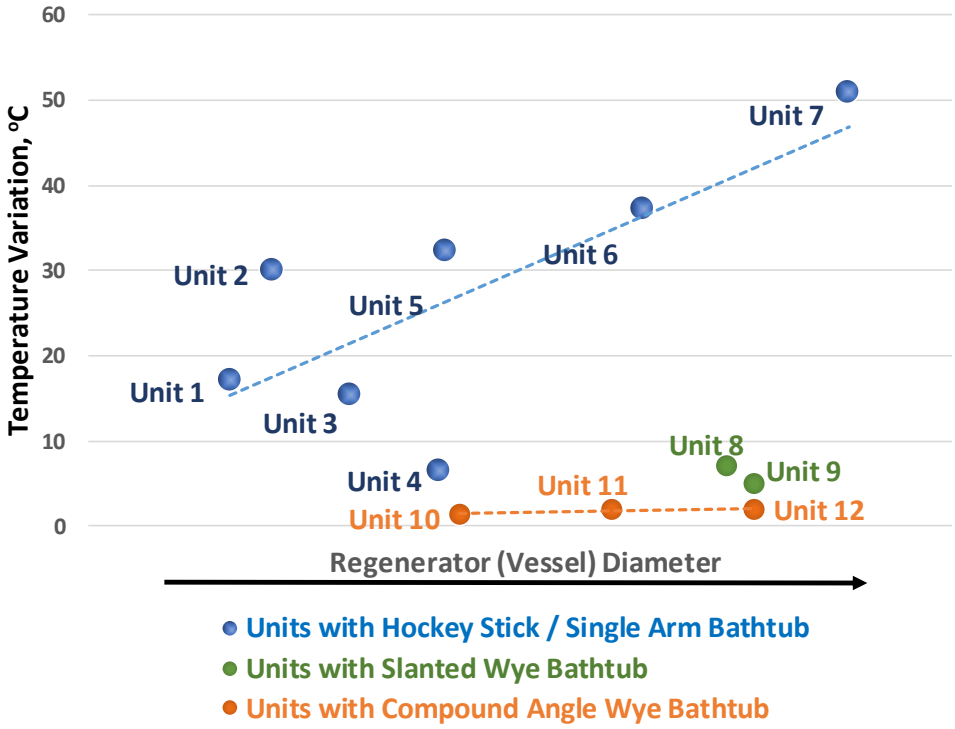


Fig. 8 Industrial data – Dense bed temperature variation vs. distributor type

Summary

Computational modeling is playing an increasingly important role in understanding gas and particle flow dynamics in the FCC process, enabling designers to offer low-risk, high value improvements to clients. Occasionally cold flow models were built, which are expensive and time consuming, and they do provide both qualitative and quantitative results to some extent. The latest generation of CFD modelling tools enables rapid exploration of different configurations and homing in on the best solution. Compared to cold flow testing, these tools allow a deeper

understanding of what is happening at all points in the system. Existing designs were modeled, and changes were made to achieve the desired catalyst flow patterns. This design, optimized solely using CFD, has been verified in several large commercial regenerators.

Acknowledgement

The authors would like to acknowledge the TechnipFMC FCC Alliance members, Axens, IFPEN and Total, for their valuable engagement and efforts to bring innovative solutions and technologies to address the challenges being faced by FCC operators.

PTF Membership

To continue receiving the PTF newsletters (3 issues per year) and stay current with particle technology events and news, please make sure to renew/ start your membership by either:

- Checking Particle Technology Forum when renewing your AIChE membership annually,
- Becoming a PTF lifetime member so that you don't have to renew membership every year

Become a PTF only member

(Annually $15, Lifetime $150)

If you don't see the PT membership in your renewal screen, you can choose "Update Membership Options" and add PTF to your order.

You can also contact AIChE customer service at 800-242-4363 (US);

203-702-7660 (Outside the US); or email customerservice@aiche.org

for membership questions and help.

- PTF Membership Committee

Atomic Layer Deposition on Particles: Scalable Production of Nanostructured Materials

J. Ruud van Ommen

Professor, Department of Chemical Engineering

Delft University of Technology, The Netherlands

j.r.vanommen@tudelft.nl

Abstract

Atomic layer deposition (ALD) is an excellent technique to make nanostructured particles: particles of which the surface is either covered by an ultrathin film or by nanoclusters, with applications in, for example, energy and health. ALD is suited to produce such nanostructured particles with very high precision. Using specialized reactors, we can produce large amounts of particles, even up to the ton-scale. This enables the application in a broad range of products including Li-ion batteries, pharmaceuticals and fuel cells.

Nanostructured particles

As we know, particles or powders are applied in many production processes. Sometimes, the powder itself is the end product, but also many engineering materials require particles as building blocks. Examples are limestone powder in concrete and carbon black particles in rubber tires. For a number of the global grand challenges we are facing, such as the supply of sustainable energy, providing clean drinking water, and advanced pharmaceuticals tailored to the patient, advanced materials will play a key role. With the rise of nanoscience, many novel nanostructured materials with superior properties have been proposed. They are often based on nanostructured particles (particles with orderly arranged elements at the nanoscale) as their building blocks. There are seemingly opposing demands when manufacturing nanostructured particles for such applications: on the one hand, we need precision at the nanoscale, while at the same time large quantities are required to fulfil the market needs. ALD is a technology that can very well combine nanoscale precision and large-scale production [1].

Atomic Layer Deposition

In ALD, we expose the substrate to be coated not simultaneously, but consecutively to the reactant gases. Typically two reactants are used, and the sequencing is repeated a number of times. ALD is normally carried out at elevated temperature (often in the range of 120° to 300° C). In the first step, Reactant A – typically a metal atom with ligands – is fed to the reaction chamber. This reactant is binding irreversibly to certain surface groups of the substrate, such as hydroxyl or oxygen groups. In the second step, the system is purged, e.g. by a nitrogen flow. In the third step, Reactant B – typically an oxidizing or reducing compound – is fed to the reaction chamber, removing the remaining ligands from the surface. Finally, in step four the system is purged again. With these four steps, a single ALD cycle is completed (see Fig. 1) and less than one monolayer of material has been deposited.

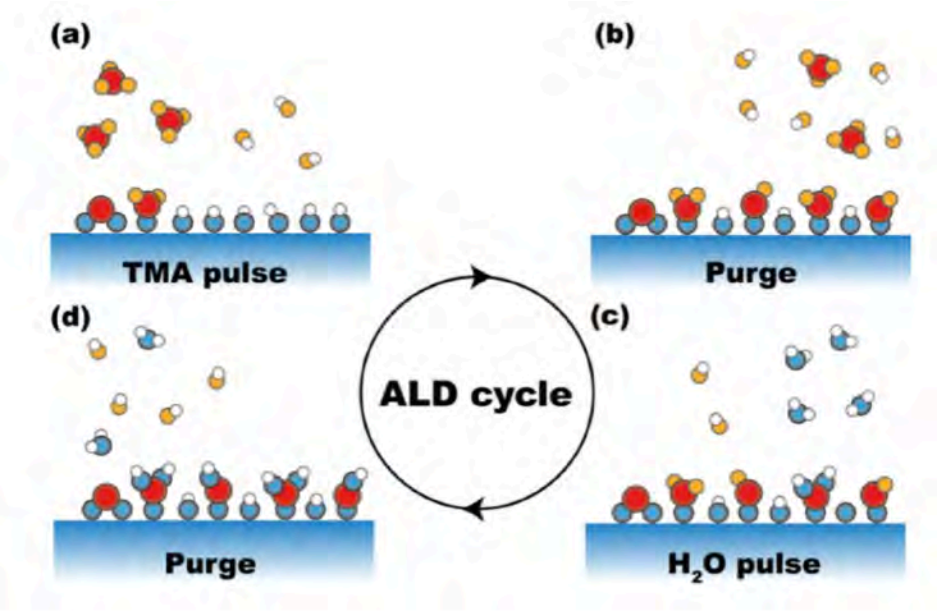


Fig. 1 Schematic representation of an ALD reaction: Al_2O_3 ALD based on trimethylaluminum (TMA, Reactant A) and H_2O (Reactant B): (a) exposure of the substrate surface to TMA and reactions between TMA and surface active sites (e.g., –OH and oxygen bridges); (b) purging of excess TMA and reaction by-product (i.e., CH_4); (c) exposure of the substrate surface to H_2O and reaction between H2O and precursor ligands; (d) purging of excess H_2O and reaction by-product (i.e., CH_4); the four steps (a) to (d) compose one ALD cycle [2].

After this, step one can be carried out again. This cycling of the four steps is repeated until the required amount of material has been grown on the surface. This can be in the form of a film, typically with a very homogeneous thickness. However, several combinations of substrate and grown materials do not yield a film, but show so-called island growth: islands or nanoparticles are formed at the surface. For example, noble metals on ceramic oxide substrates often show this behaviour (see Fig. 2).

When the reactants are purely organic precursors, yielding an organic coating, it is called molecular layer deposition (MLD) instead. It is also possible to have a hybrid approach, e.g. when reactant A is metal precursor and reactant B is an organic molecule. This yields a coating which contains both metal atoms as well as organic bonds.

The reason that ALD (and also MLD) have such a great scalability is that a gas easily fills a whole reactor volume containing the materials that need to be coated. It does not rely on a spray or a laser beam to reach the surface, like in some other methods for nanoscale coating. On the other hand, the binary nature of ALD (the A-B sequencing) makes that we keep very good control over the size of the coating.

Applying ALD to particles

Research into ALD on particles already started several decades ago [3,4], but has started to obtain more attention in the past two decades [5,6]. For research purposes, some grains of powders could be put on a wafer or in a holder, and be coated in a regular ALD reactor, like used for

coating wafers in the semiconductor industry. However, when a larger amount of material needs to be coated, it is much more attractive to apply a tailored reactor. In the early days of ALD, often packed beds have been applied: a vessel filled with a stagnant mass of particles, through which the reactant gases are blown. This has the disadvantage that the contacting between particles and reactant is not optimal, and that it is hard to remove the reaction heat. These days, more often reactors with moving particles are used, either by rotating the reactor vessel or by fluidizing the particles [7]. We use the latter approach: we fill a column with the powder we aim to coat, and blow an upward flow of nitrogen through it to fluidize the powder. Then we add the reactants A and B alternatingly to the nitrogen flow (see figure 3). We found that in this way we are able to coat the surface of all particles in a very homogeneous way. Even when the base particles are nanoparticles, this proves to work. In that case, the particles form large, very open agglomerates in which the surface area of the individual particles is still very well reachable. So we are actually not fluidizing individual nanoparticles, but rather nanoparticle agglomerates. Unlike most ALD processes, we operate our fluidized-bed reactors at atmospheric pressure: most of the gas in the reactor consists of nitrogen, to which we add small amounts of the ALD reactants [1].

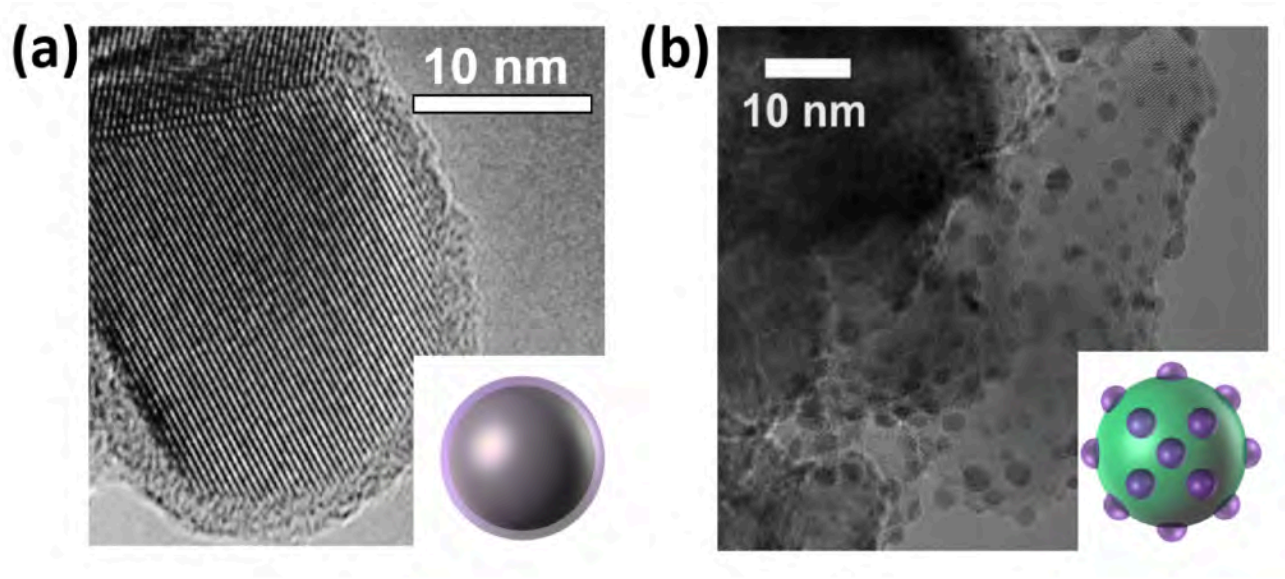


Fig. 2. The two main growth modes of ALD are: (a) conformal growth and (b) island growth. The figures show a transmission electron microscope photograph of alumina on titania and platinum on titania, respectively. The insets show a cartoon of the structure.

With this approach of ALD on particles, we have already obtained very good results in several areas. A first one is in improving batteries: everyone will have the experience that after some time, the battery capacity of a laptop or mobile phone is going down. We have been showing that by coating the particles that form the cathode of Li-ion batteries, the life time of these batteries can be greatly enhanced (Fig. 4.a) [6]. In pharmaceutics, you typically would like an active compound to dissolve slowly in the patient's body: a sudden high peak value is often quite unhealthy, and can cause severe side-effects. Coating pharmaceutical powders with ALD slows down the release (Fig.

4.b). In addition, we found that these coated powders stay stable for a longer time when storing them, and flow more easily when processing them [8]. A third application is in fuel cells: they rely on the scarce, expensive metal platinum. Using ALD, you can spread the platinum much more evenly, greatly enhancing its activity (Fig. 4.c). This enables to reduce the amount of platinum needed. This last example is not limited to fuel cells, but can be applied to all kind of catalysts [9].

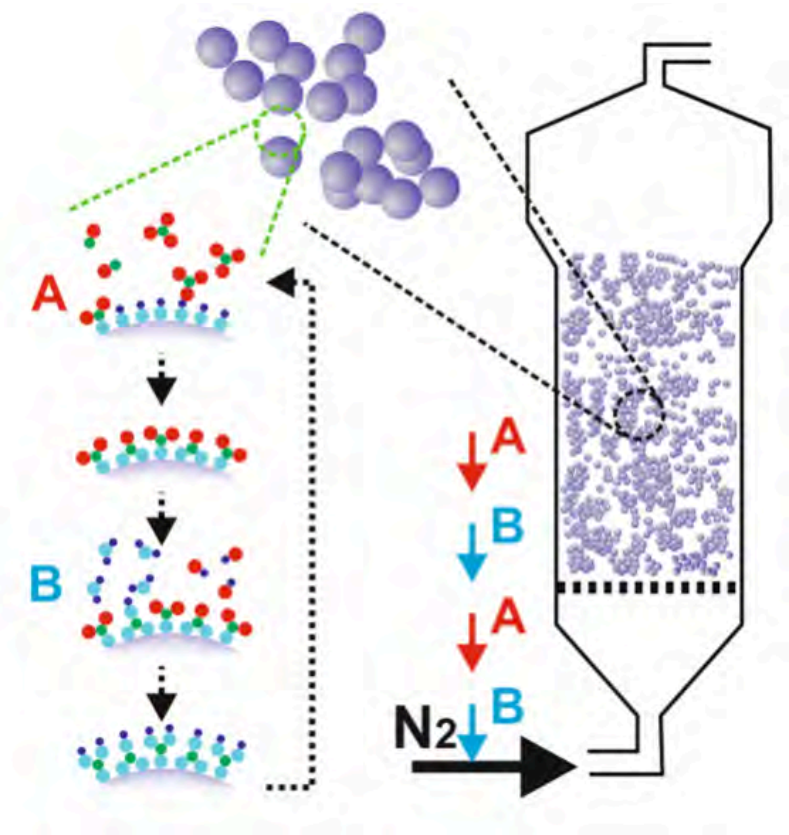


Fig. 3 A fluidized-bed-reactor for ALD. The particles are fluidized by nitrogen; the ALD reactants are added to the nitrogen flow in order to coat the particles.

Currently, we typically produce 1 g up to 100 g of the coated material in our lab-scale fluidized beds. This could also easily be done in larger fluidized beds to produce kilograms or even tonnes of material. However, you then produce it batch-wise (one amount after the other), while in many industrial processes, continuous production is preferred. We have also been developing an approach for that: the so-called pneumatic transport reactor. In this reactor, the particles are blown through a long tube, and the precursor is added along the way [10]. This indeed leads to a continuous flow of nanostructured particles. Delft IMP (which stands for Delft Intensified Materials Production), a spin-off company from our group, is working on further scaling up this approach. They are part of the start-up ecosystem of Delft University of Technology (YES!Delft), and have a reactor that can produce more than 100 kg per day. They are currently working to take this to the tonne-scale.

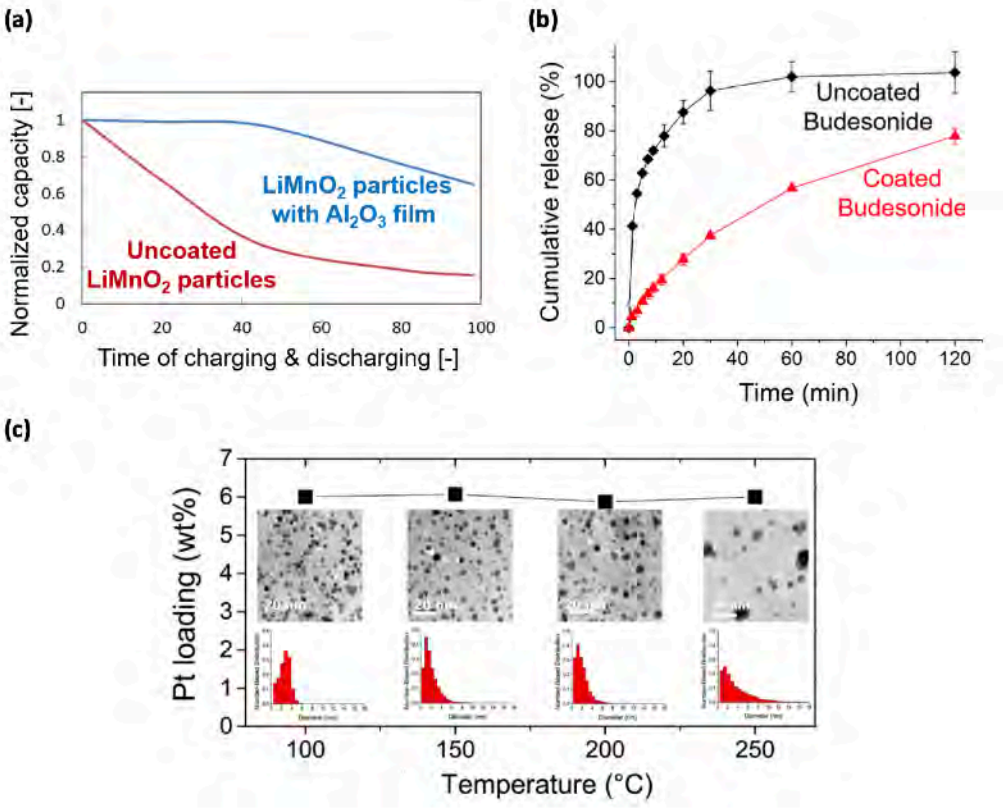


Fig. 4 Some application examples of ALD: (a) enhancing the life time of cathode particles in Li-ion batteries, (b) slow-release of a pharmaceutical compound, (c) making a fuel cell catalyst with ALD at different temperatures. At lower temperatures, the Pt loading is maintained, but a more attractive size distribution is obtained.

Since ALD has so many different applications, we will continue to work on it in my lab. It can, for example, be used to make novel electrocatalysts for the e-Refinery (https://www.tudelft.nl/e-refinery/), and also in the Health area we see plenty of new opportunities.

References

[1] J. R. van Ommen, A. Goulas, *Mater. Today Chem.* 2019, 14, 100183.

[2] H. Van Bui, F. Grillo, J. R. van Ommen, *Chem. Comm.* 2017, 53, 45.

[3] S. V. Yakovlev, A. A. Malygin, S. I. Koltsov, V. B. Aleskovskii, Yu G. Chesnokov, and I. O. Protodyakonov, *J. Appl. Chem. USSR*, 1979, 52, 959.

[4] M. Lindblad, L.P Lindfors, T. Suntola, T. *Catal. Lett.*, 1994, 27, 323.

[5] D. M. King, J. A. Spencer II, X. Liang, L. F. Hakim, A. W. Weimer, Surf. Coat. Technol. 2007, 201, 9163.

[6] R. Beetstra, U. Lafont, J. Nijenhuis, E. M. Kelder, J. R. van Ommen, *Chem. Vap. Deposition*, 2009, 15, 227.

[7] D. Longrie, D. Deduytsche, C. Detavernier. *J. Vac. Sci. Technol. A* 2014, 32, 010802.

[8] D. Zhang, D. La Zara, M. J. Quayle, G. Petersson, J. R. van Ommen, S. Folestad, *ACS Appl. Bio Mater.*, 2019, 2, 1518.

[9] F. Grillo, H. Van Bui, J. A. Moulijn, M.T. Kreutzer, J.R. van Ommen, *J. Phys. Chem. Lett.* 2017, 8, 975.

[10] J. R. van Ommen, D. Kooijman, M. D. Niet, M. Talebi, A. Goulas, *J. Vac. Sci. Technol. A* 2015, 33, 021513.

PTF Award and Dinner Sponsors

Lifetime Achievement Award

Thomas Baron Award

PTF Service Award

Particle Processing Award

Lectureship Award

Young Professional Award

George Klinzing Best Ph.D. Award

PTF Dinner

Student Travel Grants

***Thanks to MERCK for sponsoring the 2019 Student Poster Awards**

A Publicly Accessible, Web-Data Interface of PSRI Fluidization Data for CFD Validation

Casey (Wyatt) LaMarche, Ben Freireich, Ray Cocco

Particulate Solid Research Inc. (PSRI)

Chicago, Illinois, USA

Computational fluid dynamics (CFD) is an umbrella term used here to refer to solving the flow of fluids (including solid-particle flows like fluidized beds) spatially and/or temporally via physical models. CFD has been a focus of significant research resources as it offers to potentially reduce costs and increase revenue for a wide range of fluid and particle-based industrial operations, e.g., providing insight into the behavior of fluidized systems for improved troubleshooting existing systems, designing and operating new operations.

One of the biggest obstacles to the widespread use of CFD in industrial operations is a lack of widely agreed upon validation data and the validity of the physical models used in the simulations. For some fluids, the validity of physical models is widely accepted, for example, using the Navier Stokes' equation to simulate the motion of the single-phase Newtonian liquid water. However, a universal framework for predicting the behavior of particle-based fluids (like fluidized FCC particles) currently does not exist.

Our recent literature study[1] (A publicly available version of the PSRI membership report SA-29 is in preparation) assessing the state-of-the-art for modeling drag in CFD revealed significant inconsistencies in models used for predicting fluidized particle flow. One of the findings of this literature study is the systemic lack of comparison of CFD simulation results to experimental data without "tuning." In the past, PSRI[2] and NETL[3] provided CFD challenge problems as an opportunity for comparison between simulation and experimental results. The experimental apparatus (e.g., system schematics, relevant dimensions), material properties (e.g. particle size, particle density), and operating conditions (e.g., superficial gas velocity) were provided. The objective was to challenge participants to use the experimental inputs to setup CFD simulations. The simulation outputs were submitted to PSRI or NETL to be compared to the experimental results. The results of the last large-scale challenge problem (NETL and PSRI) was published in 2014[3]. They demonstrated a continued poor predictive capability of CFD. Even CFD simulations that predicted results accurately for some measurements predicted inaccurately for others. For example, in some cases, the solids mass flux was predicted well, but the solids velocity was not.

One theory for the persistent mismatch between CFD predictions and measurements of large-scale systems concerns the resolution of the numerical grid. It is assumed that computational cells are too large to simulate all of the gradients relevant to the flow field. One approach to addressing the possible source of mismatch has been to predict large-scale simulation results via sub-grid CFD models (e.g., energy-minimization multi-scale (EMMS) [4] and filter-based approaches [5]). Another theory for the extensive lack of validation is due to missing physics in the CFD, e.g., cohesion for Geldart group A materials.

While reasonably accurate validation of CFD models have been reported previously, these same models have been shown to be less accurate with other physical properties, boundary conditions or initial conditions. Often, variation to the drag model and/or coefficients were required when the flow regime changed. CFD has not demonstrated quantitative accuracy in multiple flow regimes or with a different particulate material. A study to compare the accuracy of a single drag model for predicting flow purposes has not yet been reported. For example, a study to compare the accuracy of CFD with a specific drag model to predict the flow of the same material in different experimental systems, or the different materials in the same system needs to be undertaken. Hence assessing the validity of a single drag model in various flow regimes or for various material properties is not possible with the current state of the literature and available data.

PSRI has performed such experiments and is launching a new web-data interface to bridge the gap between available experimental data and the need for a wide range of CFD validation conditions. PSRI is making the web-data interface available to the public for no-cost. To access the PSRI web-data portal, users first go to www.psri.org and create a free account. Once a PSRI website login is successfully created, the user can access the web-data interface via https://psri.org/tools/webdata/ and selecting "sign in with myPSRI". Users can download data acquired with various materials in at least two of PSRI's experimental units. Descriptions and CAD files of the experimental system and properties of the materials are also available. A snapshot of the web-data interface is provided in Figure 1. Experimental data is currently available for public use on this new web-data interface for more than 30 different materials and at least five flow regimes per material access to measurements corresponding to more than 150 experimental conditions.

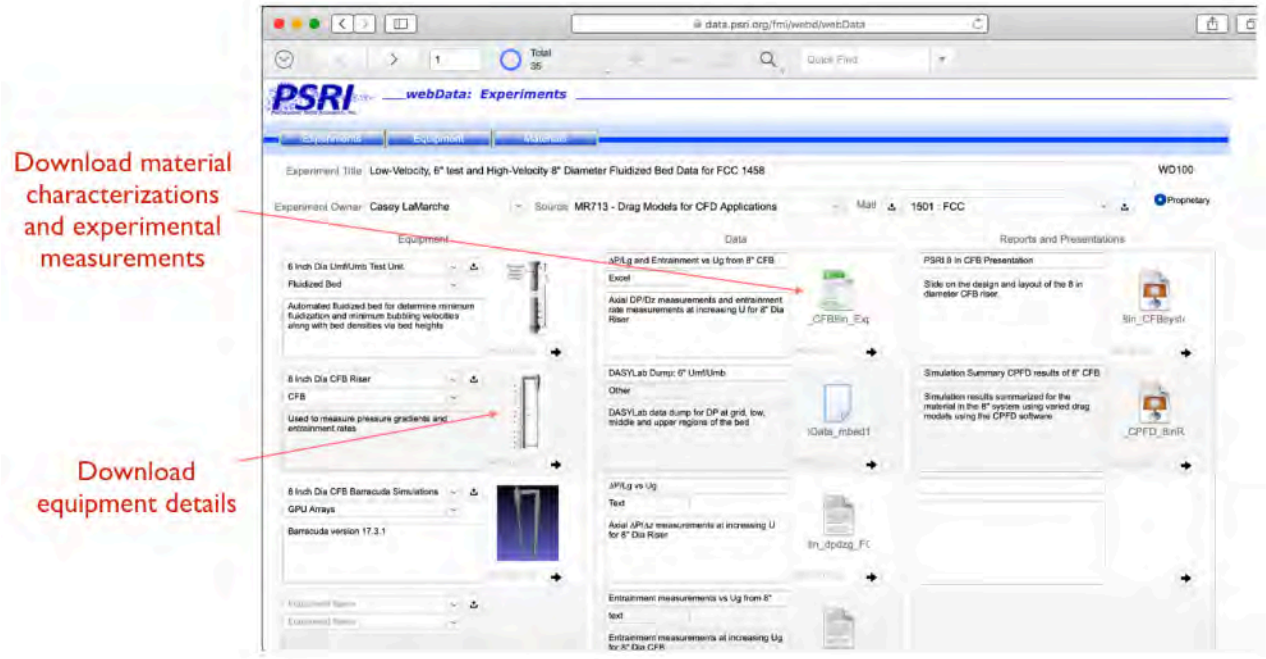


*Fig. 1 Snapshot of web-data interface version 1.0 (**beta**)*

Measurements are provided for experiments performed on the same materials in two different systems, such that the same material can be simulated in different fluidization regimes (discussed

below). Figure 2 provides diagrams of PSRI's higher- and lower-velocity experimental systems used for the data provided in the web-data interface. The higher-velocity (Figure 2a) unit is 20.3 cm in diameter and 330 cm tall. The higher-velocity system is designed to operate as a turbulent fluidized bed for most (Geldart Group A) materials. The flow exiting the top of the higher-velocity unit flows through a cyclone. In other words, the solids that entrain from the bed are recirculated back to the bottom of the bed. Pressure gradient and entrainment rate measurements are reported for the higher-velocity tests performed at different (constant) superficial air velocities. The lower-velocity unit (Figure 2b) is designed to measure the fluidization (increasing gas velocity) and defluidization (decreasing gas velocity) tests around the minimum fluidization and minimum bubbling velocities. Pressure gradient and bed height measurements in the 15.2 cm diameter, 1.5 m tall, lower-velocity unit.

PSRI is proving the measurements from experiments from the higher-velocity and a lower-velocity test unit. The flow regimes of the measurements available in the web-data interface are plotted in Figure 3 using Zenz coordinates[6]:

$$d^* = Ar^{\frac{1}{3}} = d\left[\frac{\rho_f(\rho_s - \rho_f)g}{\mu^2}\right]^{\frac{1}{3}} \quad \text{and} \quad u^* = \frac{Re}{d^*}$$

where d^* is the Zenz particle diameter, Ar is the Archimedes number, d is the particle size, ρ_f is the fluid density, ρ_s is the particle density, g is the acceleration of gravity, μ is the gas viscosity, u^* is the Zenz velocity, and $Re = \rho_f u d/\mu$ is the particle Reynolds number. The unified regime map in Figure 3 includes a correlation for the dimensionless minimum fluidization velocity (green line labeled Umf^*) and the dimensionless terminal velocity (orange line labeled u_t^*). Vertical black lines are used to signify separation between materials from different Geldart's classifications (C, AC, B, and D). The blue and red circles are associated with measurements from the higher- and lower-velocity system, respectively.

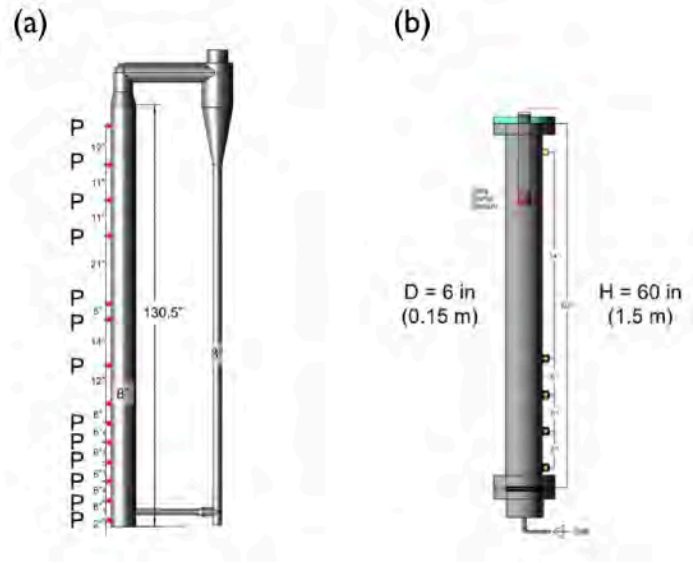


Fig. 2 Schematic of (a) higher-velocity unit and (b) lower-velocity unit

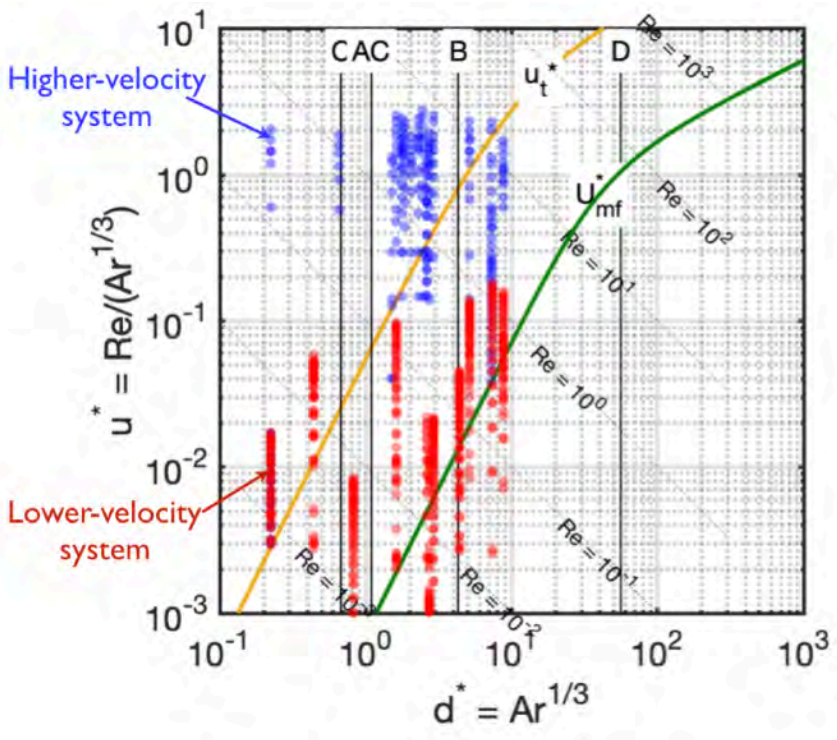


Fig. 3 PSRI's parameter space of flow regimes associated with the measurements provided in the web data reported on the unified regime map.

The aim of this work is to provide experimental measurements that can be used for robust validation of CFD models. The accuracy of model predictions for various materials in the same experimental system can now be compared. Additionally, the influence of experimental system setup and flow regime on the accuracy of model predictions can also be assessed.

References

[1] LaMarche CQ, Freireich B. Particle drag law experimental validation state of the art review. *Particulate Solid Research, Inc. State of the Art.* 2019;SA-29.

[2] Knowlton T, Geldart D, Matsen J, King D. Comparison of CFB hydrodynamic models. *PSRI challenge problem at the Eighth international fludization conference*. France1995.

[3] Panday R, Shadle LJ, Shahnam M, et al. Challenge problem: 1. Model validation of circulating fluidized beds. *Powder Technol.* Jun 01 2014;258(C):370-391.

[4] Yang N, Wang W, Ge W, Li J. CFD simulation of concurrent-up gas-solid flow in circulating fluidized beds with structure-dependent drag coefficient. *Chem. Eng. J.* Dec 2003;96(1-3):71-80.

[5] Igci Y, Andrews AT, Sundaresan S, Pannala S, O'Brien T. Filtered two-fluid models for fluidized gas-particle suspensions. *AIChE J.* 2008;54(6):1431-1448.

[6] Zenz FA, Othmer DA. *Fluidization and Fluid-Particle Systems*. New York: Reinhold Publishing; 1960.

AIChE PTF Executive Committee Elections

The election will begin on August 31, 2020 and will close on October 16, 2020.

The Executive Committee, according to the PTF by-laws, has equal representation between academics and individuals working in other sectors that interface with the field of particle technology. The Executive Committee members act as a liaison to the PTF and play an important role in improving PTF via activities such as recruiting new members/officers, judging posters at the annual meetings, and helping in other PTF standing committees.

You will be able to cast your vote online. A notification will be sent to all members with a link to the ballot. You are able to review each candidate's biography by clicking on his or her name. Once you have made your selections(s), remember to click "**Vote**". You will be voting for **two candidates from each position**, Industry and Academia.

If you have any problems acceding the ballot, please contact AIChE Customer Service at following email address: customerservice@aiche.org

Michael Molnar, The Dow Chemical Co.

Executive Committee - Industrial Member Representative

Particle Technology Forum

Candidates for Academic Member Representatives:

Bodhi Chaudhuri is a Professor of Pharmaceutics, Chemical Engineering and Materials Science at UConn. He got his PhD in Mechanical Engineering from NJIT after obtaining his MS and BS both in Chemical Engineering from IISc, Bangalore and Jadavpur University, Kolkata respectively. He performed postdoctoral research in Chemical Engineering at Rutgers and has 3 years of industrial experience. He has published more than 60 journal articles, book chapters, conference proceedings and delivered 45 invited talks in industry/academia in US and abroad. He is an editorial board member of several international journals including *Advanced Powder Technology*. He and his colleagues have garnered more than $10MM of funding from federal, industrial, and private foundations, for research in powder processing, multiphase flow, machine learning and continuous manufacturing of pharmaceuticals. He routinely consults to pharmaceutical, engineering, and biotechnology companies. He actively participates in activities of AIChE as PTF-session chair/co-chairs whilst organizing several international conferences. He received Young Investigator Award from FDA amongst several other prestigious awards. He acted as the Technical Advisor to Epygen Biopharmaceuticals from 2008-2014. He served as the grant review panel member for NSF and ACS. He held the Visiting Professor positions in University of Copenhagen, National University of Singapore, and Monash University, Australia. Congressman Joe Courtney applauded his group's research efforts in US-Congressional Report in 2011.

Harry Knickle is a Professor Emeritus of Chemical Engineering at the University of Rhode Island where he taught nearly every course including undergraduate and graduate level. Dr. Knickle earned a Bachelor's degree in Mechanical Engineering at the University of Massachusetts and a MS and PhD in Nuclear Engineering at Rennselaer Polytechnic University. He worked at Pittsburgh Energy on Coal Liquefaction and studies the movement on coal particles in bubble column reactors. He received a grant to continue the study for an additional three years. He also worked at DuPont's Titanium Dioxide Plant and studied the reaction of titanium dioxide with chlorine. He has received two NATO Grants and studied conversion of biomaterials and junk oil (ships bottoms) to usable fuel oil in the Ukraine. He has presented three papers on this subject at AIChE meetings. Bioparticle size is very important in this process. He has published three major papers on the Aluminum Air battery. These have more than 20,000 views cited on Mendeley. Harry is a member of AIChE, ASEE, and ECS professional societies.

Silvina Tommasone is a full professor at the Department of Chemical and Biochemical Engineering at Rutgers. She has over twenty years of experience in modeling of particulate and molecular systems. Since joining Rutgers, she has worked on experimental nanoparticle synthesis, characterization of pharmaceutical materials, and catalyst particles, and flow dynamics of granular materials. Silvina has authored more than 70 peer reviewed publications, 3 patents, more than 100 conference presentations, and numerous non-peer-reviewed publications, and she has secured federal (from NSF and NIH), state, and industrial research funding exceeding $8M. Her research and scientific accomplishments are well cited with *H-Index of 23* in Google Scholar, and have been recognized through several scientific awards including the NSF-NIH IGERT Award in Nanopharmaceutical Engineering and Science and the Board of Trustees Research Award for Scholarly Excellence from Rutgers University. She is an active faculty member of the Catalyst Manufacturing Consortium at Rutgers and the Pharmaceutical Engineering Program. In parallel to and aligned with her research pursuits, Dr. Tomassone has been recognized as an accomplished teacher and proficient educator through several teaching awards, including the 2017 Professor of the Year in the Chemical and Biochemical Engineering Department, the 2011 Excellence in Teaching Award in the Chemical and Biochemical Engineering Department, and the 2010 Excellence in Teaching 2010 Chemical and Biochemical Engineering Award. She is a senior member of the American Institute of Chemical Engineers and has served as Vice Chair of Area 3 Session at the AIChE Particle Technology Forum from 2007 to 2011.

Andrew Tong is an Assistant Professor of Practice in the Department of Chemical and Biomolecular Engineering at The Ohio State University, with research interests in chemical looping-based gasification and combustion processes, moving beds, and sensor development for gas-solids flow characterization. Andrew joined the faculty at The Ohio State University in 2015. He is a chemical engineering graduate of The Ohio State University (B.S. 2008, M.S. 2011, and PhD. 2014). Andrew is a member of both AIChE and the AIChE Particle Technology Forum, and he serves as a representative of the Carbon Utilization Research Council (CURC). Andrew has authored twenty-seven (27) peer-reviewed publications and three book chapters, and he has been an active inventor with two patent cases granted to date.

Candidates for Industrial Member Representatives:

Scott C. Brown is currently a Principal Research and Development Engineer at the Chemours Company, where he serves as a corporate expert in particle characterization, surface & interfacial phenomena, and nanotechnologies. His roles span from product development and external innovation to product sustainability and international policy development for emerging technologies. Dr. Brown is active in the international standards and science policy communities. He serves as Vice Chair of the Nanomaterial Expert Team for Business at the Organization of Economic Cooperation and Development (OECD), Chair of the American Chemistry Council's (ACC) Nanotechnology Panel, Convener of the Nanotechnology Liaison Coordination Group for ISO TC 229, Chair of Joint Working Group 1 for the US delegation to ISO TC229, and is leading several efforts on particle nomenclature in both ISO and IUPAC. Before Chemours, Dr. Brown was a Sr. Research Scientist in DuPont, where he led the Corporate Particle Characterization Laboratories and developed several new approaches for the advanced functional characterization of particulate materials and interfaces, as well as a research faculty member in the Particle Engineering Research Center at the University of Florida. During and prior to this time, Dr. Brown was very active in the international particle science and technology community and participated in key international coordination efforts such as Professor Ko Higashitani's Core-to-Core program sponsored by the Japanese Society for the Promotion of Science. Scott C. Brown graduated from the University of Florida [BS in Chemical Engineering and PhD in Materials Science and Engineering]. He has published more than 10 book chapters, and 60 journal articles covering a wide range of topics in particle technologies.

Mayank Kashyap is a Staff Scientist and subject matter expert (SME) in Particle Technology and Fluidization (PT&F) at SABIC. Mayank has over fifteen years of theoretical, practical, experimental, and computational research experience in PT&F. At SABIC, he leads PT&F research and plant support activities and provides fundamental insight and technical guidance on the operation and design of fluidized bed reactors and solids handling equipment, globally. Mayank has held several leadership positions in the AIChE PTF, including Board Member, Student Workshop Chair, Executive Committee Member, Newsletter Editor, and *Fundamentals of Fluidization I* Session Co-Chair. He was instrumental in establishing the AIChE PTF SABIC Young Professional Award. In addition, he was an Advisory Board member, Area Chair of Education, and Guest Editor for the Special Edition of Powder Technology Journal, for the 8th World Congress on Particle Technology. He served on the elected Technical Committee (TC) at Particulate Solid Research Inc. (PSRI), from 2014-2015. Mayank received Ph.D. in Chemical Engineering from Illinois Institute of Technology (IIT) in 2010. He has published eight (8) first-author papers in international journals, filed eight (8) patent applications, and co-authored a book. He has delivered over twenty presentations at international conferences. Mayank has been honored for his contributions with thirteen awards and recognitions from various organizations, including *2019 SABIC Year-End-Award, 2018 IIT Outstanding Young Alumnus Award*, *2016 SABIC PETCHEM Best Project Award*, *2011* and *2012 Ascend to Excellence (APEX) Awards*, and the *2012 AIChE PTF George Klinzing Best Ph.D. Award in Particle Technology*.

Madhusudhan Kodam is the Solids Processing Technology Leader in Corteva Agriscience providing technical support for both manufacturing and R&D in various solids processing technologies. Prior to Corteva, Madhu has been with Dow for almost eight years. He is involved in solving a wide variety of problems related to particle technology, ranging from caking and flowability of bulk solids to pneumatic conveying, fluidization, and other two-phase flow problems. He received his PhD in mechanical engineering from Purdue University, where he developed novel contact-detection algorithms for true pharmaceutical tablet shapes and different attrition mechanisms. His research interests include continuum modeling of bulk solid flows and the application of fundamentals for solving bulk solid flow problems. As part of AIChE's PTF, Dr. Kodam served as the Co-Chair and the Area Chair of the Area 3C, Solids Processing and Handling and chaired several sessions in PTF over the last 10 years. He is currently the Webmaster for the Particle Technology Forum of AIChE.

Casey (Wyatt) LaMarche is a Project Leader at Particulate Solid Research Inc. (PSRI). Prior to joining PSRI, Casey was a postdoctoral research assistant at the University of Colorado in Prof. Christine Hrenya's lab. Casey obtained his PhD in Chemical Engineering from University of Florida and studied the interaction of turbulent sub-sonic jets with dense particle beds with applications to landing rockets on the Moon, Mars and asteroids. Casey's current research projects at PSRI are aimed at developing better first-principals-based understanding of the influence of drag and cohesion on fluidized-bed behavior in various fluidization regimes. Casey has over 15 peer-reviewed publications and presented more than 20 presentations in the field of particle technology. He teaches a session on modeling for fluidization applications during the PSRI Fluidization seminar and a webinar on modeling discrete element method for PSRI members. Casey is currently a co-chair of the fluidization area in the Particle Technology Forum of the AIChE Annual Meeting and has chaired several conference sessions in past AIChE meetings. He has also served as a judge for the undergraduate poster session at the *8th World Congress on Particle Technology*. Casey has also mentored more than 18 undergraduate researchers for research projects focused on particle technology.

Satish K. Nune holds a Ph.D. in Materials Chemistry, which he earned from the University of Hyderabad in India in 2004. He has extensive experience in nanomaterial synthesis using green methods. To tackle the increasing energy challenges, Satish at Pacific Northwest National Laboratories (PNNL) has been pursuing development of various hybrid nanostructured materials with engineered porosity for rare earth metals separations, subsurface imaging, thermal energy storage, gas separation, water management, alkane/alkene separation, and energy storage applications. His research encompasses materials design relating to the microstructure of materials, their synthesis and processing of nanoscale porous materials, and their functionalized analogues with varied properties for biology and energy related applications. His work on improving colloidal stability of porous nanoparticles and magnesium production from sea water has been licensed to industry, and his research is regarded with numerous citations (>3320) from research groups worldwide with an *h-index* 27 (70 Peer Reviewed Publications, 13 Patents, and 21 DOE Reports). Dr. Nune is internationally recognized as an innovator in the development of hybrid nanostructured porous nanomaterials for water management, metal extraction from geothermal waters, and separation applications. As a candidate for Executive Committee, his goal is to bring the AICHE's and PTF vision into an exciting reality.

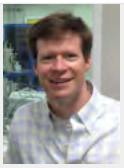
Andrés D. Orlando earned his Bachelor of Science in Mechanical Engineering and Doctorate degree with a focus on Granular and Powder Mechanics from Clarkson University. Prior to joining Jenike & Johanson, Inc. in 2012, he spent a year as a Post-Doctoral Research Associate at the University of Southern California, where he continued his research in the mechanics of granular and powder flow. As a Senior Project Engineer with Jenike & Johanson, Inc., he is regularly involved in troubleshooting and developing recommendations for powder handling equipment across a wide range of industries. He is also active in presenting short courses and lectures regarding bulk solids and powder flow technologies, primarily through AIChE. Dr. Orlando is also a licensed professional engineer.

Karla Sperati is Associate Director with Dow, Inc.'s Logistics Technology Center, specialized in particulate solids handling and industrial packaging. Since 1997, Karla held several technical roles related to Manufacturing and Engineering in Dow Plastics Business, were she led the design of the finishing area of twelve (12) Polyethylene manufacturing plants and participated in the commissioning and startup of facilities in Asia, Europe and North America. Karla is co-inventor in 2 US Patents and author of several issues of Dow internal literature related to packaging materials and solids handling processes. She is member of the AIChE and its Particle Technology Forum (PTF). She is the chair of session 03C02 of the AIChE 2020 Annual Meeting. Karla graduated with a Bachelor's degree in Chemical Engineering from Universidad Nacional del Litoral (Santa Fe, Argentina) with a Master's in Business Administration from Northwood University (Michigan, USA).

Jung-Sheng (JS) Wu is a particle processing expert in the Corporate Research Laboratory at 3M. He has extensive industrial particle process development experiences in high energy bead milling, high pressure dispersing, nanoparticle synthesis/surface modification, precision nano-dispersion coating, and emulsification. He has also led projects in carbon fiber composite processing, induction heating, hybrid aerogel synthesis, UV processing, and microreplication. His research since 2002 has been applied in various product platforms, such as infrared-control window films, 3M Matrix Resin, and optical films. He obtained his PhD in Chemical Engineering from the Massachusetts Institute of Technology and his MS/BS from National Taiwan University. He is the current holder of 36 issued or applied US patents. He has been an active AIChE member since 1999, served as NSEF Directory of Technology/Webmaster since 2010, and chaired annual meeting sections. He serves as Direct-at-Large of the 2019-2020 NESF Executive Committee.

Particle Technology Forum Organization

✦ *Officers*

Chair Dr. Bruce Hook bdhook@dow.com	
Co-Chair Dr. Jim Gilchrist gilchrist@lehigh.edu	
Treasurer Dr. Benjamin Glasser bglasser@rutgers.edu	
Past Chair Dr. Raj Dave dave@njit.edu	

✦ *Executive Committee*

Industry	
Michael Molnar michael.molnar@dow.com	
Willie Hendrickson whendrickson@aveka.com	
Dr. Brenda Remy brenda.remy@bms.com	
Dr. Mayank Kashyap mkashyap@sabic.com	

Academic	
Dr. Heather Emady heather.emady@asu.edu	
Dr. Aaron Moment ajm2293@columbia.edu	
Dr. Ah-Hyung Alissa Park ap2622@columbia.edu	
Dr. Richard Lueptow r-lueptow@northwestern.edu	

✦ *Liaisons and Committee Chairs*

CTOC Liaison	Dr. Reza Mostofi	reza.mostofi@honeywell.com
Nominating Committee Chair	Dr. Michael Molnar	michael.molnar@dow.com
PTF Newsletter Committee Chair	Dr. Mayank Kashyap	mkashyap@sabic.com
PTF Webmaster	Dr. Madhusudhan Kodam	madhusudhan.kodam@corteva.com
PTF Student Workshop Chair	Dr. Mayank Kashyap	mkashyap@sabic.com
PTF Programming Chair	Dr. Ben Freireich	ben.freireich@psri.org
PTF Dinner Sponsorship	Dr. Jim Gilchrist	gilchrist@lehigh.edu
PTF Awards Sponsorship	Dr. Reddy Karri	reddy.karri@psri.org
PTF Education Committee Chair	Dr. Shrikant Dhodapkar	sdhodapkar@dow.com
FPST 2020 Chair	Dr. Heather Emady	heather.emady@asu.edu
Staff Liaison	Ms. Darlene Schuster	darls@aiche.org
	Ms. Diane Cappiella	dianc@aiche.org
Accounting	Ms. Leila Mendoza	leilm@aiche.org

✦ *Programming Leadership*

Group 3A: Particle Production and Characterization	**Group 3D: Nanoparticles**
Chair: Dr. Bryan Ennis bryan.ennis@powdernotes.com Co-chair: Dr. Heather Emady heather.emady@asu.edu	Chair: Dr. Timothy Brenza timothy.brenza@sdsmt.edu Co-chair: Dr. Eirini Goudeli
Group 3B: Fluidization and Fluid-Particle Systems	**Group 3E: Energetics**
Chair: Dr. Jia Wei Chew jchew@ntu.edu.sg Co-chair: Dr. Casey LaMarche casey.lamarche@psri.org	Chair: Dr. Travis Sipper tsippel@iastate.edu
Group 3C: Solids Flow, Handling and Processing	
Chair: Dr. Rich Lueptow r-lueptow@northwestern.edu Co-chair: Dr. Yi Fan	