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 doing well, and are hanging in there as we see potential end in sight to the global pandemic that has affected our lives in numerous ways. COVID-19 has not only disrupted our day-to-day lives, but has also resulted in slowing down the global economy. Fortunately, innovative technologies

Message from the Chair

Greetings!

I hope you are as relieved as I am that we are beginning to round the corner and hopefully leave the pandemic in our past. As we move into a new year with the promise of (some) things eventually returning to normal, I hope you and your families and friends fair well.

Let me start by introducing myself. I've served as a professor in the department of chemical and biomolecular engineering at Lehigh University since 2004. I graduated from Washington University in St. Louis in 1997 and worked on drying of agglomerated microencapsulated dyes, my first introduction to granular systems. I attended Northwestern University and studied with Professor Julio Ottino on chaotic mixing of dry granular materials in rotating tumblers. A postdoctoral research appointment at University of Illinois in Materials Science and Engineering with Professor Jennifer Lewis (now at Harvard), took me into the direction of suspension transport and colloidal assembly. My *Laboratory for Particle Mixing and Self-Organization* now sits at the intersection of particle hydrodynamics, interfacial science, and rheology with new directions working with magnetic Janus particles and functional and 3D structured particle-based coatings (though combined with strong foundation built through decades of fundamental research have brought several vaccines in our arsenal that are expected to help us achieve herd immunity against the disease in the not too distant future. We all want to return to some sort of normalcy, as we are getting tired from the *pandemic fatigue syndrome*. However, I would like to reemphasize my personal views that it "still" remains our individual and collaborative responsibility to continue following the public health guidelines pertaining to COVID-19 from reliable health officials and sources.

"To lose patience is to lose the battle." - Mahatma Gandhi

As you may be aware, the 2021 AIChE Annual Meeting will be hybrid, i.e. one-week in-person in Boston, followed by a week, virtually. This newsletter includes the announcement from AIChE regarding the meeting. The newsletter also highlights technical contributions from three 2020 AIChE PTF award recipients, call for 2021 PTF Award nominations, and new PTF organization.

If you would like to contribute to the 2021 Summer newsletter, please contact me as soon as possible with your

Bagnold stress remains near and dear to me). I've served the PTF "from the bottom up", chairing sessions, organizing Area 3C, and serving on the EC over 10 years. I have also served as an EC member and Chair of Area 1J - Fluid Mechanics and an EC member of the North American Mixing Forum of the AIChE.

When I was elected, I knew exactly the image that I would like to symbolize my term as PTF Chair – ***a ski chairlift***. I chose this for the obvious reason that I am a skiing *fanatic*, typically heading out west to the Rockies a couple of times a year with my family to upgrade from the local Pocono Mountains. For the PTF, the symbolism of my choice is rich. A chairlift is not static – it continuously moves people from lower to higher heights, such is the goal of the PTF. Chairlifts take skiers and snowboarders to a clearer vista, just as the PTF aims to offer a vantage point that overlooks the entire particulate industry. Riding a chairlift is a relished moment of pause, perhaps a chance to discuss the ski conditions and the last run, jumps and the heroics, the stumbles and the falls, and to make a plan for the next trip down the mountain. It is a time learn more about the person sitting next to you. Similarly, PTF is a place for us to come together, get to know each other, and plan for a stronger professional network through conferences and social interactions to help guide our members through their careers.

After a year of relative isolation, our early career members need all the help they can get to establish their professional network. Based on input from the PTF community, we have launched a new initiatives including increasing diversity, equity, and inclusion efforts and continue outreach activities to newer generations of particle technologists. One such activity was held on February 25th where Dr. Mena and Dr. Mwasame, the last two Klinzing Best Ph.D. awardees, gave outstanding presentations on their work in particle technology, now hosted on the PTF website. We hope to have more of these interactions and we are always open to suggestions for improvement and advancement of the forum.

My gratitude to this newsletter's editor, Dr. Mayank Kashyap, for creating another informative newsletter and all members of the executive committee who keep programming and events running smoothly. Finally, I'm grateful to Bruce Hook, former PTF Chair, for a smooth transition in handing me the idea.

***"You make a living by what you get. You make a life by what you give."* - Winston Churchill**

As a matter of fact, this is the fourth newsletter released during the ongoing pandemic. However, it is my sincere hope that the next newsletter will come in the waning days of the pandemic that has already been in our lives for over a year.

***"Only he who has seen better days and lives to see better days again knows their full value."* - Mark Twain**

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

Mayank Kashyap, SABIC

Editor, PTF Newsletter

baton. We have worked closely over the last couple of years and his mentorship through this process was extremely valuable.

Hope to see you in person (or virtually) in Boston this November!

Regards,

James Gilchrist, Professor, Lehigh University

Chair, The Particle Technology Forum of AIChE

Email, Website, Twitter: @Gilchrist_Lab, LinkedIn

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.

2021 AIChE Annual Meeting - Hybrid

Boston (November 7-11, 2021) and Virtual (November 15-19, 2021)

A Message from AIChE Sent on March 29, 2021

Dear Colleague,

We are holding our upcoming 2021 AIChE® Annual Meeting in Boston at the John B. Hynes Convention Center, the Marriott Boston Copley Place, and Sheraton Boston, as well as in the virtual world for those unable to attend in person. After the past year, bringing together our engineering community has never been so critical. This hybrid meeting is being designed to bring you the best of both worlds, and will take place over a two-week period, from November 7-11 in person and from November 15-19 virtually.

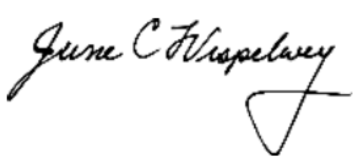
As everyone knows, nothing beats a live experience and we look forward to offering an excellent program in Boston. But it's important to us that we provide a virtual experience too. Our in-person sessions will be recorded and made available for viewing on the virtual platform for all attendees. So whether you "fly, drive or click in," we are building a great conference.

The program's theme "Building the Bridge in 21st Century Education: Chemical Engineering Industry + Academia" applies now more than ever! Our program includes a special discussion on new learning paradigms and will also encompass AIChE's highest lectures presented by Arup Chakraborty (MIT), Eric Shaqfeh (Stanford) and David Schaffer (UC Berkeley), 700+ sessions programmed by our divisions and forums and topical conferences, including the new program on Material Interfaces as Energy Solutions.

For attendees joining us in Boston, please note that your safety is our primary concern. AIChE is working with the venues to adhere to all local and national directives for social distancing and sanitizing protocols.

For now, keep an eye out for updates by email, social media and our conference website. We are happy to answer any questions—just email us at programming@aiche.org.

We are excited to see you all in Boston or virtually!



June C. Wispelwey

Executive Director and CEO, AIChE

2020 AIChE Particle Technology Forum Awards

Elsevier PTF Lifetime Achievement Award

Multiphase CFD on Emerging Computing Technologies

Madhava Syamlal

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Over the last decade, computational hardware and software have been undergoing some dramatic changes. The use of such emerging technologies for speeding up gas-solids flow computations is being explored by the National Energy Technology Laboratory (NETL). This article discusses the progress being made in the usage of three technologies: exascale computers, wafer-scale processors, and TensorFlow software.

ELSEVIER

MFIX: introducing NETL's open source multiphase CFD software

Although none of the efforts discussed here are extensions of an existing code, they originate from **MFIX**, an open source multiphase computational fluid dynamics (CFD) software suite, developed at NETL over the past three decades. Currently, MFIX has over 6,700 registered users worldwide, is downloaded over 3,900 times per year, and is cited over 400 times per year. And all these numbers are increasing each year. MFIX users at NETL and elsewhere have successfully used the software for numerous scientific studies and engineering applications. Currently, for example, at NETL, MFIX is being applied for the development of a bench-scale fluidized bed unit for coating particles used for in situ flow visualization in large-scale combustors, the design of the 23 MWth gasifier being developed by University of Alaska-Fairbanks in partnership with industry, the development and troubleshooting of the entrained flow pyrolysis reactor and the catalytic vapor-phase upgrading unit at the National Renewable Energy Laboratory, and the development of a lab-scale chemical looping reactor at NETL.

Exascale computing for enabling industry relevant CFD-DEM simulations

An epoch-making event in high performance computing (HPC) will occur later this year with the arrival of the **Frontier** supercomputer at Oak Ridge National Laboratory (ORNL). It will be the first exascale computer in the U.S., capable of over 1.5x 10^{18} floating-point operations per second and will likely be the fastest supercomputer in the world when it becomes operational.

The U.S. Department of Energy (DOE) has been preparing over the last decade, in anticipation of the arrival of Frontier and other exascale computers. It was known early on that scaling up existing HPC architectures would not be feasible because of the large increase in power consumption. Therefore, a step change in the HPC architecture that makes exascale computing affordable was anticipated. This meant that existing HPC application codes may not run efficiently on the new HPC architectures; legacy codes may not run at all. To ensure that critical DOE application codes are ready by the time exascale hardware becomes available, a joint effort of two DOE offices—the Office of Science and the National Nuclear Security Administration—launched the **Exascale Computing Project (ECP)** in 2016 [1,2].

ECP selected 24 applications in the areas of chemistry and materials, earth and space science, energy, national security, data analytics and optimization, and crosscutting algorithmic methods. One of the **ECP-Energy** applications is MFIX-Exa, a CFD-discrete element model (DEM) code that will run efficiently on current HPC systems and exascale computers.

ECP required that each application define a challenge problem at the start of the seven-year project and successfully demonstrate its solution by the end of the project. The MFIX-Exa challenge problem is NETL's 50 kW chemical looping reactor (CLR) [3], a technology that can reduce CO_2 emissions in power generation or hydrogen production. The challenge problem simulation will track 5 billion DEM particles in the full-loop CLR geometry, covering various gas-solids flow regimes (bubbling bed, riser, cyclone, standpipe, and L-valve) and include chemical reactions and interphase mass, momentum, and energy transfer. This represents roughly a 1000x increase in the CFD-DEM capability compared with the state-of-the-art in 2017.

Although MFIX-Exa builds on the multiphase modeling expertise embodied in NETL's classic MFIX-DEM code, the core methodology has been both re-designed and re-implemented. The foundation for MFIX-Exa is **AMReX** developed by the ECP AMReX Co-Design Center that supports at least four other ECP applications: large-scale simulations of cosmic structure formation, modeling of advanced particle accelerators, combustion simulations to advance understanding of fundamental turbulence-chemistry interactions, and modeling of stellar explosions. To date, the MFIX-Exa team has made the following progress:

- Implemented a modern method-of-lines projection method for the fluid flow solver.
- Incorporated capabilities for heat and mass transfer, species composition, and chemical reactions.
- Added a lower-fidelity particle-in-cell (PIC) method for determining initial conditions that will reduce the time required for CFD-DEM simulations to reach a stationary state.
- Implemented dynamic load-balancing strategies for DEM calculations and a dual-grid approach that allows independent optimization of CFD and DEM workloads on compute cores.
- Performed weak scaling studies using nearly 30% of ORNL's Summit HPC resources, the second fastest supercomputer in the world.
- Leveraged the AMReX embedded boundary capability for the creation complex geometries, such as that of a CLR.

- •Developed numerous verification cases. Verification and validation simulations are continually being conducted. Some of the results can be found at **MFIX-Exa results gallery**.

A defining characteristic of exascale machines is the predominance of graphical processing units (GPUs) that deliver high floating-point rates at a lower power consumption than central processing units (CPU). Each node of Frontier, for example, will consist of one Advanced Micro Devices (AMD) EPYC™ CPU and four AMD Radeon Instinct™ GPUs. It is a non-trivial task to fully utilize the computational power available on such CPU-GPU architectures, exploiting the fine-grained parallelism on each node, partitioning the work between the CPU and GPUs on a node, and performing parallel computations across multiple nodes. Although AMReX framework shields the MFIX-Exa developers from much of the architectural considerations, some of the optimization must be done within MFIX-Exa code. Recently, the MFIX-Exa team participated in a 12-week virtual **GPU Hackathon** where they worked with experts from the National Energy Research Scientific Computing Center, Hewlett Packard Enterprise, and NVIDIA to improve on-node GPU performance of critical DEM calculations. The team identified and fixed several performance bottlenecks. As a result, a total speedup of 3.1x was observed for DEM calculations on the Summit supercomputer.

MFIX-Exa will accelerate the development of gas-solids reactors for the removal of CO_2 from point sources, such as fossil-fuel based power plants and industrial processes, or directly from the atmosphere. The step change in the CFD-DEM capability provided by MFIX-Exa may enable the solving of a new class of problems in chemicals, petroleum, pharmaceutical, agriculture, and energy industries. For additional information on MFIX-Exa and its applications take a listen to the **Let's Talk Exascale Podcast**.

Exploring the use of the new wafer-scale processors

For most computing tasks, including CFD, existing supercomputers only deliver a very low fraction (0.5-3.1%) of their peak floating-point performance [4]. This stems from the low operational intensity (floating-point operations per byte of data) of various computational tasks. When the operational intensity is low, computational speed (floating-point operations per second) is controlled by the speed at which data reaches the processors (bytes per second) rather than the speed at which data is processed. And memory access speed—measured in terms of bandwidth and latency of memory fetches from the cache, memory, or network—has been steadily falling behind as processor speeds increased over the last 25 years [5].

The above limitation, arising from the low memory access speed in comparison with processor speed, is being overcome by emerging hardware technology called wafer-scale processors [6]. These processors use an entirely new fabrication methodology. Normally, computer chips are fabricated by cutting pieces out of a large silicon wafer, usually 12" in diameter. Wafer-scale processor is the idea that the whole wafer is converted into a chip. That enables the compute cores to be close by and to be connected by numerous wires etched into the wafer, which reduces the latency and increases the bandwidth. Also, shorter wires reduce power consumption, enabling wafer-scale processors to do energy efficient computing. There are, of course, many technical challenges that must be overcome: fabricating the large number of wires that connect the compute cores, remapping the wires around defective cores that inevitably occur at wafer scale, delivering the required power, and removing the heat generated. Cerebras Systems has overcome these challenges and brought the Cerebras CS-1 system to market. The technical specifications of CS-1 are compared with the Joule 2.0 supercomputer at NETL in Table 1.

While the CS-1 was developed to be an artificial intelligence (AI) engine, its hardware arrangement of a two-dimensional array of compute cores is ideal for mapping structured CFD grids. To explore the potential gains from that, NETL teamed up with Cerebras Systems and explored the prospect of running MFIX on CS-1. As a first step, the team developed a BiCGStab solver, a linear equation solver used in MFIX and other CFD codes, for CS-1 [4]. Necessitated by the low memory capacity of CS-1, the BiCGStab solver used mixed precision arithmetic: single precision (32-bit) for the 4 dot products and half precision (16-bit) for the 40 addition and multiplication operations per iteration per mesh point. Remarkably, the solver achieved 0.86 PFlop/s on a CS-1 for the solution of a linear system arising from a 7-point stencil on a 600x595x1536 mesh, achieving about one third of the machine's peak performance.

	Joule 2.0	CS-1
Physical Size Ratio	52	1
Compute Cores	66,560	400,000
Memory Bandwidth (TB/s)	0.256	9,600
Interconnect Bandwidth (Tb/s)	0.1	100,000
Memory (TB)	160	0.018
Power Consumption (kW)	425	20

Only a rough comparison with the performance of MFIX BiCGStab solver is possible because MFIX uses double precision (64-bit) arithmetic. For a linear system arising from a 7-point stencil on 370x370x370 mesh, the MFIX BiCGStab solver achieved 0.001 double precision PFlop/s, achieving only about 0.35% of the peak performance Joule 2.0 cores used. In contrast, the CS-1 BiCGStab solver achieved 371 mixed precision PFlop/s, achieving about 30% of the peak performance of CS-1 cores used.

Furthermore, Rocki et al. [4] evaluated the prospects of conducting CFD simulations on CS-1. The necessary operations in the MFIX algorithm were counted and categorized as vector merge operations, floating-point operations, square root, divide, and neighbor transport operations. The cycle counts for each operation were estimated. The residual calculations were ignored because they could be overlapped with other computations. Based on the performance estimates, the wall time per time step was estimated to be roughly two microseconds per mesh point. Assuming a problem size of 600x600x600 and 15 non-linear iterations per time step, it was estimated that 80–125 time steps could be conducted per second. Compared with an MFIX run on a 16,384-core partition of the Joule 2.0 supercomputer, a CS-1 run is likely to be 200x faster.

MFIX-AI: leveraging emerging AI/ML computing technologies

Dramatic advancements have also occurred in AI/machine learning (ML) software technology over the last decade. For example, the widely used open source platform for ML, **TensorFlow** from

Google, has transformed the development of AI/ML applications. NETL has been exploring its use as a platform to support a future generation of MFIX [7]. Usage of TensorFlow for CFD calculations has been reported in the literature (e.g., [8]). TensorFlow is optimized for large-scale computations, including parallel computing and GPU acceleration. A code based on TensorFlow can be written in a GPU-hardware agnostic manner, which helps rapid development and easy maintenance of the code for multiple and heterogenous computing hardware. Furthermore, TensorFlow could enable inclusion of ML models in MFIX and generation of ML models from MFIX data. The new code is called MFIX-AI.

Existing MFIX routines for the problem set up were used as the front end of MFIX-AI. They were connected to the TensorFlow code through a series of wrappers: Fortran to C to Python to TensorFlow [7]. The computational engine of MFIX-PIC was translated into dataflow graphs required by TensorFlow. The graphs are made up of nodes (operation objects) that represent units of computation and links (tensor objects) that represent the units of data that flow between nodes. The execution of the graphs is optimized at compile time, allowing the TensorFlow code to run fast on multiple computing devices in parallel. A first-generation PIC solver has been developed. For a bubbling fluidized bed simulation of 16.8 million parcels over a 3.8-million-cells mesh, MFIX-AI was found to run about 10x faster than MFIX-PIC.

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Thomas Baron Award in Fluid-Particle Systems
Honoring the Band: A Sampler of Recent Hits...

Christine Hrenya

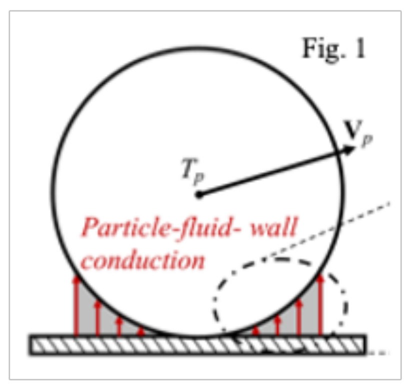
Professor, University of Colorado - Boulder

What an honor it was to receive the 2020 Thomas Baron Award sponsored by Shell. In preparing for the award lecture, I reflected quite a bit on my career, and particularly on all of my group members over the decades, whose diligent efforts led to the scientific achievements being recognized. It would simply not be possible without them, period. In that spirit, the lecture highlighted the group's recent contributions rather than choosing just one.

Heat transfer: Indirect conduction, *not* indirection



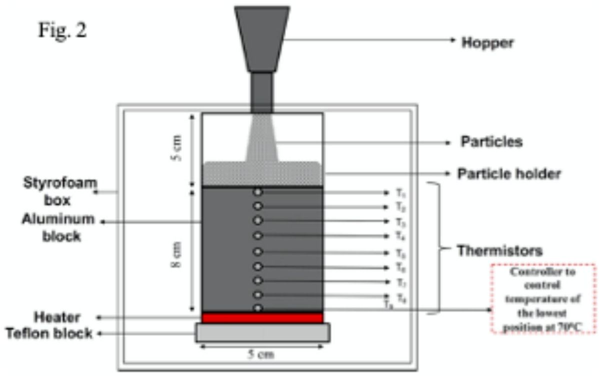

Left to right:
Dr. Aaron Lattanzi,
Prof. Aaron Morris
Ipsita Mishra
Dr. Wyatt C. Q. LaMarche



Motivated by the promise of using solid particles as a heat transfer "fluid" in concentrating solar power (CSP) systems, we focused on heat transfer in a prototype receiver. The particles, which are interior to the receiver, flow around the outside of hollow heat-exchange pipes. The interior surface of the hollow pipes is heated directly via radiation from the sun. An estimate of relevant dimensionless groups wall-to-particle heat transfer plays an important role, and particularly *indirect conduction* – i.e., conduction across the interstitial gas in small distances between the particle and wall (Fig 1).

For decades, the go-to particle-level (*DEM*) model for indirect conduction has been that of Rong & Horio (1999). It contains three assumptions: static fluid, isothermal particle, and one-dimensional heat transfer. Because this model had never been validated, we set up an experiment measuring the heat transfer in a static bed of particles (Fig 2). The DEM simulations matched the experiments within 10% when the Biot number Bi < 0.015; otherwise, the isothermal assumption deteriorates

Fig. 2



(Mishra, Lattanzi, LaMarche, Morris & Hrenya, *AIChE J.* **65** 2019).

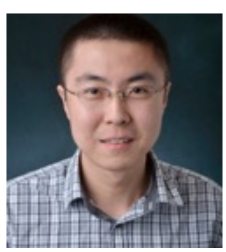
Next, a new *continuum* description for particle-wall conduction (direct and indirect) was developed based on DEM simulations using the Rong & Horio model. Past continuum approaches to describing such heat transfer suffered two deficiencies: (i) effective conductivities were not a function of particle size, contrary to past experiments and DEM simulations, and (ii) Nusselt (Nu) numbers were not a function of solids fraction, since they were developed for packed beds. Here, we adapted the idea of a particle distribution function, which is commonly used in kinetic theories to account for solid-fraction (particle exclusion) effects. Namely, a Nu correlation that incorporates a novel "particle-wall" distribution function was developed, and shown to be universal over a large range of physical properties (Morris, Pannala, Ma & Hrenya; *Int. J. Heat Mass Transfer* **89** 2015 and *Solar Energy* **130** 2016).

Next, we added one more layer of complexity by also considering the effects of convection (along with conduction) on *continuum* descriptions of particle-wall heat transfer. DEM was no longer a suitable choice for the ideal data set on which to base such descriptions since the Rong & Horio model inherently assumed a static fluid. Accordingly, novel direct numerical simulations (DNS) with heat transfer were developed (Lattanzi, Yin & Hrenya; *J. Comp. Phys. X* **1** 2019 and *Int. J. Heat Mass Transfer* **131** 2019). The results indicated that the critical length scale is the thermal boundary layer thickness of wall. With this recognition, a new Nu correlation was developed for heat transfer in excess of the standard Ranz & Marshall correlation for local, unbounded convection (Lattanzi, Yin & Hrenya, *J. Fluid Mech.*, **889** 2020).

We are grateful to our collaborators Dr. Zhiwen Ma, Dr. Sreekanth Pannala, and Prof. Xiaolong Yin, as well as our funding sources – DOE SunShot program and the National Science Foundation.

DEM: The need for speed






Left to right:
Dr. Steven Dahl
Dr. Wyatt C. Q. LaMarche
Dr. Peiyuan Liu
Dr. William Fullmer

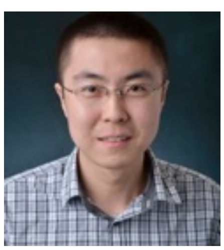
Not surprisingly, a recent industrial survey indicated that the largest bottleneck to greater use of DEM (discrete element method) on par with that of CFD is its high computational overhead (Cocco, Fullmer, Liu & Hrenya, *Chem. Eng. Prog.* Sep 2017). To address this need, we partnered with computational scientists at Univ. CO and NREL to improve the speed of DEM simulations. A related objective that my group has focused on is the uncertainty quantification (UQ) of DEM simulations – i.e., essentially determining error bars for the simulations. Due to the high computational cost of even a single DEM simulation, running the number of simulations required by the gold-standard UQ approach of Roy and Oberkampf is formidable, at best, with today's computational resources.

Fig. 3

So, we set out to develop a simpler-and faster-UQ method, and to experimentally validate it. The latter is tricky since the validation requires comparison with the computationally-intensive standard UQ. Our approach, which we coined the very, very small-scale challenge problem (VVSSCP), was to design a fast experiment (<10 s) with a small number of particles (order of 1000); Fig. 3 shows the resulting segregation experiment in which a larger intruder, starting at the bottom, finds its way to the top of the bed. Particle characterization is also a key aspect of accurate UQ, so experiments were developed to measure the particle size, restitution coefficient and friction coefficient distributions (LaMarche, Miller, Liu & Hrenya, *AIChE J.* **6** 2016 and LaMarche, Liu, Kellogg & Hrenya, *Chem. Eng. J.*, **310** 2017). *The particle characterization experiments are simple, inexpensive, and fit on a benchtop, so we encourage all experimentalists to measure and report these quantities, without which a complete (DEM or continuum) model validation – one with no estimated inputs – is not possible*. The results of our two simplified UQ approaches for the segregation experiment compared favorably with those of the standard approach, but with a computational savings of ~95% (reduced-order UQ) and ~70% (conservative UQ) (LaMarche, Dahl, Fullmer & Hrenya *under review* and Dahl, LaMarche, Fullmer, Liu & Hrenya *under review*).

We are grateful to our collaborators – Dr. Thomas Hauser, Dr. Ray Cocco, Dr. Allan Issangya, and Prof. Jonathan Higham - as well as DOE NETL for funding.

Cohesion: We got caught in a sticky situation

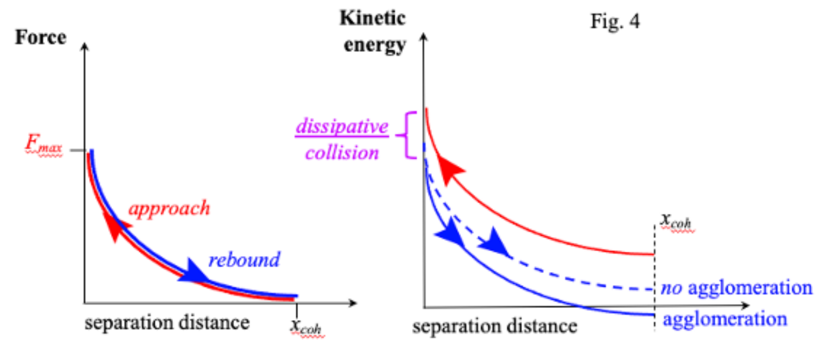



Left to right:
Dr. Wyatt C. Q. LaMarche
Dr. Peiyuan Liu
Dr. Kevin Kellogg
Ipsita Mishra

The same industrial survey mentioned above (Cocco, Fullmer, Liu & Hrenya, *Chem. Eng. Prog.* Sep 2017) also queried respondents as to which physical enhancements are most needed in DEM models. More than 50% responded that cohesion, and the corresponding prediction of agglomeration, was the DEM capability they most wanted to see improved. This response is not surprising, given that correlations for agglomerate size can differ by an order magnitude (Shabanian et al., *Int. Rev. ChE* 2012).

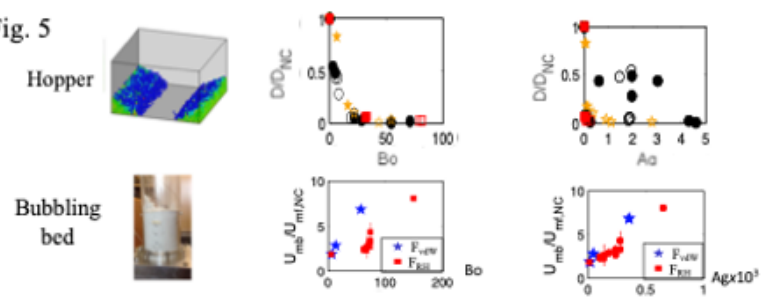
Perhaps even more surprising is that some of the aforementioned correlations for agglomeration size are based on force balances, while others are based on energy balances. This force vs. energy approach to describing cohesion is a decades-long debate that came into stark view when it initially appeared that our new continuum theory for cohesive systems (Kellogg, Liu, LaMarche, and Hrenya, *J. Fluid Mech.* **832** 2017) was at odds with Geldart's chart – a sticky situation indeed! Namely, our new theory indicated that an energy description was most appropriate, whereas the regime boundary between Groups C and A on Geldart's chart could be captured by a dimensionless group based on force (Molerus, *Powd. Tech.* **33** 1982).

The resolution of this force vs. energy quandary was spurred by a consideration of the force and kinetic energy profiles as two cohesive particles approach each other and then rebound – see Fig. 4. Namely, the force vs. particle separation does not display a hysteresis, whereas the corresponding kinetic energy profile does display a hysteresis due to the dissipation nature of the collision (inelastic and/or frictional). Without dissipation, even in the presence of cohesion, particles would not agglomerate. We therefore hypothesized that flows sustained, multi-particle contacts ("dense") would be dominated by force arguments, as agglomeration is ill-defined in such systems. On the flip side, systems characterized by brief contacts ("dilute") would be best described by energy balances, as agglomeration is not ill-defined in such systems.



To probe this hypothesis, we examined the potential collapse of system behavior with two dimensionless groups – a force-based generalized Bond number (Bo_G) and a new, energy-based Agglomeration number (Ag). We tested a wide range of systems (bubbling beds, risers, hopper flow, simple shear, etc.) and sources of cohesion (van der Waals, capillary condensation, etc.) using both simulations and experiments. The results – enduring-contact systems collapse with Bo_G but not Ag and vice versa for systems dominated by brief contacts – provide support for our hypothesis; see Fig. 5 for examples (LaMarche, Liu, Kellogg, Lattanzi & Hrenya, *AIChE J.* submitted). The results also shed light on the apparent discrepancy between our new continuum theory and the Geldart chart. Namely, when the source of cohesion is van der Waals force (as is the case for Geldart's chart), the characteristic force and energy are proportional, so collapse with both Bo_G and Ag is fortuitious.

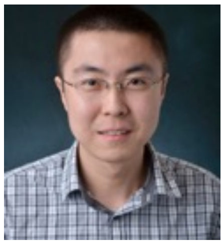
Fig. 5



We are grateful to our collaborators, Mike Molnar and Abhi Shetty, and well as those entities who supported this work – Dow, National Science Foundation and Anton Paar.

Clustering: Attractive couples, and the unattractive

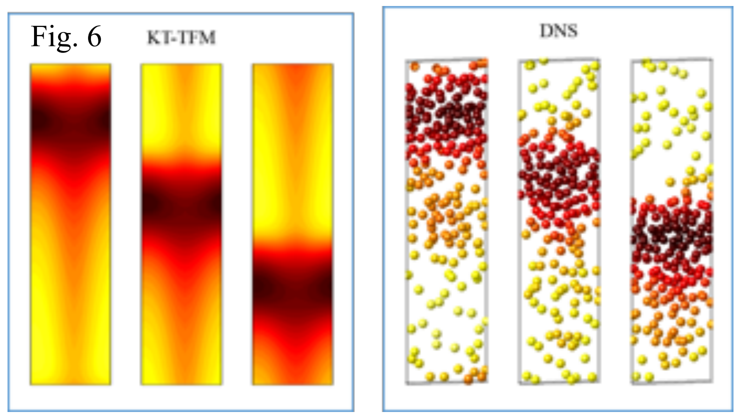
As used here, clustering refers to the hydrodynamic instability in gas-solid flows that is characterized by a relatively dense collection of particles that moves in space and time, with such clusters continually forming and dissolving. The presence of clusters, which have no single-phase counterpart, can be traced to dissipative collisions between particles (inelasticity, friction, etc.) and/or the interaction of the gas and solid phases (Fullmer and Hrenya, *Ann. Rev. Fluid Mech*. **49** 2017). Unlike agglomeration, as mentioned above, which arises from particle-particle cohesion, hydrodynamic clusters occur even without cohesion.



Left to right:

Dr. William Fullmer

Dr. Peiyuan Liu



The ability of kinetic-theory-based models to predict clustering has been well documented over the last several decades. Largely due to computational constraints, what was less clear is the quantitative ability of such models to predict clustering. Two assumptions inherent in the kinetic-theory-based models – a high Stokes number (particle inertia/viscous fluid effects) and low Knudsen number (small spatial gradients of flow variables) – had not been deeply probed. The latter assumption is particularly vexing, since a high concentration gradient is known to exist perpendicular to the surface of a cluster (due to the high concentration of particles within cluster compared to just outside its surface). Here we used direction numerical simulations (DNS) of clustering systems to assess the accuracy of kinetic-theory-based predictions. As pictured in Fig. 6, the results showed strong agreement between DNS and kinetic-theory predictions for high St (as expected) even when the low-Kn assumption is violated (Fullmer, Liu, Yin & Hrenya *J. Fluid Mech*. **823** 2017). This result is reminiscent of what is observed in rarefied gases and a welcome, albeit fortuitous, finding for gas-solid systems, since kinetic theories beyond Navier-Stokes order are extremely complex.

We next considered more complex systems, and specifically the addition of cohesion to clustering systems. We hypothesized that the presence of clusters would enhance agglomeration since within a cluster, (i) collision rates increased and (ii) particle impact velocities decreased. We were humbled when the opposite was observed – i.e., attractive couples broke up unexpectedly (Fig. 7). Further investigation revealed that this cluster-induced agglomeration traced to the cluster interface, where the impact velocities between falling clusters and upward-moving particles was quite high (Liu & Hrenya, Phys. Rev. Lett., **121** 2018)

We thank our collaborators – Dr. Xiaolong Yin and Guodong Liu –as well as funding from NSF and Dow.

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PSRI Fluidization and Fluid Particle Systems Award

Shaping the Process, Slots, Sound, Swages, Statistics: Opportunities and Insights in Fluidization and Fluid-Particle Systems

Clive Davies

Professor, Massey University

Fluidization became embedded in my professional life while, as PhD student at Imperial College, London, in the early 1970s, I faced the challenge of designing and constructing a 600 mm diameter fluidized bed to be the second stage of a two-stage combustor for residual fuel oil; ridiculous headspace and footprint constraints, bubbles, jets, soot, fouling, high temperatures, and more. But exciting times, bubbles and models and the elegant reminder from Derek Geldart -his 1973 paper- that different powders have different characteristic fluidization properties.

Another high temperature process opportunity took me to New Zealand. My post-doc project, Acetylene Manufacture by a High Intensity Electric Arc Process, had high temperatures, but no fluidization. But, through a social connection, I maintained some activity in fluidization applications with a paper *Fluidized Bed Coating of Conifer Needles with Glass Beads for Determination of Leaf Surface Area*. Conifer needles do not have a circular cross-section, and a fluidized bed enhances the efficacy of a glass bead method where a leaf or conifer needle is coated with ballotini, and a weight: area calibration used to find foliage area.

Yet another high temperature opportunity took me from University of Canterbury to Department of Scientific and Industrial Research (DSIR). My (first) project was to build a pilot plant for submerged combustion smelting of (highly refractory) titaniferous beach sand. This entailed using a water cooled lance to burn pulverised coal with oxygen beneath the surface of molten beach sand, and required a continuous flow of coal, controllable to a specified flow rate. The quest for reliable flow rate measurements in particulate systems soon became a consuming and life-long interest. In this case, the solution lay in careful design of a continuous blow tank system constructed to deliver the coal to the lance, and the simple expedient of extracting flow rate from the rate of change of the pressure drop across a fluidised blow tank feeder; the feeder operated at 60-100 kPa gauge, and accurate mass flow measurements were achieved by eliminating fluctuations and cycling in the pressure of the fluidizing air supply to the blow tank.

Shortly after joining DSIR in 1979, in addition to existing project commitments, I was given the opportunity to contribute to solutions to a pressing dairy industry problem: some (dry powder) products were being contaminated by metal fragments originating in process equipment. The long term approach was to eliminate metal-metal contact during processing and handling; in the short term, removal of fragments from existing stock was considered, but never implemented on material for human consumption. One of the glaring sources of contamination was the vertical augers used in many processes. I suggested "air-lift" technology as a solution, and my first design was continuous *pot feeder* with downward-blowing spargers for the fluidizing air (to satisfy clean in place requirements) which sat on the process floor; *déjà vu* here, ridiculous headspace and footprint constraints, but a full scale prototype did function well. However, before the first plant tests were complete, I realised that the *pot feeder* could be reconfigured as a *pipe feeder* (simpler, cheaper, easier to operate and clean) in which an aerated head of solids, analogous to an L-valve, fed a vertical lift tube sitting on the process floor, with the lift air blowing into the bottom of the lift tube; see Figure 1. This design of *pipe feeder* replaced all the offending augers throughout New Zealand, and continues to be used in new processing plant. None of this work could be directly published in the open literature, but the *pipe feeder* was used in experiments on the use of swages in a pipe wall to reduce pressure drop in vertical pneumatic conveying. Figure 2 shows, from left to right, a (laboratory) pipe feeder, a photograph of a swage in the wall of a stainless steel tube, and results for three different swage spacings; the tube diameter in this case was 150 mm. The use of swages to re–entrain material after a bend(s) in a horizontal conveying circuit, with accompanying pressure drop reduction, was also demonstrated in the laboratory.

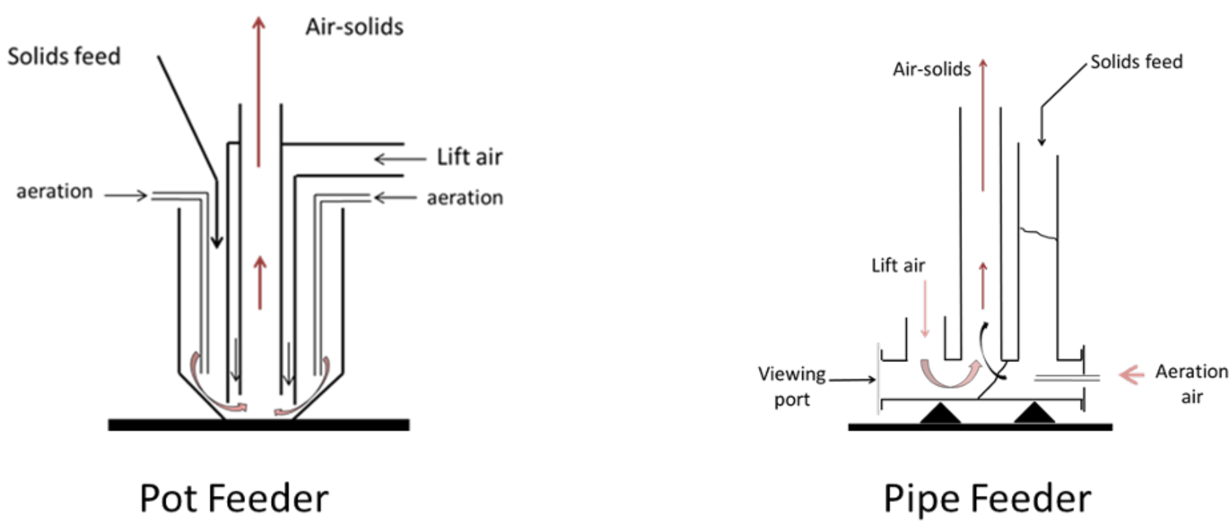

Fig 1. Schematic diagram of *pot feeder* and *pipe feeder*

Numerous and extended visits to dairy factories all over New Zealand in the mid-1980s while commissioning new equipment, exposed me to the demanding requirements of industrial practice, and also highlighted the lack of reliable and robust instrumentation for *in-line* measurement of key dry powder process parameters. Particularly useful, I felt, would be means for measuring flow rate in bulk flows, and in conveying lines, and also bulk density.

The flowrate of a granular material, moving under gravity, through an opening is proportional to the bulk density of the material, acceleration due to gravity, the dimensions of the flow opening, and a correction related to the size of the particles; the functional relationship between these parameters and flow rate is independent of orientation. The concept of a long narrow vertical slot in the wall of a container paved the way to "The Slot Flow Meter". In outline, an inflow to the container reaches an equilibrium height in the slot; flow rate (for a narrow shot) is linearly proportional to height;

height is proportional to the mass of material in the container; load cells measure the mass; thus flowrate is proportional to the mass of material in the container. Investigations of flow through vertical slots, including flows with a free surface, showed that weighing a discharge vessel with a slot in its side, had promise as a method for measuring flow rate. The slot flow meter found almost immediate application at University of Cambridge in measuring flow rates in circulating beds, and has been used in (non-fluidization) applications in the minerals industry in Australia.

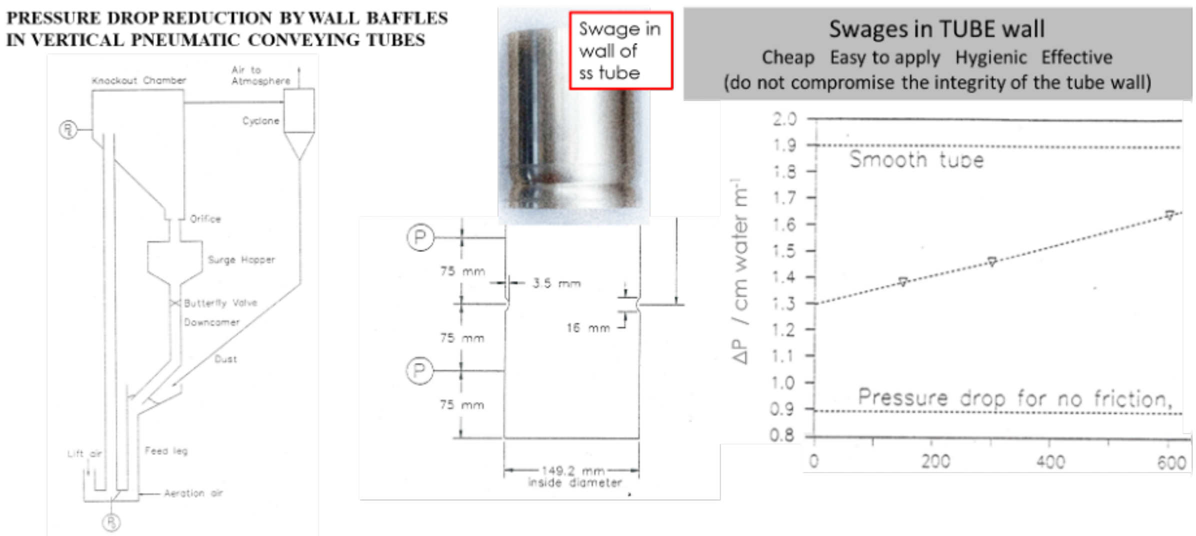

Fig 2. Pressure drop reduction using swaged indentations in the wall of a vertical conveying tube

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During the development of the slot flow meter, I realised that a flow from a slot much wider than the particle diameter, feeding a continuously weighed vessel with a narrow slot, could enable continuous estimates of particle size; this applies to both fluidized and un-fluidized material, and the approach is illustrated in Figure 3 which shows a schematic of apparatus for the fluidized case, and some results for the response to a step change in particle size.

Slot flow monitoring of particle size exploiting edge effects in orifice flow: An instrument concept. Both bulk (un-fluidized) and fluidized versions developed. Some results from fluidized version shown below

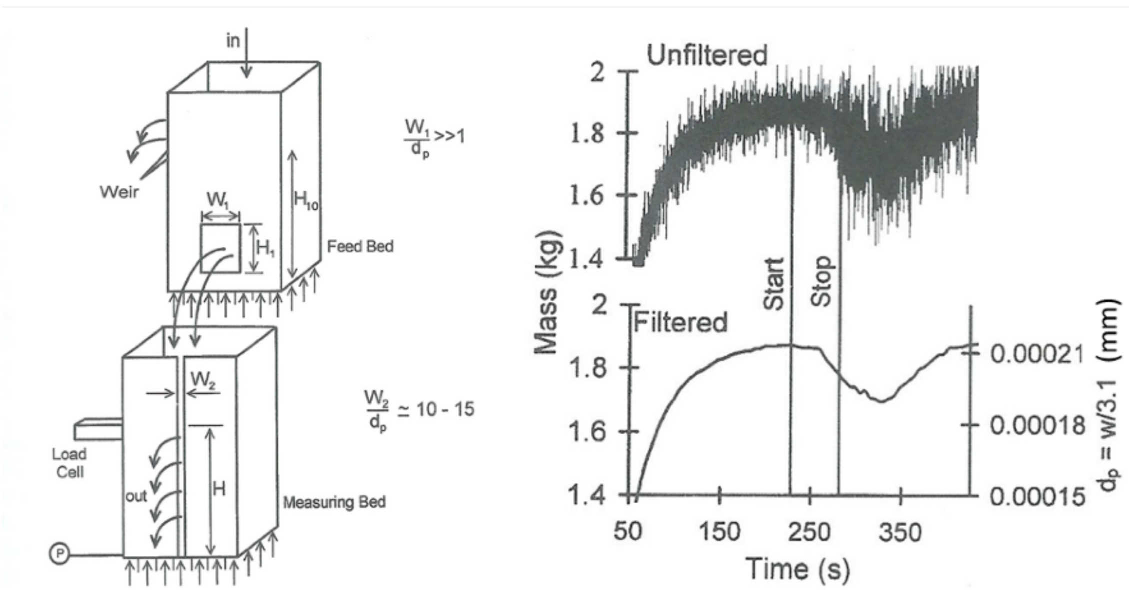

Fig 3. Slot-flow apparatus for measuring particle size (left), and response to a step change in particle size (graph on the right); particle size is indicated on the right vertical axis of the graph

$$V_{TOT} = \frac{\sum_{i=1-n} (x_i - \bar{x})^2}{(n-1)}$$ Total Variance x_i (Pressure), from ΔP record

$$V_{HI} = \frac{\sum_{i=2-n} (x_i - x_{i-1})^2}{(n-1)}$$ High Speed Variance (mean square successive difference)

$$\frac{V_{TOT}}{V_{HI}} \approx \frac{1}{2(1-\rho)}$$ T^{-1} ρ (correlation between successive data points)

I noted above an interest in in-line measurement of bulk density of dry powders. While pursuing this, it was apparent that the information in the fluctuating signal from a prototype density instrument could be correlated with a variety of different physical properties of the test powder. A particularly powerful, yet computationally simple statistical parameter is the ratio, $\mathbf{T^{-1}}$, of the Total Variance to the Mean Square Successive difference (see below) which was proposed by von Neumann, and has found utility and application in many quite different physical systems.

Decreasing estimates of the ratio $\mathbf{T^{-1}}$ reflect decreasing correlation between successive data values. Examination of some of my own historical data on pressure fluctuations for silica sands having mean diameters that placed them close to the Geldart A/B boundary, provided indications of distinct change at or close to estimates of U_{mf} or U_{mb}. But there were no supporting experimental measurements of U_{mf} and U_{mb}, so no substantive conclusions could be drawn. This omission has been partially rectified following experiments with lactose powders, some sand samples, glass ballotini, and refractory dust. U_{mf} was measured by the pressure drop method, and U_{mb} determined visually ($U_{mb,v}$). Figure 4 is a plot of the ratio of the total variance to the mean square successive difference, $\mathbf{T^{-1}}$, against superficial velocity, U, normalised with respect to $U_{mb,v}$; *maximum* values of $\mathbf{T^{-1}}$ occur at or close to $U = U_{mb,v}$, *i.e.* $\{U / U_{mb,v}\} = 1$, and are shown by the symbol **X**.

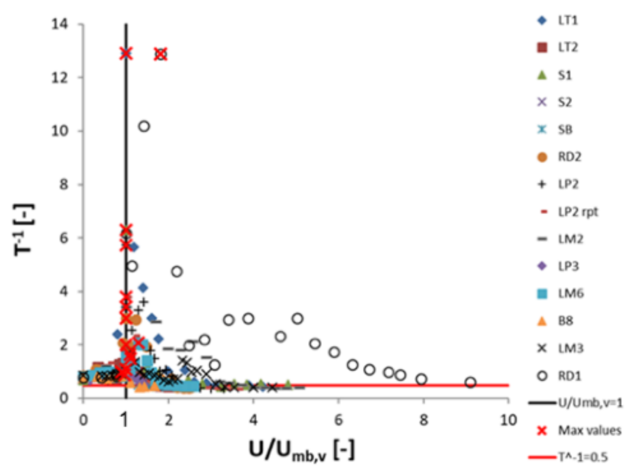

Fig 4. T^{-1} as a function of normalised superficial velocity

Augers were not the only source of contamination of dairy powders through metal-metal contact. Rotary valves are extensively used as feeders in (dilute) pneumatic conveying lines in the dairy industry, and venturi feeders were seen as potential alternatives in some situations. A test rig constructed for venturi investigations paved the way to opportunities for exploring approaches to measuring flowrates in pneumatic conveying. Beginning in 1991 a number of approaches were used to extract information from pressure signals, starting with correlations of pressure fluctuation data, and subsequently using cross correlation methods, and (finally) time of flight and attenuation of applied acoustic waves. A spinoff was an indication that the attenuation of the applied acoustic signals could be used to indicate particle size.

The effect of rotation rate on the behaviour of powder in a rotating drum has been the focus of considerable research attention, but the effect of the physical properties of a powder on flow behaviour is not well documented. Exploratory experiments with powders from the four Geldart Groups, using apparatus that tracked avalanche motion, showed significant differences in the behaviours for the different Groups. An investigation of an A/B and a C/A powder, using Speckle

Visibility Spectrometry, revealed powder avalanche dissipation was dominant for the A/B powder while collisional dissipation was more important for the C/A powder.

I am fortunate to have been active at a time when the workplace offered a variety of exciting technical challenges, as well as opportunities for professional development and service. I am grateful for the support I have had over many years from mentors both in academia and industry and acknowledge contributions from colleagues and students without which much of this would not have been possible.

Author's note: I have not put in references to the work in this article, but can provide further information on request. The link below is to a recording of my Award Lecture:

https://webcast.massey.ac.nz/Mediasite/Play/14df8faacb7a453c9588b9ee157097611d

2021 PTF Award Nominations - Now Open

Dear PTF Members:

We are announcing the 2021 PTF awards. The nomination information, award criteria, and previous winners for each of these awards are found in the links below:

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

Key information for this year is below:

The Nomination process is a single step. The full package (a single PDF document) is due by **Friday, May 28th, 2021**, containing items specific to each award.

•If the nominee has previously received any award from PTF, an explicit statement of new accomplishments or work over and above those cited for the earlier award(s) must be included (maximum of 1 double spaced page).

•Selected bibliography (including major papers published, books, and patents)

•In a given year, the same person cannot win more than one PTF award

•Wait period for nomination after previous award

•A former PTF award winner cannot be nominated for another award for at least three years after receiving any previous PTF award

•It is required that the nominators are current PTF members

•Nominees are not required to be PTF members

•For the PTF Lifetime Achievement Award, one of the support letters must be from a former PTF Lifetime Achievement Award winner.

•Except for the PTF Service Award, the Executive Committee has released the nominee PTF membership requirement. PTF membership is still expected for the PTF Service Award.

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

- S.B. Reddy Karri

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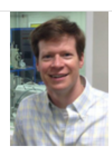
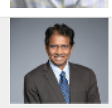
Chair Dr. Jim Gilchrist gilchrist@lehigh.edu	
Co-Chair Dr. S.B. Reddy Karri reddy.karri@psri.org	
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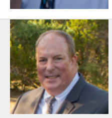
Past Chair Dr. Bruce Hook bdhook@dow.com	

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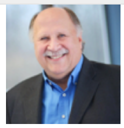
Willie Hendrickson whendrickson@aveka.com	
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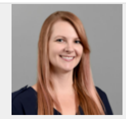
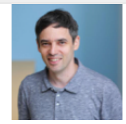
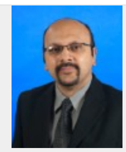
Dr. Heather Emady heather.emady@asu.edu	
Dr. Aaron Moment ajm2293@columbia.edu	
Dr. Bodhi Chaudhuri body.chaudhuri@uconn.edu	
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