



The PTF Newsletter

Editorial:

The summaries of award lectures and the pictures of the Award Dinner in this issue once again remind us of our vibrant and active organization. Let us continue to contribute towards its success.



Shrikant Dhodapkar

The Dow Chemical Company

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2016 AIChE Annual Meeting

November 13-18, 2016

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Presented by Dr. Stefan Heinrich, *Hamburg University of Technology*

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"Effective Use of Discrete Element Method (DEM) Modeling of Particle Attrition Applications and Understanding Unforeseen Consequences with Attrition Reduction Design Techniques"

Presented by Dr. John Carson, *Jenike & Johanson*

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Letter from The Chair



This is the election year and no I am not talking about the US elections. What I am bringing your attention to are another important set of elections related to our profession. As all other elections, it is important to practice our rights as a member of the society and voice our concerns and even bring our ideas to practice. I encourage each and every one of you to do your part this year and vote. So what is going on at AIChE and PTF this year?

First there is the AIChE constitution. The AIChE constitution serves as the primary governing document for the institute. This year, AIChE's Board of Directors will be asking us to approve proposed changes to the Institute's Constitution. These changes are set to: - confirm with the latest regulatory requirements, - modernize and streamline institute processes and - enhance AIChE's responsiveness. The voting will happen in fall 2016 and it is very important for all members to participate and carry the AIChE toward its new chapter.

Second is the PTF bylaws. We at PTF have also been working hard to review the bylaws and the proposed amendment will be send out to the members for review and voting at our business meeting in San Francisco. There are some outdated items that need to be revised and also some modernization that need to be included. So look out for the email containing these updates and vote in November. I would like to take this opportunity to thank Ben Freireich and Bruce Hook for their time and effort to review and proposed the revisions and also thank the other officers for their constructive discussion and feedback.

The last one is also related to PTF. This is a year that we elect our new Executive Committee members. Please consider getting involved with PTF business and nominate yourself. This is a great opportunity to

work with other PTF devotees who are volunteering to improve and move forward what PTF pioneers have started. We are a small forum and new voices and fresh ideas are always welcomed in our EC. We are seeking two new members from academia and two from industry for a 4 year term. A separate email will be sent out later and there are some more information elsewhere in this issue. If you have any question, please feel free to contact me at reza.mostofi@uop.com and I will be happy to provide more information.

What else is going on in the PTF world? Thanks to Raj Dave, Jim Gilchrist and Bruce Hook, we are also re-vamping and standardizing our PTF awards process and procedure. The main reason for this was to create a written document which is clear and easy to implement and follow. It was a big job to collect all the past information and talk to all the involved people and eventually come up with a final document. In future, this may have to be revised as well, but we were looking for a starting point at this time. There is also some more information about this unified process in this issue. Again for more information, please contact me.

We also have teams who have worked on ways to increase our membership, contact companies for advertisements and create programs to use that revenue for student outreach programs, run the students' workshop and also identify members for AIChE fellow nomination. Recently, Ben Glasser has agreed to take on the treasurer role after Alissa Park has decided to help in a different capacity. A big thank you to Alissa for taking care of the PTF financial side for the past years.

So many things going on in the background. The newsletter has also experienced some changes and improvements. An Editorial Advisory Committee for the PTF Newsletter was formed to facilitate greater participation of our membership and help to cover a broad interest of all members. Shrikant Dhodapkar will serve as the Newsletter editor for the next 5 years.

As always, if you have any comments, please send it to me or any other EC member listed on the last few pages of this newsletter.

Happy voting!

Reza Mostofi

UOP, A Honeywell Co.

PTF Award Lecture 2015

Reflections on 50 years in bulk solids handling

John W. Carson, Ph.D.
Jenike & Johanson, Inc.

November 10, 2015



INTRODUCTION

I'm appreciative of Tim Bell and Dr. Greg Mehos for nominating me, and to the selection committee for honoring me in this way. I understand that I'm the 20th recipient of this award but only the 5th industrial recipient. Previous industrial recipients were: Reg Davies, Andrew Jenike (I was honored to accept his award in 1998), Ted Knowlton, and Karl Jacob – all people I have known and respected.

Receiving this award in Salt Lake City takes on special significance, since this is where Dr. Jenike did his basic research and wrote his now-famous "Storage and Flow of Solids", Bulletin 123 of the Utah Engineering Experiment Station.

BRIEF HISTORY OF JENIKE & JOHANSON

On Jenike's 39th birthday in 1954, he decided to dedicate his life to the field of storage and flow of bulk solids. Up to then the design of bins and hoppers was a "black art", with no scientific basis. Jenike spent the next eight years at the University of Utah Engineering Experiment Station, where he developed basic theories, test equipment and design procedures. During that time he was thesis advisor to a number of graduate students, the most accomplished of whom was Jerry Johanson. Jerry completed and published his Ph.D. thesis, "Stress and Velocity Fields in the Gravity Flow of Bulk Solids", in 1962.

That same year Jenike left Utah and set up a private consulting engineering business in Winchester, MA. Johanson went to US Steel's Applied Research Laboratory in Monroeville PA. After four years there

he joined Jenike in Massachusetts, and together they formed Jenike & Johanson, Inc. (J&J).

In 1975 J&J opened its first branch office in Toronto Canada, with Dr. David Goodwill as president.

Jenike retired in 1979 at age 65, and Johanson took over as president. Under his leadership J&J opened a branch office in San Luis Obispo, CA in 1982. Three years later he left the company, and I became president.

Over the years J&J has opened four additional branch offices: Chile (1994), Australia (2012), Houston (2013), and Brazil (2014). Currently we have nearly 90 employees of whom over half are degreed engineers. We offer a wide range of services in the field of storage, flow and processing of bulk solids: testing, consulting, structural design, custom fabrication, capital projects, simulation and modeling, training and forensic services.

"BE AT THE RIGHT PLACE AT THE RIGHT TIME"

During my three-plus years as a graduate student at MIT I worked there 12 months a year except for one summer when I was employed by Kennecott Copper's Ledge-mont Laboratory in Lexington MA. Over lunch one day I asked one of the senior executives there, "What does it take to succeed in business?" He responded, "Be at the right place at the right time". I said, "Great – but how do I know that I'm at the right place and that it's the right time?" His response, "You won't know until it's too late. Good luck!"

I feel that I have been blessed with being "at the right place at the right time" numerous times throughout my career, but never more importantly than when I was just starting out.

I grew up in a small farming community in northern Maine. We started school mid-August each year, then closed mid-September for at least three weeks while we all went out to nearby potato fields to harvest the crop. It was hard work with little pay (25 cents for a 180-lb barrel of potatoes), but I learned

valuable lessons about commitment, frugality and the satisfaction of completing a job no matter how difficult.

My father was a clerk in a hardware store, and my mother stayed home to raise my sister, who is two years younger than I, and me. Even though my dad had only a high school education, it was important to both of my parents that my sister and I attend college. However, at my dad's meager salary, that was going to be difficult. Fortunately, I heard about the cooperative (co-op) education program at Northeastern University (NU) in Boston. This appealed to me because I could essentially pay for my way through school by working half of each year in industry and, at the same time, learn what a career in my chosen field (engineering) was all about.

My first co-op job was at US Steel's Fairless Works in Morrisville PA. Initially I worked in the engineering department of the coke plant, then later in Central Engineering. As a result of my work experience and classes that I took at NU, I changed my major twice: from chemical engineering to industrial engineering, then to mechanical engineering.

After two years working in the steel mill I knew one thing for sure: I didn't want to work in a steel mill for the rest of my life! I asked my Co-op Coordinator if there were other co-op positions available. About that time my first boss at Fairless Works was at NU interviewing graduating seniors. When he heard that I was looking to change jobs, he asked to meet with me. His first question when we met: "What do you want to do after graduation?" I told him I really didn't know for sure, but I had an interest in R&D. The next thing I knew he set up interview for me at US Steel's Applied Research Laboratory in Monroeville PA. During my interview there I met with four groups, one of which was Bulk Solids Handling Research. At the end of day I was asked, "If we offer you a co-op job here, which group do you want to work in?" I replied, "I'll work in any of them – they all sound interesting."

They offered me a position, and I accepted. I didn't know which group I would be working in until I showed up for my first day of work and I was told, "We've decided to place you in the Bulk Solids Han-

dling Research group." This was a lively, interesting group of individuals led by Henk Colijn, with Jerry Johanson as Chief Researcher. I did research on loads acting on inserts inside bins, friction plate sizing of bulk solids, and other topics.

Johanson left US Steel in 1966 to form J&J, while I stayed there to the end of my co-op and graduation from Northeastern in 1967. Since J&J was located in a suburb of Boston, I had the opportunity to meet Jenike, and he offered me a summer job between undergrad and grad school. The company was located in the basement of Jenike's house.

Upon graduation from NU I was commissioned in the US Army through the ROTC program. I applied yearly for a delay to active duty so that I could attend grad school. Each year's request was granted until June 1970 when I was told, "No more delays after this year". I hurriedly completed my PhD in October of that year.

Expecting that I had at most six to eight months before I'd have to go into the Army, I took a "short term" job with J&J upon graduation. In the spring of 1971 I received a letter from Uncle Sam saying in effect, "We have too many officers coming into the Army because the Vietnam War is winding down. Would you be interested in serving 3 to 6 months Active Duty for Training followed by a 2-year extension of your Army Reserve commitment?" I went to Jenike and asked if it was OK for me to stay. He turned my question back to me: "Do you want to stay?" I said, "Yes" -- and 45 years later I'm still there!

Looking back during my formative years of college, I was extremely fortunate to "be at the right place at the right time" on numerous occasions, although it certainly wasn't clear to me at the time.

THE FUTURE IS BRIGHT

Looking forward I am confident that the future is bright for those individuals who are currently working in this field and for those who will join in the future. I have four reasons for being optimistic.

Reason for optimism #1: The importance of this technology is as great as ever

Bulk solids handling is, by far, the world's largest industrial activity and certainly one of the most mature, having been carried out for over 2,000 years. It has been estimated that over 16 billion tons of common bulk solids are handled – often many times – every year [1]. Yet, even with all this history and wealth of experience, far too many solids handling projects still go wrong!

When visiting clients I still hear words such as:

“It's just a bin.” (Downstream equipment often does not perform as intended unless the flow of material into it is uniform and reliable.)

“There's no need to design transfer chutes. We can modify them in the field.” (Field modifications are time consuming and more limiting than designing them right the first time.)

“The supplier of some flow aid equipment we're considering is so confident it will work that he'll give us our money back if it doesn't.” (The money back will be miniscule compared to the plant downtime and cost of retrofit.)

A strong reason for the lack of understanding about this technology is that education of engineers in this field isn't much better than it was 40 or 50 years ago. We at J&J have been offering short courses in this technology through AIChE and other groups since the early 1970s. Despite the popularity of these courses, only a small fraction of engineers in industry receive such training. Most of the rest often flounder when faced with a bulk solids handling problem. This is even truer in developing areas of world, so they are ripe for introduction of this technology.

Another indication of the importance of this technology is that material-induced loads on bins and silos are still misunderstood or ignored. As a result, bins and silos fail with a frequency greater than any other structure [2]. A failing bin can release huge potential energy that can kill or seriously injure anyone nearby as well as cause significant property damage and plant interruption.

Part of the reason for this sorry state of affairs is

that most Codes and Standards in this field are very weak, especially in No. America. For example, the American Concrete Institute “Standard Practice for Design and Construction of Concrete Silos and Stacking Tubes for Storing Granular Materials” (ACI 313-97) [3] provides the following guidance to users concerning eccentric loads:

4.4.2.3 Asymmetric flow -- Pressures due to asymmetric flow from concentric or eccentric discharge openings shall be considered.

The ACI 313-97 Commentary references 13 papers that had been written on this subject before this Standard was adopted (1997), but it doesn't endorse any of them. The result: silo designers often ignore or incorrectly treat this important issue, and many silos fail when eccentric discharge occurs.

The Commentary also includes a table of typical flow properties. A common bulk solid, bituminous coal, is listed as having a coefficient of friction against steel of 0.30. The reader is provided no guidance as to the type of bituminous coal, its moisture, ash or other characteristics for which this value applies. Furthermore, there is no indication as to the type of steel: smooth carbon steel, rusty carbon steel, stainless steel (what type, what surface finish?). The reader is left with the impression that none of these variables is important – which is patently false. The footnote warns in small print,

Design parameters should preferably be determined by test and the values above used with caution.

I suspect that most users of this Standard overlook this warning.

Over a decade ago the American Society of Mechanical Engineers formed a committee to develop a standard for bin and silo design. Called “Structures for Bulk Solids”, this document has not yet received final approval. However, if/when it does it will likely be extremely limited in the conditions that it covers. For example, the current draft limits the container shapes to:

...a cylindrical section that is circular in cross-section, and a converging hopper portion beneath the cylin-

der that is either a plane flow wedge (with vertical end walls) or a right circular cone. The geometry is further defined to be symmetrical.

Bins and silos with multiple and/or off-centered outlets, transition hoppers, and other common silo configurations will not be covered by this standard.

The most comprehensive code currently in existence is British Standard BS EN 1994-1:2006 "Eurocode 1 --Actions on structures – Part 4: Silos and tanks" [4]. Yet, as complete as this code is, it still does not cover many common design conditions faced by users [5].

Clearly, bulk solids handling technology is important as ever.

Reason for optimism #2: There are many unsolved problems needing attention

The authors of a 2005 NASA [6] paper observed:

Working with soil, sand, powders, ores, cement, etc. and using hoppers are so routine, that it seems straightforward to do it on the Moon and Mars as we do it on Earth. This paper brings to the fore how little these processes are understood and the millennia-long trial-and-error practices that lead to today's massive over-design, high failure rate, and extensive incremental scaling up of industrial processes because of the inadequate predictive tools for design.

My friend Lyn Bates of Ajax Equipment has been quoted as saying:

Bulk solids technology is not rocket science – it's much more difficult than that! What's more, rocket scientists agree!

More robust and precise solution methods are needed to address many common problems: ratholing, caking, segregation, silo vibrations, properties of – and design procedures for – unusual bulk solids such as those that are anisotropic, both viscous and cohesive, or both elastic and cohesive.

The number of problems to be solved is endless.

Reason for optimism #3: DEM is providing useful insight into complex bulk solids behavior

Discrete Element Modeling (DEM) has come a long way since the turn of the century. Fifteen years ago the state-of-the-art was limited to spherical particles of varying size. Eight to ten years ago, "gluing" spheres together to create clusters was introduced. Today, modeling of more realistic particle shapes using polyhedra is possible.

While this technology holds huge potential, it is still a long way from modeling most "real" systems. For example, the number of particles in an industrial-size silo is on the order of 10^{15} , but current DEM codes are limited to on the order of 10^6 particles – nine orders of magnitude difference! At present the demands on computing power are impractical, particularly considering that the time scale is inversely proportional to particle size. Then there is the very real problem of particle cohesiveness, which has yet to be fully addressed.

One must guard against assuming that pretty pictures and videos that "look right" are sufficient to ensure that the results of a DEM run are correct. Furthermore, at best DEM can answer the question, "Why is this problem occurring", but it cannot provide guidance as to what to change to correct the problem. This is where the expertise of design engineers who have worked in this field for years comes into play.

Reason for optimism #4: There is a great group of committed individuals around the world who want to do the right thing and are passionate about this field

I have been fortunate to know and work with many who have built this field to where it is today. This includes a number who have passed away: Abraham Goldberg, Pedrag Marjanovic, Jan Novosad, Ivan Peschl, Fritz Rademacher, Brian Scarlet, Sunil de Silva, Fred Thomson, Jürgen Tomas, John Williams, Harold Wright.

Another important group who I have known and worked with includes those who have retired or semi-retired: Peter Arnold, Henk Colijn, Gisle Enstad, David Goodwill, Richard Jenkyn, Jerry Johan-

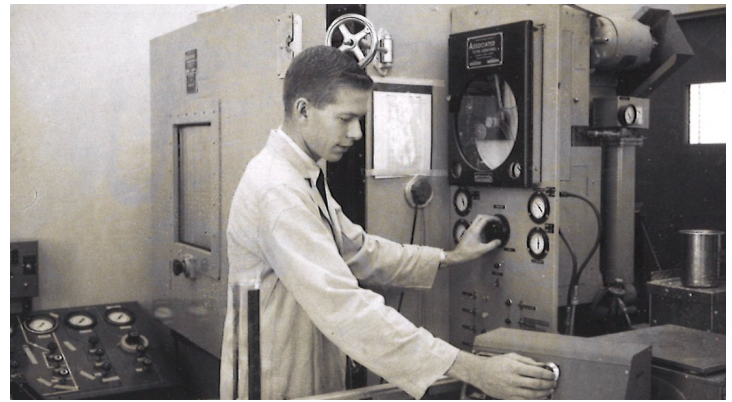
son, Alan Roberts, Michael Rotter, Jörg Schwedes.

Now the baton is being passed to a younger generation, which includes Herman Purutyan, CEO of J&J, and other members of J&J's Senior Leadership Team. The chairmanship of ASTM Subcommittee D18.24 "Characterization and handling of powders and bulk solids" has been passed to Dr. Ben Freireich of Dow Chemical, and Prof. Álvaro Ramírez of the Technical University of Madrid is now chair of the European Federation of Chemical Engineering's Working Party on Mechanics of Particulate Solids.

Given the substantial contributions of all those who have passionately devoted themselves to this field over the years and the enthusiasm and technical abilities of those who are following in their footsteps, I'm confident that the future is indeed bright.

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As a co-op student circa 1966



Jenike & Johanson's first office – the basement of Jenike's house in Winchester MA



US Steel's Applied Research Center, Monroeville PA

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CFD Simulation of Gas-Solid Flows: Poly-dispersed Systems

Hamid Arastoopour
Wanger Institute for Sustainable Energy Research



Illinois Institute of Technology, Chicago, IL

Introduction

Our research team in recent years has focused in mathematical modeling and numerical analysis of poly-dispersed systems using the Computational Fluid Dynamics (CFD) Eulerian approach and kinetic theory (Gidaspow, 1994). In our research, we considered two types of poly-dispersed systems: first, flow of a multi-type particle phase without particle property variation, and, second, a fluid-particle flow system when the particle phase property distribution is changing.

Modeling and Simulation of Multi-type Particle Flow

Particles with property distribution flow significantly different from uniform particles. For example, Arastoopour et al. (1982) showed that particle size has a great effect on the pressure drop and choking velocity and particles segregate along the vertical transport line. Savage and Sayed (1984) showed that the stresses in a shear cell for a mono-size mixture of polystyrene beads were about five times higher than those for a binary mixture. Jenkins and Mancini (1987) extended the kinetic theory of dense gases to a binary mixture of idealized granular material for the low dissipation case. Then Iddir and Arastoopour (2005) extended the kinetic theory for granular flow for mixtures of multi-type particles assuming a non-Maxwellian velocity distribution. Each type of particle was considered as a separate phase with a different velocity and granular temperature. The Iddir and Arastoopour (2005) model was applied to the simulation of simple shear flow of a

binary solid mixture with the same density sheared between two infinite parallel plates. Our calculated values showed a good agreement with the molecular dynamic simulation results of Galvin et al. (2005). Later on, this model was incorporated in the MFIX code and used by Benyahia (2008) to study the flow of multi-type particles in the riser section of the circulating fluidized bed systems.

Modeling and Numerical Solution of Fluid-Particle Processes with Continuous Variation in Particle Properties (CFD-PBE Solution)

To account for continuous variation in particle size density distribution due to phenomena such as chemical reaction, agglomeration, breakage, attrition, and growth, an approach to solve Population Balance Equations (PBE) linked with CFD is needed. PBE is a balance equation based on the number density function that accounts for the spatial and temporal evolutions of the particulate phase internal variable distribution function in a single control volume (Ramkrishna, 2000). This equation is an integro-differential equation that involves both integrals and derivatives of the distribution functions. The most promising method of solution at the present time for CFD/PBE equations is the method of moments. The method of moments, such as the Quadrature method, QMOM (Marchisio et al., 2003 and 2005) is based on solving the distribution function transport equation in terms of its lower order moments. Strumendo and Arastoopour (2008 and 2010) introduced a new version of method of moments called Finite size domain Complete set of trial functions Method of Moments (FCMOM), with unique advantages including fast convergence to the exact solution, and provision of the solution of PBE in terms of the moments of the distribution and the reconstructed distribution function itself. This makes FCMOM distinct from other available approaches.

Population Balance Equation: The Population Balance Equation (PBE) is a balance equation based on

the number density function $f(\xi; \mathbf{x}, t)$, where ξ and \mathbf{x} are internal and external coordinates, respectively. Depending on the system of interest, the number density function $f(\xi; \mathbf{x}, t)$ may have only one internal coordinate (i.e., particle size) or multiple coordinates, such as particle size and surface area.

For an inhomogeneous particulate system, the general governing equation becomes

$$\frac{\partial f(\xi; \mathbf{x}, t)}{\partial t} + \frac{\partial}{\partial x_i} [v_{p,i}(\xi; \mathbf{x}, t) f(\xi; \mathbf{x}, t)] + \frac{\partial}{\partial \xi_j} \left[\frac{\partial \xi_j}{\partial t} f(\xi; \mathbf{x}, t) \right] - \frac{\partial}{\partial x_i} \left[D_{pt,i}(\xi; \mathbf{x}, t) \frac{f(\xi; \mathbf{x}, t)}{\partial x_i} \right] = h(\xi; \mathbf{x}, t)$$

The terms on the left-hand side are the accumulation term, the convective term with respect to the external coordinate, the convective term with respect to the internal coordinate, and the diffusive term, respectively. v_p and D_{pt} are the particle phase velocity and the turbulent diffusivity, respectively, which generally are functions of time, location, and internal coordinates. The source term $h(\xi; \mathbf{x}, t)$ on the right-hand side accounts for the net rate of introduction of new particles into the system.

FCMOM Approach: In FCMOM, the size distribution function is presented as an explicit series expansion by a complete system of orthonormal functions. Thus, first the number density function $f(\xi, \mathbf{x}, t)$ in PBE is approximated by set of orthogonal functions (e.g., Legendre polynomials), then PBE is reformulated in the standard interval $[-1, +1]$ by a coordinate transformation, instead of in the $[0, \infty]$ range, and is expressed in terms of the moments of number density function:

$$\bar{f}(\bar{\xi}; \mathbf{x}, t) \approx \sum_{n=0}^{M-1} c_n(t, \mathbf{x}) \phi_n(\bar{\xi})$$

Where,

$$\bar{\xi} = \frac{\{\xi - [\xi_{\min}(t) + \xi_{\max}(t)]/2\}}{[\xi_{\min}(t) + \xi_{\max}(t)]/2}$$

:

$$\bar{\xi} \in [-1, +1]$$

$$\mu_i = \int_0^\infty \xi^i \cdot f(\xi; \mathbf{x}, t) d\xi$$

With coefficients c_n can be expressed in terms of the moments as:

$$c_n = \sqrt{\frac{2n+1}{2}} \cdot \frac{1}{2^n} \sum_{v=0}^n (-1)^{n-v} \cdot \frac{(2v)!}{[(2v-n)!]} \cdot \left\{ \frac{1}{[(n-v)!] \cdot [(v)!]} \right\} \cdot \mu_{2v-n}$$

$\phi_n(\bar{\xi})$ are the orthonormal functions associated

with the Legendre Polynomials $P_n(\bar{\xi})$ as:

$$\phi_n(\bar{\xi}) = \sqrt{\frac{2n+1}{2}} \cdot P_n(\bar{\xi})$$

Then, a set of transport equations for the moments of the distribution function, f , could be derived from the general PBE in the interval of $[-1, +1]$,

$$\frac{\partial \mu_i}{\partial t} + v_{p,j} \frac{\partial \mu_i}{\partial x_j} - \frac{\partial}{\partial x_j} \left[\int_{-1}^{+1} D'_{pt} \frac{\partial \bar{f}}{\partial x_j} (\bar{\xi})^i d\bar{\xi} \right] = -(M_{ct} + IG) + S$$

On the right-hand side of the moments evolution equations, M_{ct} is due to the coordinate transformation, IG is due to the Integration of the Growth term, and S is the Source term due to the aggregation and breakage (for more details, see Strumendo and Arastoopour, 2008 and 2010). FCMOM numerical results for particle growth, nucleation, and aggregation were verified with analytical solutions (Strumendo and Arastoopour, 2008).

CFD-PBE Coupling for Gas-Particle Flow Systems:

To develop a coupled CFD-PBE model, the PBE equation was solved using FCMOM and the results were linked to a commercial CFD code (ANSYS Fluent 13.0). Figure 1 describes our CFD-PBE algorithm (Abbasi and Arastoopour, 2013).

CFD essentially provides phasic velocities and volume fractions in every iteration. Then, this infor-

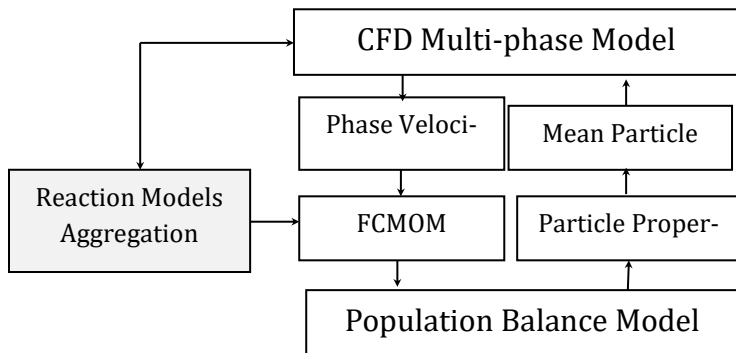


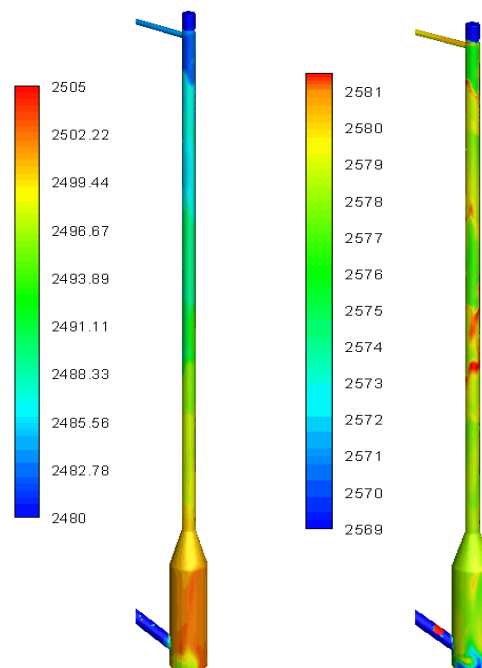
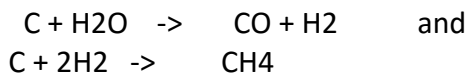
Figure 1. CFD-PBE Coupling Algorithm (FCMOM-ANSYS Coupling)

mation, along with information regarding particle property variation, is provided to PBE to use FCMOM to calculate the moments of the distribution function. This function provides particle properties at each computational cell that are reported back to the CFD model to be used in calculations of particle phase and interphase exchange properties and forces. The coupled FCMOM-ANSYS model was employed in simulations of coalescence of water droplets in an oil-water emulsion flow in backward-facing step geometry and the results compared well with those obtained by the QMOM approach (Abbasi and Arastoopour, 2013).

Simulation of CO₂ Sorption: The main objective of this study was to use the FCMOM approach to account for the variation of particle phase density due to the chemical reaction for CO₂ removal using MgO-based solid sorbents in a riser section of a circulating fluidized bed reactor. The solid sorbent has a minimum density of 2480 kg/m³ (fresh sorbent) and a maximum density of 2830 kg/m³ (fully reacted sorbent). The density growth rate was calculated based on the carbonation reaction rate and treated as a linear growth term. The mean density value was calculated as the ratio of the second moment of the distribution function to the first moment of the distribution function. Figure 2 shows the mean and minimum density contours that correspond to the front of the fresh sorbent in the reactor after 10 seconds of operation (Abbasi et al., 2015).

Simulation of Particle Size Changes during Coal Char Gasification Process: The objective of this case study was to conduct a two-dimensional simulation for studying the effect of particle size de-

crease during the gasification of coal char on the hydrodynamics of the fluidized bed reactor. The following reactions were considered:



Solid Minimum Density (kg/m³)

Solid Mean Density (kg/m³)

Figure 2. Contours of the instantaneous minimum and mean density of the solid phase at t=10 sec.

A heterogeneous reaction expression based on the shrinking core model was developed and used in our model. Figure 3 shows the calculated coal char particle decrease from 450 microns to 220 microns during 30 seconds of gasification using our coupled FCMOM-CFD code. Figure 4 shows the contours of solid volume and hydrodynamics of the fluidized bed during the coal char gasification process. This figure clearly shows the gradual variation of flow regimes from a no bubbling expanded packed bed to a bubbling fluidized regime after 30 seconds of char gasification.

Acknowledgment

Thanks to our research team at IIT in recent years, especially: Professors Abbasian and Strumendo and Drs. Abbasi, Benyahia, and Iddir, and Mr. Ghadirian.

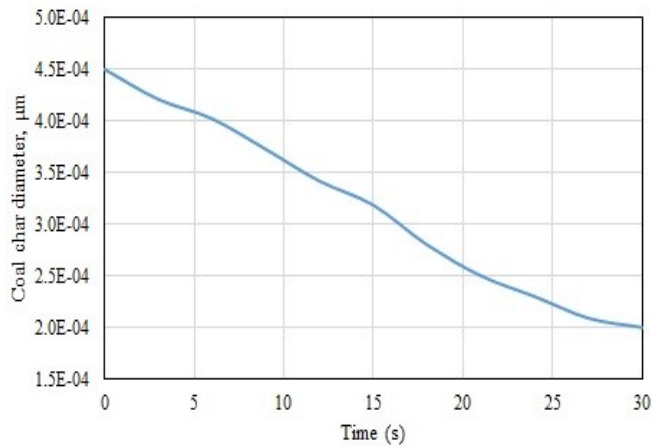


Figure 3. Simulation of the average coal char particle size variation during gasification

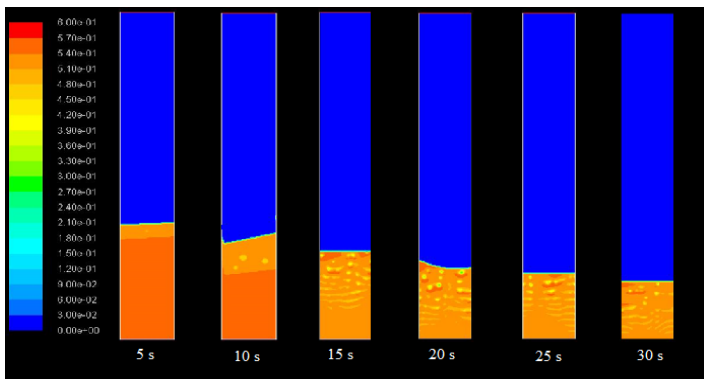


Figure 4. Variation in solid volume fraction and fluidization behavior during the coal char gasification process

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Fluidization of Geldart Group C Powders

Rajesh N. Davé

New Jersey Center for Engineered Particulates (NJCEP)

New Jersey Institute of Technology, Newark, NJ



The Challenge

Fine cohesive powders are extremely difficult to fluidize and generally form cracks, channels or “rat holes” or even lift as a solid plug when exposed to the fluidizing gas. Prof. Geldart¹ has classified such fine powders as group C powders based on empirical observations. Poor behavior of group C powders is attributed to the large interparticle forces arising mainly from Van der Waals attraction, which can be up to a million times greater than the force of gravity when the particle size goes down to a few microns resulting in fine particles forming agglomerates. Past research indicates that agglomerate fluidization may be possible for group C particles if either the process or the nature of powders (e.g., nanopowders²) facilitate formation of mostly mono-sized agglomerates. However, the nature of agglomerate formation is dynamic and very unstable and results in only partial fluidization or even defluidization. In order to improve the stability of the fluidization of cohesive group C particles, external forces may be employed, such as vibration, centrifugal force, magnetic assistance, acoustic and electric fields, or by addition of inert large sized particles³. These approaches have some merits, but due to the need for external excitations or addition of other materials (such as magnets or coarse powders) within the bed, pose practical limitations, and may hinder or interfere with subsequent powder processing such as film coating, granulation, etc.

Why are Fine Powders Cohesive?

Although, it is generally known that fine powders are cohesive, saying that a 10 mm particle is more cohesive than a 100 mm particle is at the best ambiguous

or at the worst, incorrect. To make this point, it is better to discuss this in terms of the interparticle forces, which may include, electrostatic, capillary, Van der Waals, etc. Typically for gas fluidization, Van der Waals attraction is the dominant component, which is linearly dependent on the contacting surface chemistry (i.e., material property represented by the Hamaker constant or surface energy) and contact radius. It follows that the magnitude of Van der Waals attraction actually decreases as particle size becomes smaller, hence saying that smaller particles are more cohesive appears to be a contradiction. On the other hand, as the size of the particle becomes smaller, its body force, typically its weight due to gravity, greatly reduces. This leads to a higher ratio of interparticle force to individual particle’s weight for finer particles, represented through a dimensionless granular Bond number, Bo_g . Thus it is indeed more precise to say that fine powders have a higher Bond number, which causes high level of agglomeration and poor fluidization behavior.

Geldart’s fluidization phase map is shown in Figure 1, where a curved band depicts the empirically derived boundary between groups A and C. It was noted by Masimilla et al⁴ and later by Rietema⁵ that the theoretical estimates did not match the empirical boundary between groups A and C, unless the surface roughness was accounted for when typical group A particles such as fluidized bed cracking catalysts (FCC) were considered. They recommend using the size of the asperities rather than the particle size to calculate the adhesion force because they claimed that most particles have a rough surface with radii of curvature of about 100 nm. Such work from decades ago forms the basis of not only understanding the nature of particle fluidization but also potential mitigation of the poor fluidization behavior. Combined with the concept of granular Bond number, it is easy to see why two most fundamentally based practical solutions to improved fluidization of fine powders aim at reducing the Bond number^{6,3}. The first approach to reducing Bond number is by “increasing” particle weight, which can be done through centrifugal fluidization⁶ that allows operating at very high equivalent “g”. The second approach³, perhaps more

practical since conventional gravity driven fluidization can be employed.

Controlling Cohesion through the Particle Contact Radius and Surface Energy

There are several models considering the effect of asperity on the adhesion force and may be classified as single-asperity, e.g., Rumpf⁷ model, and multi-asperity, e.g., Chen³ model. It is useful to understand the main difference between such models. In the single asperity models such as Rumpf and others⁸⁻¹⁰, essentially the contact of a single asperity (e.g., having an equivalent rms surface roughness⁹) with a much larger sphere (or a flat surface) is considered. The major limitation of this is that the effect of spatial distribution of asperities and the contribution from multiple contacts between two contacting particles is not properly considered. As a simplistic example, the model will estimate the same contact force for a particle with only one asperity or one with many. Chen's model³ overcomes this limitation and his subsequent extensions¹¹⁻¹² overcome other limitations such as powder bed consolidation, and non-uniform size and spatial distribution of the asperities. The most important message from these models is that the interparticle adhesion is greatly influenced by both the nature of surface roughness and the intrinsic surface property such as Hamaker constant, and to a lesser extent, particle hardness and elastic modulus. This also provides two tunable parameters, contact roughness and the Hamaker constant; latter more easily represented by dispersive surface energy.

Tuning or manipulating these properties is easier said than done. Classical approaches to reducing particle adhesion include changing the surface energy through chemical treatment such as silanization. Unfortunately, this approach is unsuitable for many applications; for example, powders intended for human consumption. Moreover, generally speaking it is difficult to greatly reduce the surface energy even with a surface functionalization treatment. A better approach is to create a nano-scale surface roughness, as done using dry coating¹⁰. This superimposition, shown schematically in Figure 2, can achieve reduction in adhesion force by an order of magnitude or more; i.e., assuming R is 100 nm^4 , and r can be easily 10 nm or less¹⁰. Yang et al¹⁰ systematically

showed (Figure 3) not only how flow improvement resulting from reduced cohesion after dry coating is a strong function of surface roughness, but they also showed that even when the asperities are poly-disperse, the dominating length-scale is still that of the finest sizes. This important fact is generally under appreciated, but forms a basis for reduced interparticle forces after dry coating with nanoparticles. This is further appreciated through examining the multi-asperity model³. It was shown that the contact forces depend inversely on the amount of surface area coverage (SAC). As the SAC increases from zero (no silica coating) to 100 %, the largest drop in contact forces occurs rapidly after coating of as little as 1 % SAC as shown in Figure 4(a). Since the contact force reduction can be over one order of magnitude, Geldart group C particles may become fluidizable. This was demonstrated using silica coated cornstarch ($\sim 12 \text{ mm}$), for which as SAC increased, the fluidization quality improved and the minimum fluidization velocity also reduced³ (Figure 4(b)). Results such as these and other suggest that it is better to have SAC > 30 %. This model also indicates that there is an optimal asperity size that leads to the lowest level of contact forces. That means that if the asperities are too small, the particles behave like smooth spheres and have higher cohesive forces. Likewise, as the asperities become larger, they become micro-rough and more cohesive. Thus the best scenario is to impose a nano-scale (about 5-12 nm contact radius) surface-roughness, which is naturally achieved via dry coating (Figure 2). The reader is referred to Huang et al¹³ for the predictive aspects of dry coating of industry relevant powders. Such model based strategy allows for developing a material sparing predictive methodology for using dry coating to greatly reduce the Bond number of otherwise cohesive powders. This then leads to their improved flow¹⁰, packing¹⁴ and most importantly, fluidization^{3,15}.

Correlating Particle-scale with Bulk-scale through Granular Bond Number

The power of the model-based approach to cohesion reduction is further demonstrated by linking a bulk-scale property such as powder packing with a particle-scale property through an empirical model that is a function of the Bond number¹⁴. Five different commercial grade powders are considered as

host particles. They are irregular shaped particles of three different active pharmaceutical ingredients (APIs) and two different pharmaceutical excipients with sizes ranging from 10 to 250 μm . Six different nanoparticles as guests are considered with sizes ranging from 7 to 40 nm. For each combination of host-guest, dry coating is performed with guest amounts sufficient to achieve theoretical 100 % SAC. The packing porosities for uncoated and coated particles are measured and plotted in Figure 5(a). Naturally, significant scatter is observed. As expected from the models^{3,7-12}, the porosity decreases as the guest particle size decreases in each case, but the effect is less significant as the host particle size becomes larger. The behavior for larger host particles is an interesting outcome and suggests that the assumption of natural asperity size of 100 nm radius as done by Massimila et al⁴ is not valid for larger particle sizes. The reader is referred to Capece et al¹⁴ for an extended discussion on this. The scatter in Figure 5(a) can be greatly reduced through employing the Bond number, estimated using Chen model³, as shown in Figure 5(b). This outcome shows that the use of the granular Bond number can allow for linking particle-scale and bulk-scale properties. This approach can be also extended to other bulk-scale properties and has been recently shown to work for flow index such as the flow function coefficient. Thus the fundamentals of contact-mechanics of nano-rough particles provide both the predictive tools and practical means to achieve cohesion reduction of fine Geldart group C powders.

Fluid-bed Coating of Geldart Group C Powders

Dry coated powders have controlled nano-scale surface roughness, which could be typically 20 nm diameter or smaller. Referring back to Figure 1, three additional group A/C boundaries are drawn for surface roughness of 20, 10, and 5 nm, respectively showing how the boundary increasingly shifts towards left. Thus particles that were previously on left of the A/C boundary (at natural 200 nm roughness) can be on the right of the boundary at 20 nm or 10 nm roughness. Those dry coated powders can then behave like group A powders and can be fluidized. Consequently, dry coated cornstarch and other very fine powders can be fluidized and further processed for top-spray polymer film-coating or fluid-bed granulation^{16,17}. Un-

fortunately, fine pharmaceutical powders pose even greater challenge in fluid bed (FB) film coating due to their higher cohesion. For example, ibuprofen powders, considered as model Geldart group C powders with Sauter mean diameters of 22 μm , could not be fluidized due to severe agglomeration, solid-bridging, and poor flowability. Dry coating, applied as a pre-processing method, enabled sufficiently improved flow, hence fluidization via reduced cohesion. It is interesting to note that blending with silica, which is typically done in industry to improve flow, led to a significant increase in flow of ibuprofen powder. In fact, the angle of repose for blended and dry coated ibuprofen was almost the same. However, as shown in Figure 6, whereas uncoated ibuprofen could not be fluidized at all, even blended powder exhibited poor fluidization. In contrast, dry coated ibuprofen powders were successfully polymer film coated in a top spray fluidized bed; see an SEM of a typical individually film coated ibuprofen particle in the inset. The results indicate that while improved flow is a necessary condition for fluidization, it is not a sufficient condition.

Concluding Remarks

Examination of the governing principles for Geldart group A/C boundary along with the concept of granular Bond number reveal that there are essentially two fundamental approaches to achieving fluidization of group C powders. Clearly, the most practical approach comes from the fundamentals of contact-mechanics of nano-rough particles as done in the multi-asperity contact models^{3,11,12}. Such models provide the predictive tools and lead to practical means based on dry coating to increase the Bond number and hence achieve fluidization of fine Geldart group C powders. Of the two tunable parameters, surface energy and surface roughness, the latter has a more dominating effect. While not discussed, dry coating also alters surface energy¹⁸ and essentially, the contacting surfaces behave like the guest particles both in terms of surface energy and contact radius. Thus it generally impacts both tunable parameters, although creation of a well-defined nano-scale surface roughness is the most important and significant outcome. In future, it would be interesting to extend the correlations between the granular Bond number and powder bulk behavior, including fluidization.

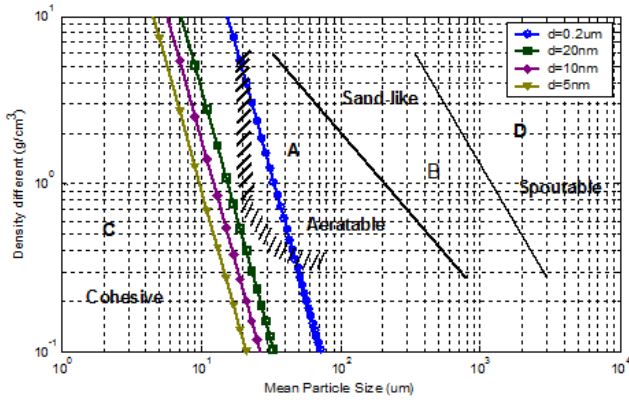


Figure 1. Geldart classification and the effect of contact radius or guest particle size on Geldart group A to C boundary shift. The blue line is the empirically derived boundary between groups A and C, assuming natural roughness equivalent to a contact radius of 100 nm.

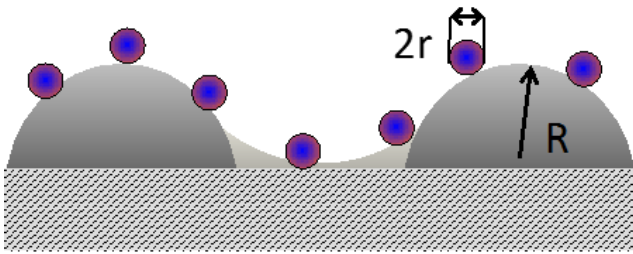


Figure 2. A cartoon depicting naturally rough surface with asperities of radius R coated with nano-particles of radius r resulting in a nano-scale surface roughness. The cohesion reduction is of the order $\sim R/r$.

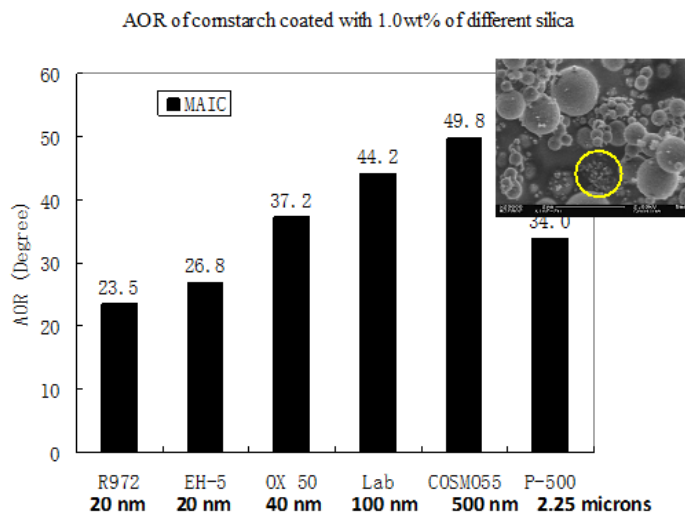


Figure 3. Validation of Rumpf⁷ and modified Rumpf model¹⁰ shows that the AoR reduces as asperity size reduces. An exception is P-500 that has volumetric averaged particle size of 2.25 μm . However, the number averaged size and an SEM (circled group of fines) reveals that many particles are under 100 nm, causing higher than expected cohesion reduction.

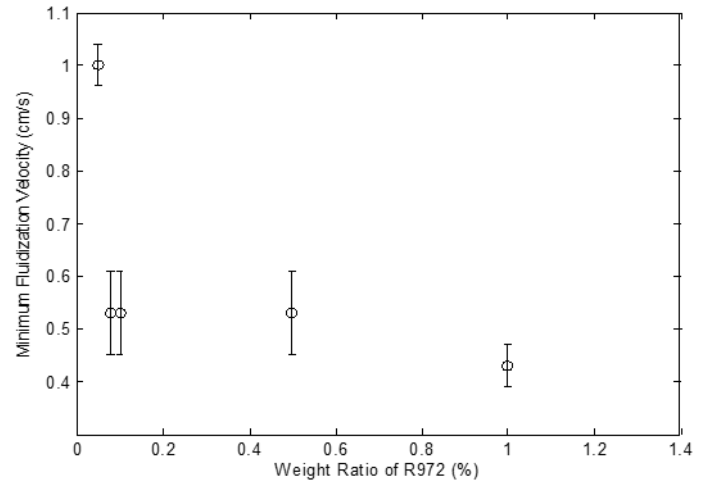
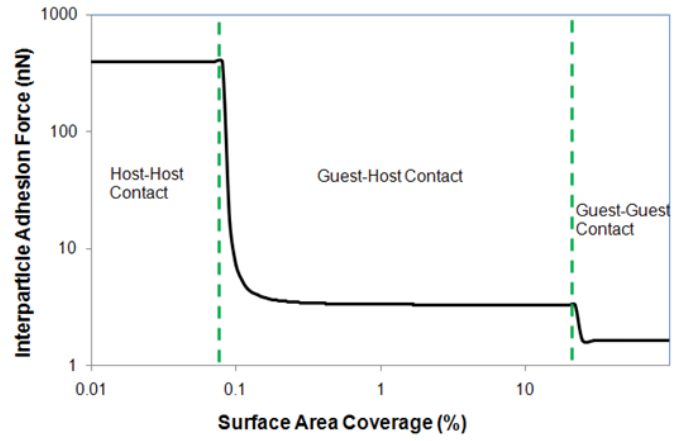


Figure 4. (a) Decrease in the interparticle contact force as a function of SAC by silica nanoparticles based on the multi-asperity model³. (b) Experimental validation based on the minimum fluidization velocity of silica coated cornstarch ($\sim 12 \mu\text{m}$).

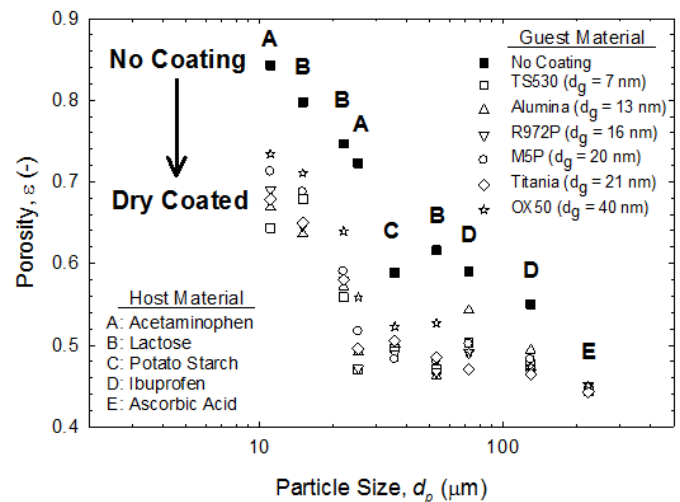


Figure 5. (a) Porosity as a function of particle size for five different host materials, uncoated, and coated with seven different nano-guest particles.

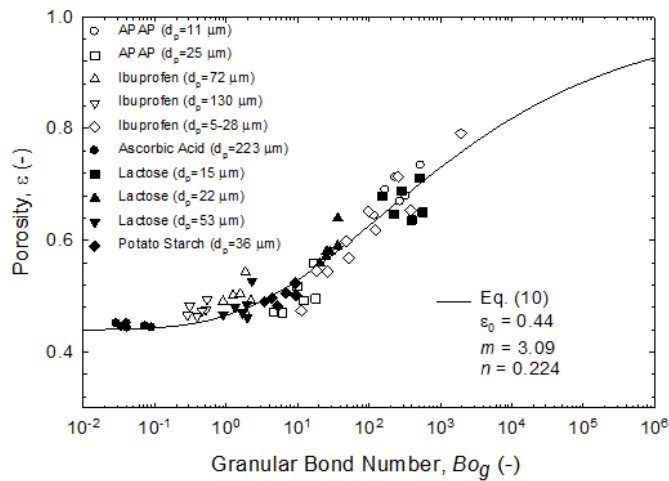


Figure 5. (b) All data may be collapsed to a single empirical curve which is a function of the granular Bond number, suggesting a strong correlation between particle-scale properties with the bulk scale behavior.

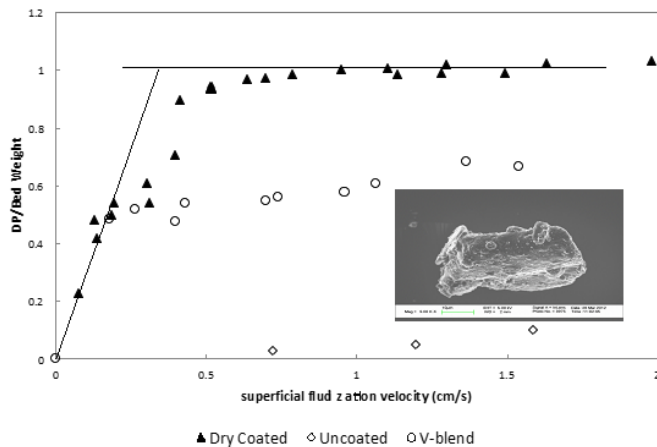


Figure 6. Fluidization behavior of uncoated, silica-blended, and silica dry-coated very fine ibuprofen. Inset shows a typical individually film coated irregular shaped ibuprofen particle.

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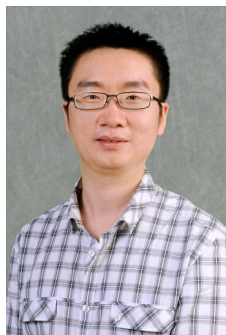


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Pushing the Boundaries for Chemical Looping Particle Development and Applications



Fanxing Li

Chemical and Biomolecular Engineering Department, North Carolina State University, Raleigh, NC 27519

Chemical looping combustion (CLC) is considered as one of the more promising approaches for carbon capture from fossil fuel combustion (Figure 1).^{1,2} In a CLC process, transition metal oxide particles, a.k.a. oxygen carriers, are used as reactive media for air separation and indirect combustion of the carbonaceous fuel. The avoidance of direct contact between air and the fuel, enabled by cyclic redox reaction of the oxygen carrier particles, results in an easy-to-sequester CO₂ stream. Unlike typical CO₂ capture approaches, which reduce the output of traditional energy conversion processes by as much as 40%, CLC integrates CO₂ separation with combustion, offering the possibility of higher efficiency than conventional combustion processes from a second-law standpoint.^{1,3} The excellent potential offered by CLC has spurred extensive research and development activities worldwide over the past few decades. While significant advancements in terms both oxygen carrier development and chemical looping reactor demonstrations have been made, the timetable for CLC commercialization remains uncertain. This is due partly to the lack of concerted CO₂ regulation efforts and the technical risk associated with CLC. For instance, economies of scale dictate that utility plants need to be operated at hundreds of megawatts scales. On the other hand, successful scale up of CLC requires a number of intertwined challenges to be addressed. Such challenges include development of oxygen carrier particles with suitable thermodynamic properties, high activity, low cost, and outstanding chemical and mechanical stabilities, en-

gineering of the particle hydrodynamic and kinetic properties for the cyclic redox operations, design of reactor systems that are capable of circulating such oxygen carrier particles at high density and flux, and development of heat recovery, power generation, and fine separation-reclaiming systems suitable for the CLC operations. As such, research and development of the chemical looping technology represents a challenging problem for nearly all aspects of particle technology. This article intends to share the recent findings with respect to oxygen carrier particle design and applications over the past four and half years. It also offers a perspective for future directions of development. Much of our research has resonated with the inspiring work conducted by my mentors and chemical looping colleagues including Prof. L.-S. Fan at the Ohio State University, Prof. Anders Lyngfelt at Chalmers University of Technology, Prof. Goetz Vesper at University of Pittsburgh, Prof. Ian Metcalf at Newcastle University, Prof. Juan Adanez of ICB-CSIC, Prof. Christoph Müller at ETH Zurich, etc, through both personal interactions and their insightful publications.

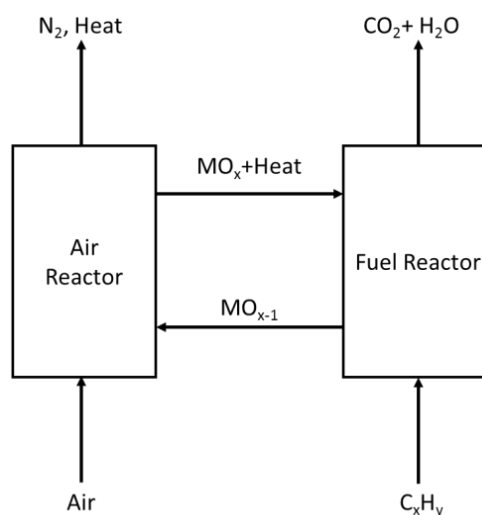


Figure 1. Schematic of the Chemical Looping Process

“Rationalization” of Oxygen Carrier Development

The solids circulation rate for a 600 MW_e CLC plant is projected to be on the order of 10⁴ tonnes/hour with solids inventories over 360 tonnes.¹ Circulation and reaction of large quantities of metal oxide particles at elevated temperatures leads to inevitable particulate

loss through attrition and elutriation. In addition, oxygen carriers can deactivate under redox cycles. Therefore, cost and robustness of the oxygen carrier are critical factors for the economic attractiveness of CLC. Two methods are generally adopted to control the cost of oxygen carrier particles, i.e. use of low-cost oxide ores or development of “synthetic” oxygen carriers with superior performance. Although the former approach can be quite effective, synthetic oxygen carriers, which can be designed based on fundamental understandings of metal oxide redox reactions, offer significant room for optimization and process intensification. For instance, although oxide ores can be orders of magnitude cheaper than synthetic oxygen carriers, it is not unrealistic to develop synthetic carriers that are significantly more active and sintering resistant for the said redox reactions. It is therefore important for the research community to continue to gain mechanistic insights for oxygen carrier design. Our recent experience on iron oxide based oxygen carrier development can serve as an example to demonstrate the importance of mechanistic understanding and basic engineering principles for oxygen carrier design and optimization:

Iron oxides, especially wustite and magnetite, are known to react relatively slowly with carbonaceous fuels and deactivate over multiple redox cycles. Stable ceramic supports, such as spinel, alumina, and titania, are often found to be effective to improve the activity and recyclability of iron oxide based oxygen carriers. Based on such findings, it is natural to conclude that the primary function of the support is to increase the surface area and sintering resistance of iron oxide. As such, supports with high surface area would be considered ideal for CLC applications. Thorough investigation of physical properties of pure and supported iron oxide over multiple redox cycles, however, provides a different picture.^{4,5} Although as-prepared iron oxide with support indeed possesses significantly larger surface area than unsupported iron oxide, its surface area readily decreases over the first few redox cycles. In the meantime, no deactivation is observed for supported iron oxide even with over an order of magnitude surface area decrease. More detailed experimental and density functional theory studies reveal that, unlike heterogeneous catalytic reactions, the rates of iron

oxide redox reactions are controlled by the diffusion of lattice oxygen (O^{2-}) (and electrons) in the oxide lattice. While sintering of iron oxide indeed is the primary cause for iron oxide deactivation, the primary role of support is to promote O^{2-} and/or electron conduction as opposed to retard sintering. With such findings in mind, it is rational to seek supports with high mixed ionic-electronic conductivity (MIEC) as opposed to those with high surface areas. Improvement in iron oxide redox activity by facilitated O^{2-} (and electron) conduction is validated by comparing supports with varying mixed conductivities. A positive correlation between iron oxide based oxygen carrier activity and mixed-conductivity of support was observed.⁶ 50-fold increase in methane oxidation activity was achieved when $La_{0.8}Sr_{0.2}FeO_{3-\delta}$ (LSF), an acceptor doped, mixed-conductive perovskite, was used to substitute an inert support in a composite form.⁷ Since the O^{2-} conductivity in iron oxides are significantly lower than MIEC supports, further decrease in the size of iron oxide can lead to further enhancement in redox activities. As such, a core-shell oxygen carrier concept was proposed to enclose iron oxide nano-particles (to reduce O^{2-} transport resistance) with a more conductive and selective LSF shell. A $Fe_2O_3@LSF$ core-shell oxygen carrier, a.k.a. redox catalyst, exhibits two orders of magnitude activity increase when compared with Fe_2O_3 supported with inert ceramics and YSZ (Yttria Stabilized Zirconia).⁸ When utilized for a chemical looping reforming process to produce syngas, 94% syngas selectivity can be achieved (Figure 2a) through controlled reduction and regeneration of the core-shell oxygen carriers.⁹ In comparison, composite Fe_2O_3 -LSF and Fe_2O_3 -inert oxide are notably less selective. The redox catalyst has been found to be chemically and structurally stable under redox cycles at high temperature.^{8,9} This highlights the importance of fundamental understanding towards the rational design and optimization of oxygen carrier particles.

Novel Applications of Oxygen Carrier Particles

The cyclic redox concept can be applied in applications beyond electric power generation. The ability to generate alternative, higher value products offers the potential to improve the economic feasibility of the chemical looping concept at smaller scales. Many nov-

el redox concepts for alternative products have been explored. For instance, H_2 can be generated through a three-step chemical looping gasification process¹, the chemical looping reforming (CLR).

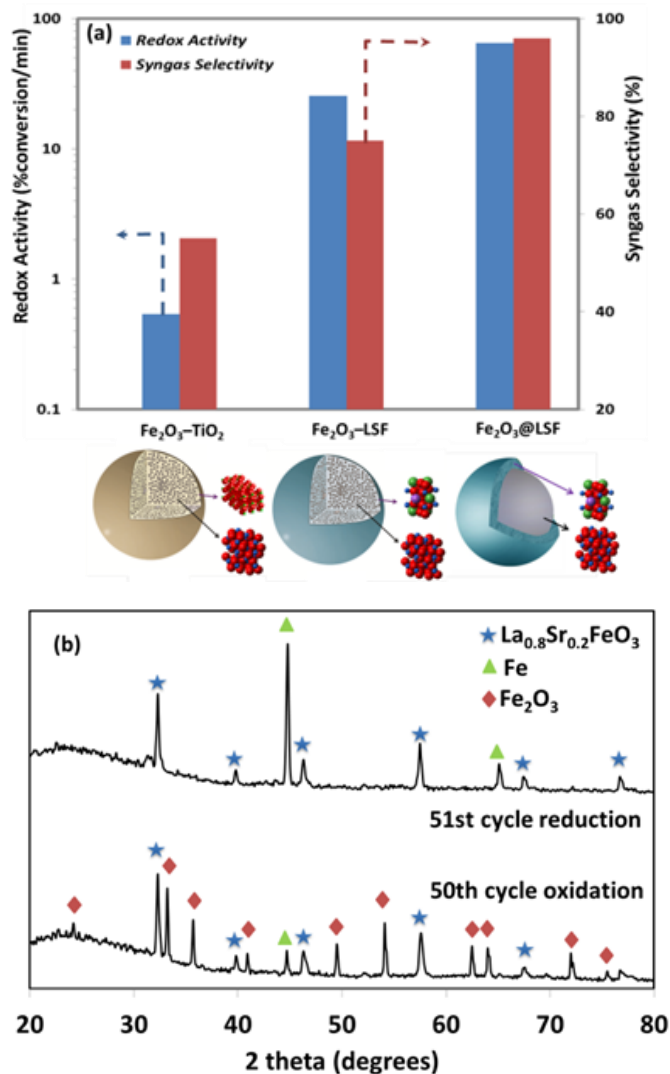


Figure 2. (a) Activity/selectivity of composite (Fe_2O_3 -inert oxide, Fe_2O_3 -LSF) and core-shell ($Fe_2O_3@LSF$) redox catalysts for CH_4 partial oxidation ($900^\circ C$, 10% CH_4 . Oxidation shows a similar trend); (b) X-Ray powder Diffraction (XRD) showing the compatibility of LSF and FeO_x phases over 50 redox cycles.⁷⁻¹⁰

and chemical looping dry reforming concepts were studied for syngas and/or CO generation from methane^{10,11}, and more recently a two-step hybrid solar-redox process for Fischer-Tropsch ready syngas and hydrogen coproduction was investigated with

promising results^{12,13}. In addition to hydrogen and CO_x products, which are thermodynamically favored, we have recently explored the use of chemical looping concept for ethylene production via oxidative dehydrogenation of ethane. Figure 3 illustrates a process schematic of the chemical looping – oxidative dehydrogenation (CL-ODH) process. In such a scheme, ethane is fed along with an oxygen carrier, a.k.a. redox catalyst, into an ODH reactor, where lattice oxygen is used to partially oxidize ethane to water and ethylene. The reduced redox catalyst is subsequently regenerated with air in the air reactor. The exothermic reaction heats the catalyst particles, which convey sensible heat into the ODH reactor. The product gas stream from the ODH unit is rapidly cooled and then compressed. This is followed with drying, acid gas removal, cooling, and fractionation to recover ethylene and other value-added products. Unreacted ethane is recycled into the ODH feed stream. CL-ODH offers several advantages over the conventional steam cracking process. For instance, H_2 product limits the equilibrium conversion of ethane in steam cracking. Selective oxidation of H_2 to H_2O , enabled by the CL-ODH redox catalyst, can lead to significantly improved single pass yield of ethylene. Increase in single-pass yield, along with H_2 combustion, result in significantly lowered molar flow rate of non-condensable gaseous products from ethane conversion.

Therefore, energy consumption for downstream compression and separation processes are decreased for CL-ODH. Moreover, steam cracking is highly endothermic. Combustion of fuel gases such as methane and hydrogen in conventional cracking leads to significant CO_2 and NO_x emissions. In comparison, CL-ODH allows auto-thermal operations through indirect combustion of hydrogen byproduct. As a result, the overall consumption is reduced by 82% (with 85% single-pass ethane conversion). Meanwhile, indirect flameless combustion of hydro-

gen in CL-ODH has the potential to reduce CO_2 and NO_x emissions by 79%. Furthermore, CL-ODH eliminates the needs for steam dilution and allows [continuous process operations](#). Compared to oxygen co-fed ODH, CL-ODH eliminates the capital and energy intensive air separation units (ASU). It also eliminates the direct contact between gaseous oxygen and ethane. Our recent studies have resulted in Mn-based redox catalyst particles with over 85% single-pass ethane conversion and close to 90% C2+ olefin yield. Scale up of the CL-ODH process is underway in collaboration with EcoCatalytic Technologies LLC and PSRI.

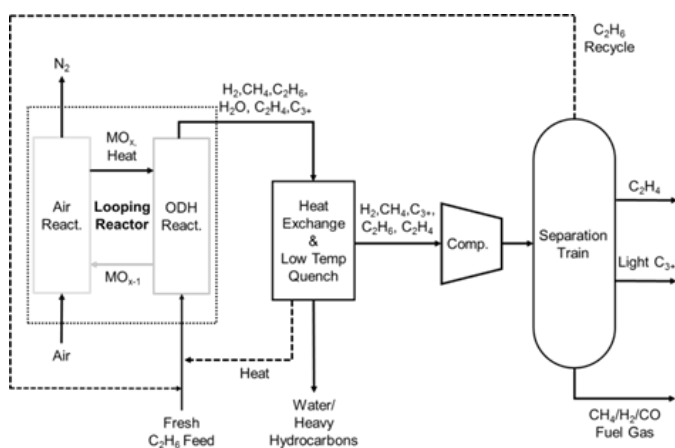


Figure 3. Chemical Looping-Oxidative Dehydrogenation of ethane (CL-ODH). The ODH reactor serves as the fuel reactor.

Oxygen Carrier Particle Development – The Path Forward

The above examples demonstrate the versatility of the chemical looping concept and the importance of fundamental understanding for oxygen carrier particle design and optimizations. While notable progresses have been made on these aspects, numerous challenges and potential pitfalls still exist. It is therefore important to learn from past experiences. The vanadium pyrophosphate (VPO) redox catalyst developed by DuPont for n-butane oxidation to maleic anhydride is one of such examples. One limitation of the VPO (redox) catalyst is its low oxygen storage capacity since the oxygen atoms available to

the redox reactions are estimated to be within 5 atomic layers from the catalyst surface. While many recently developed CLC oxygen carriers have significantly higher oxygen carrying capacities, excellent recyclability, and good attrition-resistance albeit at higher temperatures, few if any of these oxygen carriers have been tested for extended operations in large scale looping reactors due to their limited accessibility and constraints in resources. From a fundamental standpoint, metal oxide redox mechanism, fuel oxidation pathways, active sites, and primary factors that determine particle deactivation attrition mechanism are poorly understood. This is partly due to the large material design space for oxygen carriers, the complexity of the redox mechanism, and the dynamic bulk and surface reaction pathways. The latter is especially true for partial oxidation applications. For instance, the bulk and surface properties of an oxygen carrier constantly changes during the redox reactions. As a result, the reactions are highly dynamic with changing surface reaction pathways. This draws distinct contrast with heterogeneous catalytic reactions. Our recent studies of methane partial oxidation with $\text{Fe}_2\text{O}_3@LSF$ core-shell redox catalysts indicates four reaction regions with distinct mechanisms.¹⁴ Direct probing of active sites, surface intermediates and reaction pathways, however, is challenging due mainly to the low surface area of typical oxygen carriers and the high reaction temperatures required. Such mechanistic information is critical to rational design of oxygen carriers for the generation of value added chemicals and to push the boundaries for novel redox applications. Achieving such ambitious goals requires the application of fundamental knowledge, methodology, and tools in particle science and technology, heterogeneous catalysis, material science, and reaction engineering. Considering the exceptional promises offered by the chemical looping strategy, I would urge concerted efforts within the community to take on such challenging yet vastly

rewarding efforts in pushing the boundaries of chemical looping particle design and applications.

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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.
- Become a PTF lifetime member so that you don't have to renew membership every year.

Become a PTF only member (annual \$15, **lifetime \$150**)

Visit website: <http://www.aiche.org/community/divisions-forums/ptf>

If you don't see the PTF 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@aiiche.org for membership questions and help.

PTF Membership Committee

HISTORY OF PARTICLE TECHNOLOGY

Gunpowder and DuPont

Gunpowder was invented in the ninth century by the Chinese. Much of the early production was for fireworks, but over time the industry grew to support military purposes, hunting, and eventually mining. Production techniques and recipes were published in ancient texts. The best performance was found to come from a mixture of 75% saltpeter (potassium nitrate), 12.5% charcoal and 12.5% sulfur.

In 1774 King Louis XVI hired the chemist Lavoisier to increase France's ability to make high quality gunpowder. A major research effort went into improved methods for collecting and refining saltpeter, the key ingredient. Around 1785 Lavoisier took on E.I. du Pont as an apprentice. The young du Pont worked for Lavoisier for several years but eventually returned home to join his father's publishing company. In 1800, the wealthy family was threatened by the French Revolution. They set sail for America, with money and political connections but no firm plans.

After evaluating potential business ventures (including cattle ranching), du Pont realized that there were no U.S. manufacturers of high-quality gunpowder. Using French technology, he established a gunpowder manufacturing operation in Wilmington, Delaware. The location was selected for the water power from the Brandywine River and local infrastructure. The early success of the venture came from strict adherence to quality, branding, and the growth of America in those times. The War of 1812 was also helpful, as it both created demand and shut out Britain, the major foreign source of gunpowder.

Gunpowder manufacturing technology involves the processing of particles. A damp mixture in the correct proportions is finely ground and sim-

ultaneously mixed in massive rolling mills. The intimate mixture is necessary to ensure complete combustion, but the fine powder has poor air permeability. Permeability is required to provide a rapid combustion rate and its consequent rate of pressure rise. The permeability problem was solved by compaction granulation of the damp mixture. The resultant granules were screened, generating a variety of particle sizes. Different particle sizes had different handling behavior and different packed-bed permeability. This permitted the tailoring of the product to provide the required rate of pressure rise and handling properties for guns, cannons, and blasting. Flintlock rifles were primed with 0.3 mm particles, while Civil War cannons required particles as large as 13 mm.

Despite the later fame of the DuPont Company for its chemistry research, there were no substantial chemistry contributions by the firm until 1857, when Lamot du Pont developed a process to substitute the cheaper and more effective sodium nitrate for saltpeter.

Tim Bell

DuPont



Edge runner mill at the Hagley Museum in Wilmington, Delaware. Massive iron wheels grind and mix damp particles in a wooden trough. Photo from Wikipedia.

Particle Technology Forum: Organization and Roles



Reza Mostofi

UOP, A Honeywell Co.

As we are getting ready for PTF elections, it seems appropriate to highlight some of the aspects of PTF day to day business. This is not a complete list and is only compiled to provide some understanding of the executive team especially for the members who would like to serve the forum.

Awards and Banquet Dinner

- ⇒ Form award committees while avoiding conflicts
- ⇒ Collect and redistribute completed nomination packets
- ⇒ Notify all parties of the outcome
- ⇒ Collect winner information, request plaques & checks
- ⇒ Present awards at the banquet and arrange for awards talk
- ⇒ Search for nearby restaurants
- ⇒ Negotiate options and select the most appropriate one

Finance

- ⇒ Maintain financial records
- ⇒ Send invoices and collect funds from sponsors and advertisers
- ⇒ Provide PTF budget and cooperate with AIChE accounting
- ⇒ Request or issue awards checks and pay other expenses

Secretary

- ⇒ Take notes for various meetings
- ⇒ Communicate with members about EC and PTF news
- ⇒ Prepare ballots and report the votes
- ⇒ Assure compliance with the PTF bylaws
- ⇒ Review the procedures and revise if necessary

Communications: Newsletter/Website

- ⇒ Request and collect information for newsletter and website
- ⇒ Update website as the main communication front with members
- ⇒ Issue newsletter several times a year with most up to date information

Programming

- ⇒ Communicate and guide programming chairs for PTF related sessions
- ⇒ Work with AIChE planning to assure the PTF members needs are met and resolve possible issues
- ⇒ Ensure sound and creative program planning and area chairs leadership quality and succession

One-time Tasks

- ⇒ Ongoing: review awards process and update as necessary
- ⇒ Ongoing: review PTF bylaws and revise
- ⇒ Recently: revised poster session and judging process
- ⇒ Ongoing: review membership needs and develop plans on attracting more members

Executive Committee Members

- ⇒ Participate in EC meetings by phone or in person
- ⇒ Actively looking and suggesting ways to improve PTF related activities
- ⇒ Help with poster judging at the annual meeting
- ⇒ Act as a liaison to the PTF and their respective workplace and vice versa. This can include recruiting new members/officers and advertising for PTF related activities
- ⇒ Help in nominating new EC members
- ⇒ Help in other PTF standing committees

One last note is that becoming a PTF EC member would require on average somewhere between 1-7 hours per month of your time with some peak months and some months with no activity. In summary, I can assure you that there are lots of interesting works which help PTF grow, offer a great platform for your social connection, help you grow as a leader and learn something new.



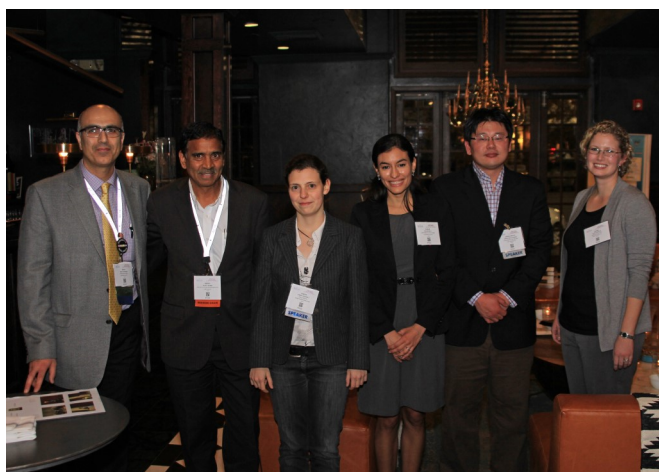
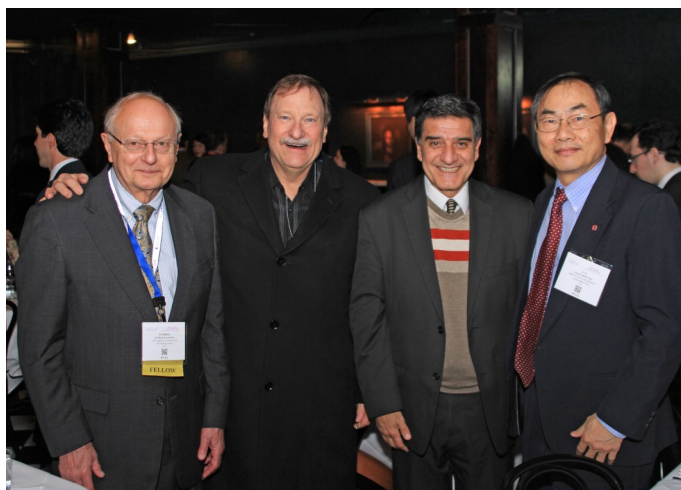
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New Ideas for the PTF Newsletter ?
Contact
Editorial Advisory Committee or
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Particle Technology Forum Awards Dinner—2015



Particle Technology Forum Awards Dinner—2015




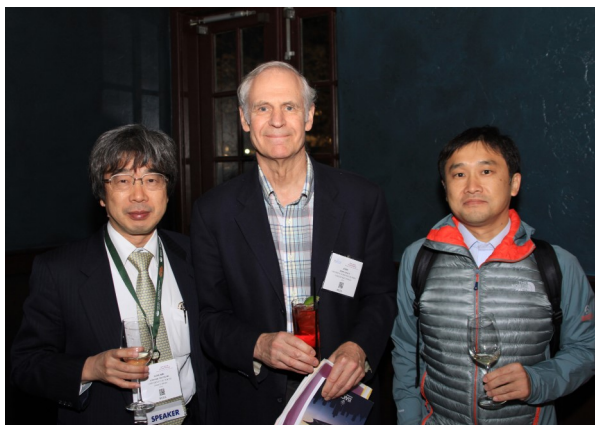
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Particle Technology Forum Awards Dinner—2015



Particle Technology Forum Awards Dinner—2015



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Frontiers in Particle Science & Technology



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Attend Frontiers in Particle Science and Technology: Mitigation & Application of Particle Attrition

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Presented by Dr. Mojtaba Ghadiri, *University of Leeds*

Industrial Keynote Address

Presented by Dr. John Carson, *Jenike & Johanson*

Confirmed speakers also include:

- Khalid Alshibli, *University of Tennessee, Knoxville*
- R. Bertrum Diemer, *University of Delaware*
- John Grace, *University of British Columbia*
- Stefan Heinrich, *Hamburg University of Technology*
- Karl Jacob, *The Dow Chemical Company*
- Paul Mort, *Procter & Gamble*
- David Potyondy, *Itasca Consulting Group, Inc.*
- Carl Wassgren, *Purdue University*
- and more.

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For the list of confirmed speakers, registration, and additional information,
please visit www.aiche.org/fpst.

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Save the Date!

The 8th World Congress on Particle Technology (WCPT8) will be held in conjunction with the 2018 AIChE Spring Meeting & 14th Global Congress on Process Safety.

On behalf of AIChE and the Particle Technology Forum (PTF), we invite you to participate, learn, teach and collaborate.

The WCPT8 conference will focus on all aspects of particle technology from fundamental research to applied successes in areas including:

- Particle Processing Technologies
- Particulate Product Engineering
- Specialty Particle Research
- Characterization & Measurement Techniques for Particles & Particulate Systems
- Modeling & Simulation of Particle Hydrodynamics & Interactions

The Call for Abstracts for the WCPT8 will open in the Spring of 2017.

For more information on programming areas, important dates, and the organizing committee, visit:

www.aiche.org/wcpt8

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KEEPING AICHE VIBRANT

Constitutions Are Living Documents

The AICHE Constitution serves as the primary governing document for the Institute. It ensures that AICHE has the ability to meet the needs of members. Next year, AICHE's Board of Directors will be asking you to approve proposed changes to the Institute's Constitution. These changes will make AICHE more vibrant, flexible and better able to adapt to the changing needs and interests of its members by:

- Conforming with the latest regulatory requirements for non-profit organizations
- Modernizing and streamlining Institute processes with best practices and new communication technologies
- Enhancing AICHE's responsiveness

Why change now?

- Implementing Best Practices:** We propose specifying term limits for Directors, Secretary, Treasurer and President; moving several provisions from the Constitution to the Bylaws (member description and eligibility, Nominating Committee and election processes); and removing obsolete references.
- Modernizing Governance:** We propose conforming Constitutional provisions to requirements of the Non-Profit Revitalization Act of 2013 under New York Not-for-Profit Corporation Law; changing the requirement for future amendments to the Constitution from 75 percent approval by a minimum of 20 percent of voting members to two-thirds of votes cast; and changing the requirement for Board petition candidates from the low threshold of support from 100 members to a more representative 2 percent of the membership.
- Reflecting Current Processes:** In the Constitution, we propose broadening Board creation of divisions, local sections and student chapters to encompass all entities, including industry technology groups, forums, and future groups; specifying that the Past President is an Officer; and changing the process for proposing an amendment from discussion at a general meeting to presentation to the membership.

AICHE is *our* professional home.

In the fall of 2016, please cast a positive vote to better position our
Institute for the future so AICHE may better serve our profession.

PTF Awards

CALL FOR NOMINATIONS

The deadline for submission of nominations has been extended to **March 30th** for the following PTF awards:

- George Klinzing Best PhD Award
- Particle Technology Forum Lifetime Achievement Award
- Thomas Baron Award
- PSRI Lectureship Award in Fluidization
- SABIC Young Professional Award

While completed packets are due by May 11th, 2016, at this time, we need your initial nominations, which are due by March 30, 2016.

We request you to make these nominations as soon as possible via using the [form](https://form.jotform.com/60587168379168) at <https://form.jotform.com/60587168379168>

Please note that the requirements for the PTF Awards have been recently changed and made consistent with the general AIChE guidelines. The details of each award can be found at the [AIChE PTF Awards webpage](#).

Raj Dave

Chair—PTF Awards Committee

Have an idea for an article or suggestions for the PTF Newsletter or Website?

Please let us know:

Shrikant Dhodapkar sdhodapkar@dow.com
Pat Spicer p.spicer@unsw.edu.au

Upcoming Conferences

Fluidization XV

A ECI Conference Series

May 22-26, 2016
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The XV Fluidization Conference welcomes delegates from academia, industry and government who share the vocation to meet societal needs, reduce the environmental footprint of our processes, while at the same time forging new business models to meet the needs of the growing global population. To meet these challenges, we bring together experts in fields beyond fluidization and powder technology and include theoreticians in computational fluid dynamics (a transverse application), nano-processing and materials, catalysis, and biopharmaceuticals.

www.engconf.org/16af



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July 24-29, 2016

Location: Stonehill College, Easton, MA

Application Deadline: **June 26, 2016**



Particle Technology Forum Organization

PTF OFFICERS

CHAIR

Dr. Reza Mostofi
reza.mostofi@uop.com



CO-CHAIR

Dr. Raj Dave
dave@adm.njit.edu



TREASURER

Dr. Benjamin Glasser
bglasser@rutgers.edu



PAST CHAIR

Dr. Jennifer S. Curtis
jcurtis@che.ufl.edu



PTF EXECUTIVE COMMITTEE (INDUSTRY)

◆ Dr. Reddy Karri
reddy.karri@psri.org



◆ Dr. Ben Freireich
BJFreireich@dow.com



◆ Dr. Bruce Hook
BDHook@dow.com
PTF—Secretary



◆ Dr. Mehrdad Kheiripour
Mehrdad.kheiripour@merck.com



PTF EXECUTIVE COMMITTEE (ACADEMIC)

◆ Dr. Benjamin Glasser
bglasser@rutgers.edu



◆ Dr. Jim Gilchrist
gilchrist@lehigh.edu



◆ Dr. Raj Dave
dave@adm.njit.edu



◆ Dr. Marc-Olivier Coppens
m.coppens@ucl.ac.uk





LIAISONS AND COMMITTEE CHAIRS

CTOC Liaison	Ray Cocco	ray.cocco@psrichicago.com
SIOC Liaison	Reza Mostofi	reza.mostofi@honeywell.com
CEOC Liaison		
Nominating Committee Chair	Alissa Park	ap2622@columbia.edu
PTF Newsletter Committee	Shrikant Dhodapkar	sdhodapkar@dow.com
PTF Webmaster	Pat Spicer	p.spicer@unsw.edu.au
PTF Student Workshop Chair	Mayank Kashyap	mkashyap@americas.sabic.com
PTF Programming Chair	Manuk Colakyan	manuk.colakyan@renmatix.com
PTF Dinner Sponsorship	Jennifer Sinclair Curtis	jscurtis@ucdavis.edu
PTF Awards Sponsorship	Reddy Karri	reddy.karri@psri.org
PTF Education Committee	Shrikant Dhodapkar	sdhodapkar@dow.com
WCPT8 Committee	Ray Cocco	ray.cocco@psrichicago.com
FPTC 2016	Ben Freireich	bjfreireich@dow.com
Staff Liaison	Darlene Schuster	darls@aiche.org
	Diane Cappiella	dianc@aiche.org
Accounting	Leila Mendoza	leilm@aiche.org
WCPT8	Stephanie Orvoine-Courvette	ginag@aiche.org
FPTC 2016	Stephanie Orvoine-Couvrette	stepo@aiche.org

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