THE PARTICLE TECHNOLOGY FORUM (PTF) NEWSLETTER

An American Institute of Chemical Engineers (AIChE) Forum

Message From The Chair

Dear Colleagues,

I hope you're enjoying the start of summer. I wanted to share a few updates from the Particle Technology Forum and highlight some of the great work happening across our community.

Planning for the AIChE Annual Meeting in Boston is progressing well. Abstract submissions have closed, and I'm happy to report that we received a strong number, slightly more than last year's meeting in San Diego. Most sessions are well populated, and our two honorary sessions are already full, thanks to the outstanding efforts of our organizers and sponsors. While a few sessions came in lighter, such as one on cohesive and non-traditional forces in fluidization, the programming team is actively working to ensure a balanced and engaging technical program.

We're also excited for our upcoming PTF Awards Banquet, which will be held at Basile Fine Italian Kitchen, just a short walk from the Marriott Copley Place and near the Green Line. The evening will feature a full restaurant buy-out, a four-course dinner (including a vegan option), a cocktail hour with passed appetizers, and a drink ticket system. It promises to be a warm, celebratory evening with friends and colleagues.

I'm pleased to share that we've had a very strong response to this year's award nominations, including a record number of submissions in some categories. For example, the George Klinzing Best PhD Award received five nominations, the most we've ever had, and a few final submissions are still being processed. We look forward to recognizing these outstanding contributions at the banquet. I'm also happy to announce that Dr. Reza Mostofi of Honeywell has been unanimously selected by the Executive Committee to receive the PTF Service Award, honoring his continued dedication to the Forum.

We are also working with AIChE to resolve some persistent issues with member email communications. If you or a colleague hasn't been receiving updates, please let us know so we can follow up and keep everyone connected.

As always, thank you to all of our volunteers and members for making this such an engaged and supportive community. If you have ideas, feedback, or would like to get more involved, I'd love to hear from you.

Warm Regards,

Maria Tomassone

PTF Chair
Professor, Department of Chemical and Biochemical Engineering
Rutgers University

A Peek At The Contents

Welcome to the website for the Particle Technology Forum!

It is your comprehensive resource to keep you informed and stay connected with the Particle Technology Forum community.

FROM THE EDITOR'S DESK

The last AIChE Annual Meeting in San Diego was intellectually exciting in the breadth and scope of its technical content, and professionally invigorating due to our ability to connect and network in person. As is the tradition, we acknowledged and celebrated the accomplishments and excellence of our peers through the PTF Award Lectures & the PTF Awards Dinner events.

The success of programming and networking events hinges on the tireless efforts of the PTF Executive and Programming Committees, along with many of our colleagues who selflessly step in to help. That is what makes our community strong and effective. Let us keep that spirit going!

On a somber note, I share with you the sad news of Dr. Ecevit Bilgili's passing away. He had been an active and prolific member of the PTF for many years. If you would like to write about him or contribute any articles related to his areas of research, please reach out to me by **July 12th**.

Shrikant Dhodapkar
Senior R&D Fellow / AIChE Fellow
The Dow Chemical Company
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PTF Website

Our website is a resource for our membership, which must be updated and enriched by the contributions from all of us. I encourage you to remain engaged by visiting the website and sharing the links with others.

Some key features...

- PTF leadership, where you can learn about the esteemed professionals guiding our initiatives.
- Stay up-to-date with upcoming events, including conferences, webinars, and workshops that offer opportunities for professional growth and networking.
- Discover our awards section to celebrate the achievements and innovations of our members who are making significant contributions to particle technology.
- Newsletters provide updates, insights, and articles to keep you informed about the latest exciting events, trends, research, and job opportunities.

If you are interested in contributing content to the newsletter or share information about upcoming events, please reach out to me (yfan5@dow.com).

Yi Fan
Senior Research Scientist
The Dow Chemical Company, TX

Past PTF Chairs

Year	PTF Chair
1992 – 1994	L. S. Fan Ohio State University
1994 – 1996	Reg Davies DuPont Company
1996 – 1998	Mike Roco NSF
1998 – 2000	Karl Jacob Dow Chemical Company
2000 – 2002	George Klinzing University of Pittsburgh
2002 – 2004	Ralph Nelson DuPont Company
2004 – 2006	Alan Weimer University of Colorado, Boulder
2006 – 2008	Shrikant Dhodapkar Dow Chemical Company
2008 – 2010	Hugo Caram Lehigh University
2010 – 2012	Raymond Cocco PSRI
2012 – 2014	Jennifer Sinclair Curtis University of Florida
2014 – 2016	Reza Mostofi UOP
2016 – 2018	Raj Dave NJIT
2018 – 2020	Bruce Hook Dow Chemical Company
2020 – 2022	Jim Gilchrist Lehigh University
2022 – 2024	Reddy Karri PSRI

PTF Award Winners 2024

Elsevier PTF Lifetime Achievement Award

Dr. Hamid Arastoopour

Henry R. Linden Professor of Engineering
Director of the Wanger Institute for Sustainable
Energy Research (WISER)
Illinois Institute of Technology, Chicago
Email: arastoopour@iit.edu

Citation: **Arastoopour is a pioneer in the development of CFD-based models for fluid-particle systems for scale-up and design of energy and sustainability related processes.**

Hamid Arastoopour is currently Henry R. Linden Professor of Engineering and Director of the Wanger Institute for Sustainable Energy Research (WISER) at Illinois Institute of Technology (IIT). Before that, he served as Dean of Armour College of Engineering and as Chairman of the Chemical and Biological Engineering Department at IIT.

Dr. Arastoopour has made significant contributions to research and education in particle technology, fluidization, and computational fluid dynamics (CFD), motivated by energy and sustainability applications. He holds 15 U.S. patents and has published three books, seven book chapters, and about 150 papers.

He is the recipient of the Sustainable Engineering Forum (SEF) Research Award, the Thomas Baron Award in Fluid/Particle Systems, the Donald Q. Kern Award in Heat Transfer and Energy Conversion, the PTF Lectureship Award in Fluidization and Fluid/Particle Systems, the Ernest W. Thiele Award, and the PTF Fluidization Process Recognition Award from the American Institute of Chemical Engineers (AIChE). He is a Fellow of the National Academy of Inventors (NAI) and AIChE. He is also the recipient of the University Excellence in Teaching Award. He has served on the editorial boards of *Powder Technology*, *Sustainability*, and *Fluids* journals.

ELSEVIER

Sponsor of the Lifetime Achievement Award

Pathway to a Sustainable Net-Zero Economy:
Examples of Particle Technology Research Contribution

Hamid Arastoopour
Linden Professor of Engineering and Director
Wanger Institute for Sustainable Energy Research (WISER)
Illinois Institute of Technology, Chicago, Illinois

Abstract

A pathway to a sustainable net-zero economy is both multi-faceted and complex and requires abundant supplies of renewable energy and water. An effective pathway aims to improve the reliability, security, and affordability of energy and water by: utilizing a least-cost strategy to reduce the negative impact of energy consumption on climate change and water availability; emphasizing the gradual decarbonization of the global energy system; increasing energy efficiency and conservation; and preserving natural resources and the environment. This paper will discuss examples of the critical role of particle technology research in the creation of a pathway to a sustainable society. Specifically, it will focus on my research group's contributions in the areas of computational fluid dynamics (CFD) simulation of CO_2 capture in circulating fluidized bed (CFB) systems; CO_2 conversion to useful products using an electrolyzer; design of thermal energy storage for concentrated solar energy (CSE) using packed, fluidized bed systems; and production of natural gas from unconsolidated hydrate reservoirs

Introduction

The pathway to a sustainable net-zero carbon society is based on providing clean and renewable energy as well as security and economic vitality and growth for global societies. The pathway to a net-zero carbon society approach would significantly impact the reversal of the adverse effects of climate including sea level rise, increased hurricane damage, and changed rainfall patterns that might dramatically affect agricultural productivity and result in more floods, droughts, and wildfires. Engineers are uniquely qualified to take the leadership role in research and development in areas such as particle technology as global energy systems continue to evolve in the historical cycle from primary reliance on wood to coal and oil to current reliance on natural gas as a transitional fuel in creating a pathway to sustainable global energy systems.

Continuous improvement in the development of devices with accurate and fast response measurements at the molecular/cellular, particle, and reactor levels, along with advances in computational capabilities, enable engineers to create more rigorous and accurate design and scale-up tools such as computational transport phenomena (CTP), molecular dynamics, and artificial intelligence, and begin to shorten the gap between laboratory and industrial scales.

Today, there is an even greater opportunity for engineers to use particle technology principles and advanced experimental tools and software to become one of the important contributors in research and development in building a pathway toward a future sustainable society and economy[1].

Examples of Particle Technology Research

Contributions of particle technology research and education may include: use of the advances in fluidization and fluid-particle research to provide an efficient design and scale-up tool for biofuel reactors, process intensification, conversion of waste to energy, and gasification processes; CO_2 capture, utilization (conversion to useful products and fuels), and sequestration; use of fluidized and packed bed systems as thermal energy storage media for concentrated solar energy (CSE); contribution to efficient wind turbine design under different environmental conditions; production of natural gas from unconsolidated hydrate reservoirs to substitute coal and oil as a transitional step toward a sustainable economy; and particle pulverization as a recycling tool for polymeric and elastomeric materials.

CO_2 Capture and Utilization

The world consumption's of non-fossil fuels is expected to grow much faster than that of fossil fuels. However, fossil fuels will continue to account for most of the energy today and for at least a couple of decades to come. The global anthropogenic CO_2 emissions from burning fossil fuels are about 90%, and only 10% is from emissions of CO_2 from forestry and other land use. All of these predictions indicate that the global emission of CO_2 and its impact on climate change will continue for many years in the near future.

Figure 1 shows our road map research for CO_2 capture and utilization. Our road map includes sorbent preparation, fundamental studies of solid flow through different regimes of fluid particle systems and circulating fluidized bed systems (CFB), computational fluid dynamics (CFD) simulation and validation using data from non-reacting experiments, simulation of high-temperature CO_2 sorption and regeneration using a CFB system followed by scale-up studies, and, finally, conversion of CO_2 to alcohols using an electrolyzer. In this study, we simulated CO_2 capture and regeneration using amine-coated particles of 115 microns in a CFB.

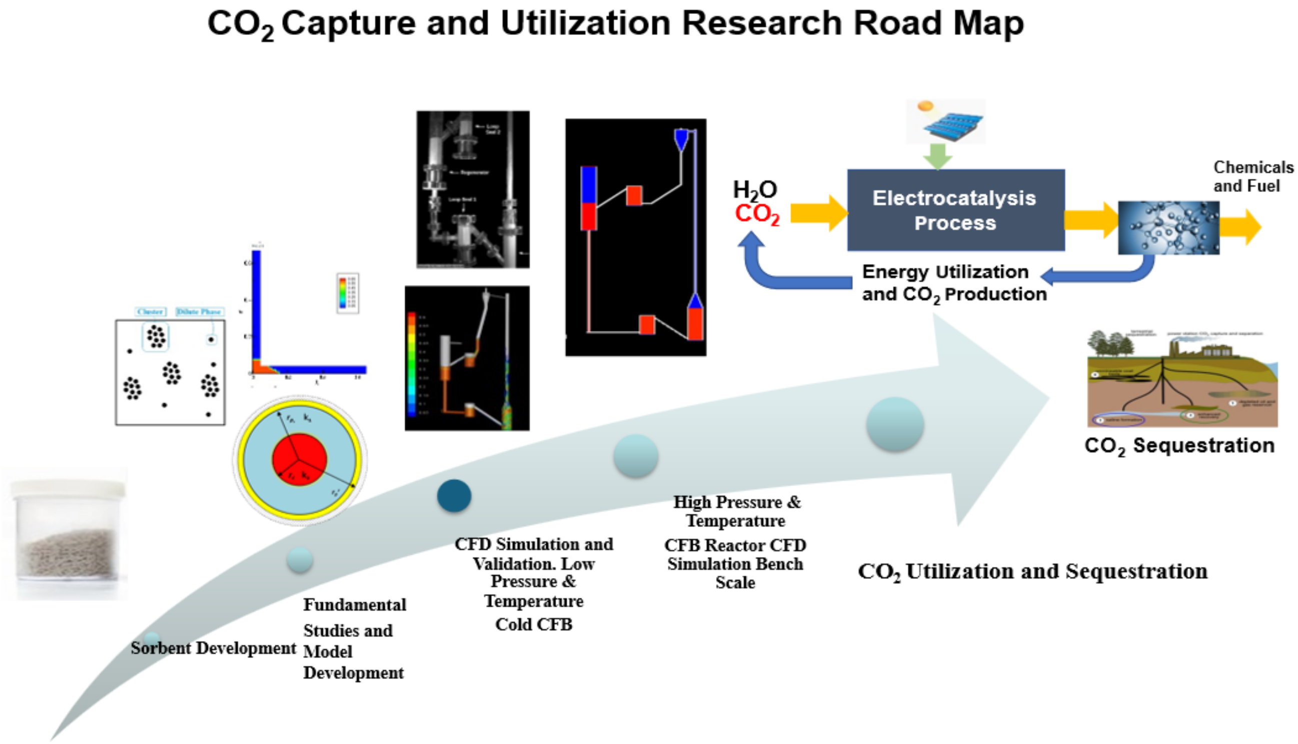
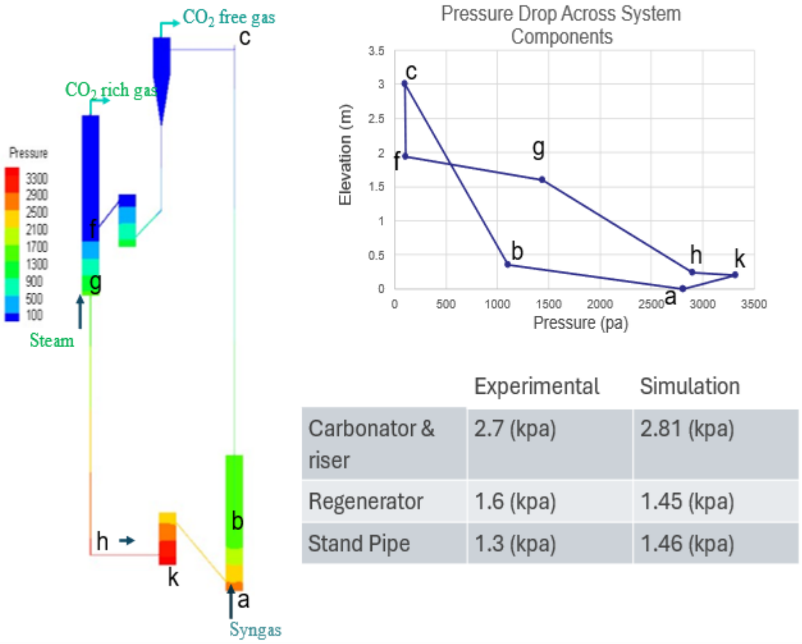


Figure 1: CO_2 capture. conversion to useful products, and sequestration research pathway.

In our CFB process, gas containing CO_2 enters the bottom of the fluidized bed absorber and reacts with fresh sorbent in the bed. The CO_2-laden particles flow up the riser and flow to the regenerator fluidized bed, where CO_2 is released from the sorbent particles by heating up the spent sorbent using concentrated solar energy or steam. The regenerated sorbent particles then move to the fluidized bed absorber to complete the loop (see Figure 2). Our simulation using ANSYS code showed not only how a CFB loop system can be used to capture CO_2 and regenerate CO_2-laden sorbents, but also the capability of the CFD approach that is based on the fundamentals of transport phenomena in the simulation, design, and scale-up of such systems. Figure 2 also shows the simulation of a pressure drop across different system components in our CFB loop and comparison with NETL experimental data[2].



	Experimental	Simulation
Carbonator & riser	2.7 (kpa)	2.81 (kpa)
Regenerator	1.6 (kpa)	1.45 (kpa)
Stand Pipe	1.3 (kpa)	1.46 (kpa)

Figure 2: Schematic diagram of the CFB process, pressure drop across system components, and comparison with the experimental data.

Figure 3 shows our simulation results for molar concentration of the carbon dioxide at the outlet of the riser during 30 seconds of the system operational time. The mole fraction of the CO$_2$ at the outlet of the riser was 2.8% after 30 seconds of operation. The molar concentration of the carbon dioxide in the injected synthetic flue gas from the bottom of the carbonator was 20%. Therefore, almost 86% of the carbon dioxide was adsorbed by solid-supported amine sorbents in the carbonation section of the circulating fluidized bed loop.

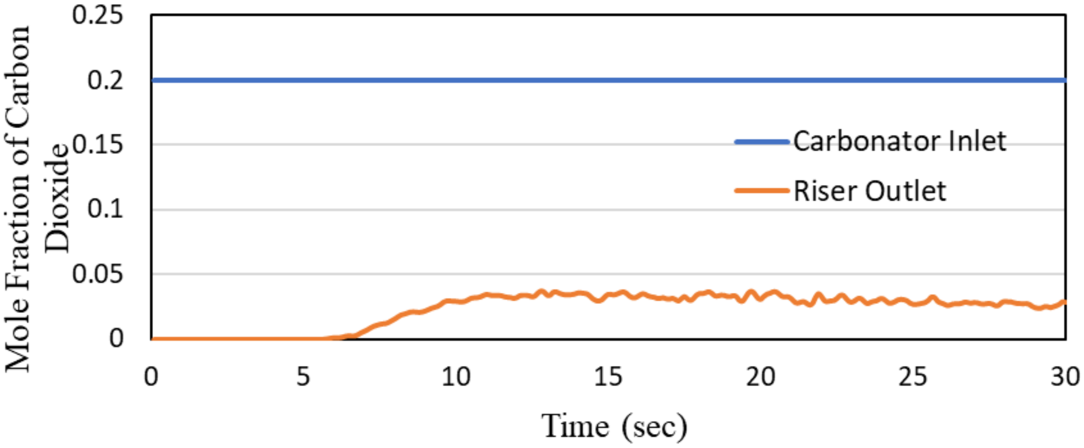


Figure 3: Simulation values of mole fraction of carbon dioxide in the gas phase at the riser inlet and carbonator outlet.

Steady state, two-phase (gas and liquid), and isothermal one- and two-dimensional models for a zero-gap electrolyzer process were developed to study the conversion of CO$_2$ to valuable products, such as ethanol and hydrogen. Figure 4 shows the schematic of a zero-gap electrolyzer. It contains two compartments, including the cathode and anode, separated by a membrane. The electrolyzer consists of seven distinct domains, including the: CO$_2$ gas flow channel (GFC), carbon gas diffusion layer (GDL), copper (Cu) catalyst layer (CL), anion exchange membrane (AEM), iridium oxide

(IrO_2) anode CL, titanium anode mesh, and electrolyte (KOH) flow channel (EFC). Humidified CO_2 enters the zero-gap electrolyzer through the GFC, diffuses through the porous carbon GDL, and reaches the Cu-catalyst surface where it is electrochemically reduced. Unconverted CO_2 and products diffuse back to the GFC, whereas, in the anode compartment, the electrolyte solution provides the necessary hydration for the operation of the zero-gap electrolyzers. It is assumed that the GDL is an ideal hydrophobic material; therefore, the liquid phase is not modeled in GFC and GDL, and cathode CL is the only common region for the gas/liquid phases where interphase species mass transfer is considered.

We conducted one-dimensional and two-dimensional simulations for a zero-gap electrolyzer using Cu as the catalyst. Figure 5 shows the comparison of our simulations with the experimental data of Wang et al[3]. Our simulations compared well with the experimental data. A comparison of the total current density simulation results of the 2-D numerical model and the 1-D numerical model of the zero-gap electrolyzer showed that the 1-D numerical model simulation that requires significantly less computational time is a very reasonable assumption for current density prediction at only lower cell potentials.

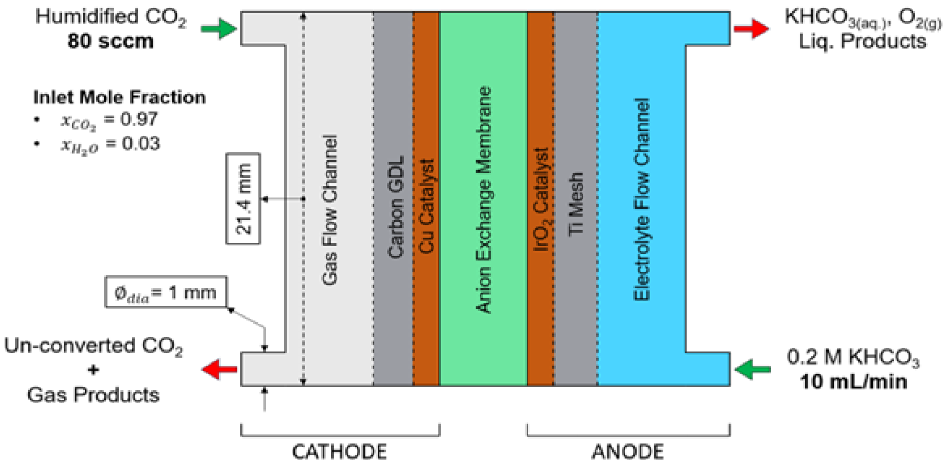


Figure 4: Schematic diagram of a zero-gap electrolyzer.

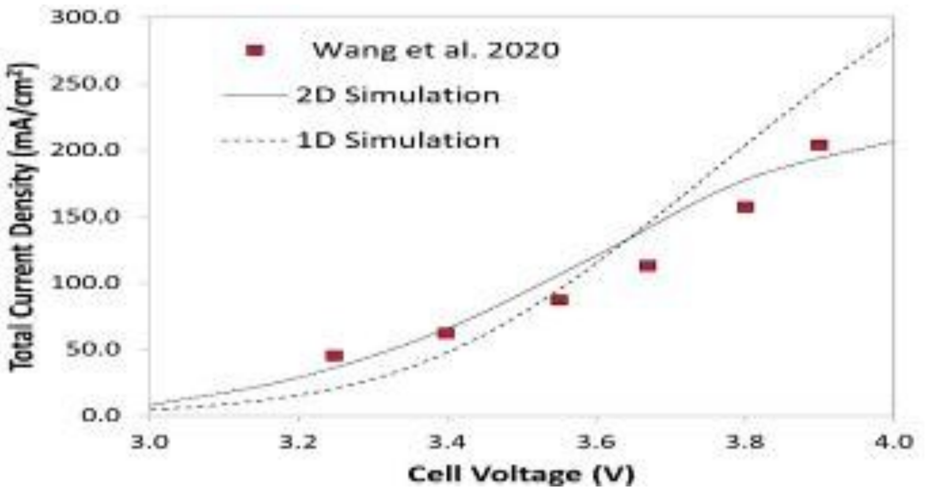


Figure 5: Comparison of our one- and two-dimensional simulations with the experimental data of Wang et al. (2020).

Storage of Concentrated Solar Energy (CSE) Using Packed and Fluidized Bed Systems

Among the renewable energy resources, solar energy, which includes photovoltaic and concentrated solar energy (CSE), is considered to be one of the main renewable sources for future energy in the world. Unlike PV systems, CSE technology captures and stores the sun's energy in the form of heat, using fluidized or packed bed systems with materials that are low cost and stable. This system approach allows CSE with thermal energy storage (TES) to deliver renewable resources to the energy grids, thereby enabling increased penetration of variable renewable energy technologies. We developed a radiative heat transfer model as well as continuity, momentum, and energy equations for the gas and particle phases. The computational fluid dynamics (CFD) approach was used to simulate concentrated solar energy (CSE) absorption and energy recovery using both a packed bed and a fluidized bed system filled with silicon carbide particles[4]. Figure 6 shows our numerical simulation of temperature of SiC at the center of the surface of a packed bed with CSE focusing on the middle of the bed compared with the experimental data of Tregambi et al[5]. Our three-dimensional numerical simulations showed that a packed bed system with a wider incident radiative energy flux distribution increases the energy absorption by a packed bed. Our simulation also showed that multiple distributions of incident energy sources enhance the capacity of CSE energy storage in the system.

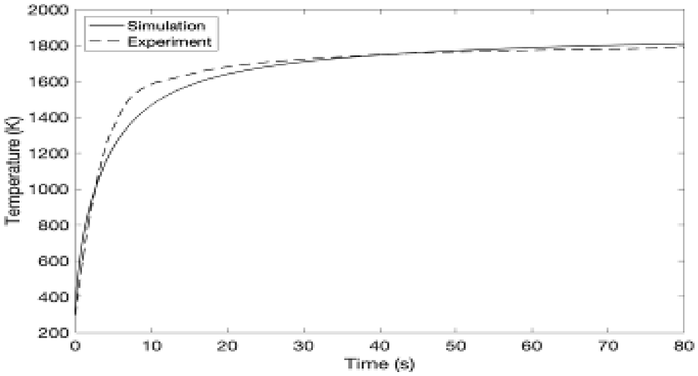
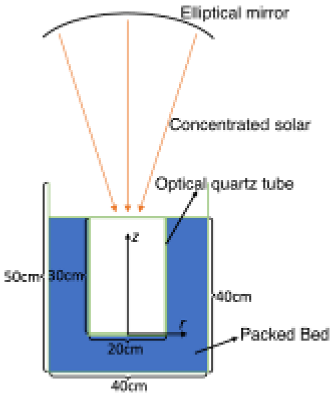


Figure 6: Comparison between simulation of the temperature of SiC at the center of the surface of the packed bed with the experimental data of Tregambi et al.

Furthermore, our numerical simulations showed that a packed bed with a novel design of an optical quartz tube (see Figure 7), where the radiative energy from the bed surface meets the surface of the optical tube at the center of the packed bed, results in additional distributed concentrated solar energy on the tube and an increase in energy absorption, storage capacity, and energy storage at higher temperature[6]. Figure 8 shows the comparison of the average temperature of the entire packed bed of SiC in the different cases. The average temperature of SiC of the packed bed with an optical quartz tube can exceed 500K at 4000 seconds, which potentially has several applications, including electric power generation and energy storage. Using a bubbling fluidized bed for CSE storage and energy recovery significantly reduces energy loss due to the lower surface temperature caused by convective energy transfer resulting from the mixing created by bubbles. The lower temperature on the surface significantly decreased the radiative energy loss from the surface to the environment.



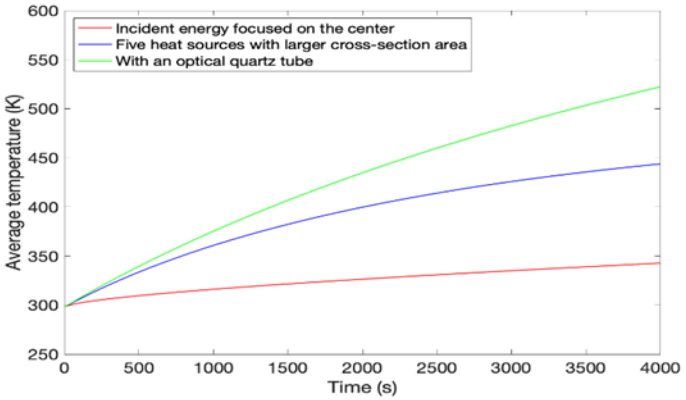


Figure 7: Schematic diagram of our novel packed bed with central optical quartz tube for CSE absorption and storage.

Figure 8: Comparison among simulations of average temperature in a packed bed with optical tube, five heat sources, and one heat source.

We developed a large-eddy simulation (LES) model and CFD model to simulate CSE absorption by a fluidized bed of silicon carbide (SiC). The results of the temperature profile of the SiC particle and corresponding volume fraction at 15 and 30 seconds after the incident CSE power of 254kW is turned on are shown in Figure 9. When the air flows into the fluidized bed, the air temperature immediately increases to approximately 1100K, equal to the initial SiC temperature, which causes the air expansion and the superficial velocity to become approximately 0.5m/s, which is about 40 times the minimum superficial velocity at that temperature[7].

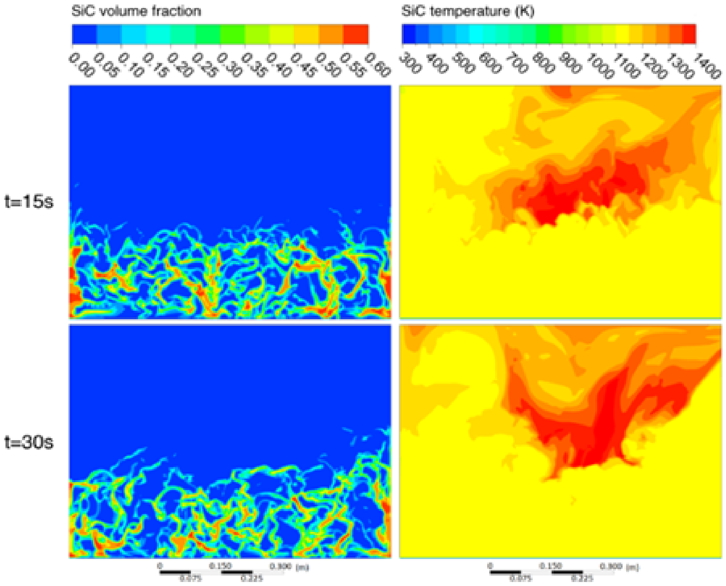


Figure 9: Temperature profile and corresponding volume fraction at 15 and 30 seconds after the incident CSE is turned on, under air inflow rate of 0.12kg/s and CSE power of 254Kw.

Production of Natural Gas from Hydrate Reserves

Natural gas from hydrates is extremely abundant as an energy resource: even the more conservative estimate of global resources is about 15 times the world's proven natural gas reserve. The challenge is that we must rely on modeling and numerical simulation of gas, hydrates, water, and solid particles to estimate the rate and extent of gas production from these unconsolidated hydrate reservoirs. Thus, we developed a four-phase flow model and numerical simulation to capture the unconsolidated flow of gas, water, hydrate, and sand. A solid viscosity constitutive model was developed to model the frictional and cohesive contributions to the solid shear stress[8]. Figure 10 (see next page) shows a simulation of the production of gas, water, and sand phases, and a comparison with the production data from the Mallik hydrate reserve. As can be seen from Figure 10, the prediction agrees well with the gas production data for this complex four-phase flow with phase change.

Concluding Remarks

Fluidization and particle technology have demonstrated the capability to make a major contribution to both the short- and long-term research and education components all of which is critical to the success of our pathway to a sustainable economy and society. The specific research and education contributions of fluid particle systems may include CO_2 capture and utilization, concentrated solar energy (CSE) storage, effect of rain and particulates on wind turbine performance, issues related to natural gas production from hydrate reservoirs, and material recycling.

- **There is no silver bullet to solve energy- and sustainability-related issues. These global issues are functions of location, time, technology, and lifestyle and require a paradigm shift in the way that we are currently thinking and living.**
- Although pursuing energy decarbonization and a net-zero carbon path is crucial, it also must be set in the wider context for sustainable growth, including water security, food availability, and human well-being. Critical inter-linkage of technical, economic, environmental, and societal factors is essential.

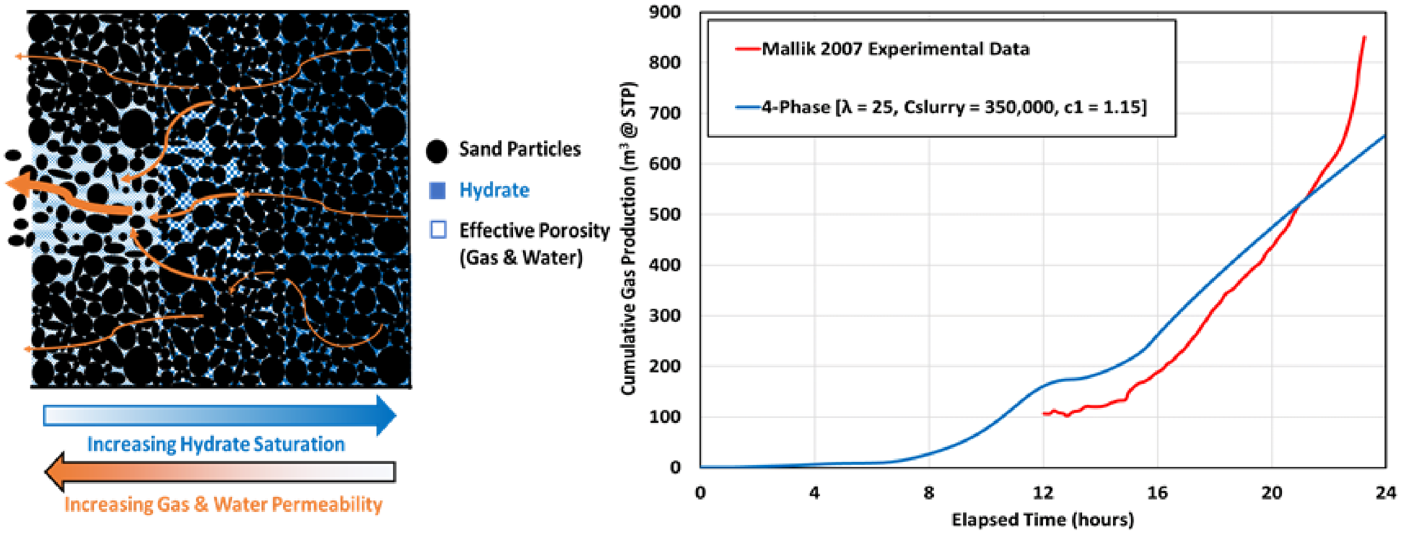


Figure 10: Simulation of the production of gas, water, and sand phases and comparison with the natural gas production data from the Mallik reserve.

References

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PTF Award Winners 2024

PSRI Fluidization and Fluid-Particle Systems Award

Dr. James Gilchrist

Ruth H. and Sam Madrid Professor

Chemical & Biomolecular Engineering

Lehigh University, Bethlehem, PA 18015

Email: gilchrist@lehigh.edu

Citation: For his research on granular mixing and segregation, rheology and microstructure of dense suspensions of complex particles, particle-based coatings, and scalable synthesis of janus particles

Dr. James Gilchrist is the Ruth H. and Sam Madrid Professor of Chemical and Biomolecular Engineering at Lehigh University. He directs the Laboratory for Particle Mixing and Self-Organization, focusing on research areas such as particle technology, rheology, transport phenomena, and interfacial science. His work has applications in active and nanostructured particle-based coatings for energy, optoelectronics, environmental engineering, and bioengineering. Dr. Gilchrist earned his B.S. in Chemical Engineering from Washington University in St. Louis and his Ph.D. from Northwestern University, where he studied chaotic mixing and segregation in granular materials under Julio M. Ottino. Before joining Lehigh University in 2004, he was a postdoctoral research associate in the Department of Materials Science and Engineering at the University of Illinois with Jennifer Lewis (now at Harvard University). Dr. Gilchrist served as chair of AIChE's Fluid Mechanics and Particle Technology Forum, and he is currently chair of AIChE's EBPC and sits on the executive committees of the International Society of Coating Science and Technology and the International Polymer Colloids Group. He was a visiting professor in the Department of Chemical Engineering at the California Institute of Technology for the 2011-2012 academic year and a Visiting Professorial Fellow at the University of New South Wales in 2016. His research group has published over 60 peer-reviewed articles and patents and has delivered more than 70 invited talks. His work has received continuous funding from the NSF since 2006, as well as support from the DOE, DoD, NASA, ACS PRF, and various state and local sources. Dr. Gilchrist has been honored with the North American Mixing Forum Young Faculty Award, the ACS PRF Doctoral New Investigator Award, and multiple Lehigh University accolades, including the 2024 P.C. Rossin College of Engineering Experiential Learning Excellence Award. In 2022, he was named a Fellow of the AIChE.

PSRI
Particulate Solid Research, Inc.

Sponsor of the Lectureship in Fluidization Award

Granular dynamics of magnetically responsive Janus particles with adjustable torque and friction

James F. Gilchrist
Ruth H. and Sam Madrid Professor of Chemical and Biomolecular Engineering
Lehigh University, Bethlehem, PA, USA

Our recent work on granular materials starts with a simple question: "Does the flow of field responsive particles with imposed torque exhibit classical granular mechanics and dynamics?" In the particle technology community, the answer is somewhat obvious when considering the large range of physical behavior exhibited by particulate matter whether the interactions are field driven or resulting from dissipation from potential energy through kinetic energy and friction in dense flows. At the same time, there are limited, semi-empirical descriptions of the rheology of dense flowing powders. These are primarily limited to freely flowing Geldart B that exhibit freely flowing grains and a minimal role of the interstitial fluid other than mediating the frictional contacts between particles. These flows dominate many pharmaceutical, chemical, food and agricultural, cosmetic, energy, and mineral and construction-related processes and natural systems of sand, silt, and soils. My doctoral research investigated mixing and segregation of granular materials[1–4], where complex pattern formation of segregating materials simply followed the underlying kinematics of the flow, even when chaotic advection dominated. My research moved on to nanoparticle self-assembly and suspension rheology and the science and engineering of granular mechanics moved on without me and I remained a passive observer of the field. Yet, I was instantly drawn back to this area on a day when members of my group, Dr. Samuel Wilson-Whitford and an undergraduate student, were manipulating a vial of magnetically-responsive particles we developed as a paint additive. When I heard them comment, "the particles look like they roll uphill when we rotate a magnet near them!" my own perspective of granular systems was shaken, and it opened a rabbit hole of unexplored physics and engineering[5].

Until recently, there has been surprisingly little overlap between the well-established granular mechanics field and the recent broad interest in active systems. Mechanics and the signatures of overarching non-equilibrium thermodynamic principles dominate both areas. Active systems, defined as those that inject and dissipate energy at the constituent scale, have been studied primarily in living systems, and synthetic mimics therein, such as suspensions of swimming microorganisms, mechanics of dense cellular clusters, and living polymers. The key difference between active and purely dissipative systems is the role of stress. Cells migrate under tension[6] and collective motion of swimmers can exhibit negative viscosity[7]. Energy is both expended and dissipated locally. At the intersection of passive and active systems are responsive systems that individually respond in a prescribed way and translate and dissipate energy at the constituent level in a directed manner. The system responds in a way that can collectively be considered an active system with emergent dynamics that are not simply field responsive. Emergent dynamics arise that mimic phase behavior and order found in soft condensed matter and occasionally thermodynamic principles can be loosely applied in general or semi-empirical ways.

The system presented in Fig. 1 is a dense system of ~50 mm PMMA particles having one hemisphere coated in 100 nm of iron that oxidizes into ferromagnetic iron oxide. These are "Janus particles", coined by Pierre de Gennes[8], comprised of two hemispheres of functionality and their use in our other applications have been published previously[9,10]. Many prior studies of magnetically-responsive systems consider wholly magnetic particles such as iron flakes with high coefficient of friction or core-shell μ systems of particles where a magnetic seed particle is coated in another material where magnetic dipoles are always separated. In water or ethanol and with no applied magnetic field, these Janus particles flow with a low coefficient of friction, μ, characterized by their angle of repose, θ, where the coefficient of friction is related to the ratio of shear stress, τ , and normal stress, σ , in the Mohr-Coulomb yield criterion, $\mu = \tau/\sigma = tan(\theta) + c/\sigma$, where c is the particle cohesion.

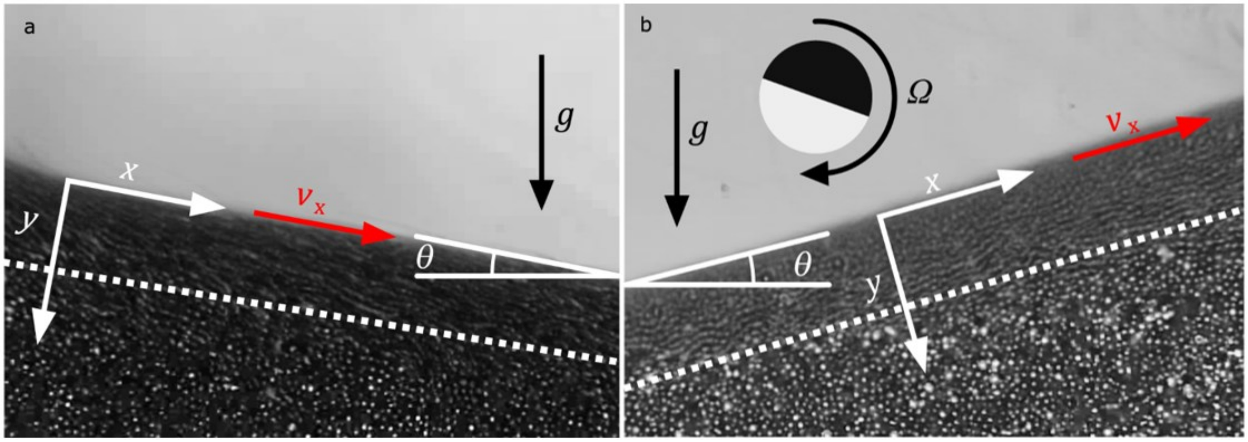

Fig. 1 (adapted from prior work[5]): a) Magnetically-responsive Janus particles flow under the influence of gravity with a characteristic angle of repose, θ , and near-surface flow. b) With an applied rotating magnetic field, these same particles spontaneously flow uphill as granular media with attenuated cohesion providing friction.

When a magnet is brought close to these particles, they have attractive forces that can generate a significant yield stress[11]. If these forces are mediated and the field is applied as to generate a torque on each particle, these particles spontaneously flow with kinematics that scale as granular materials. They flow uphill with a negative angle of repose and either eventually stagnate into a static pile or they have sufficient stress to fluidize. These systems have kinematics (Fig. 2) that scale with their maximum velocity, which increases with magnetic force,(β/β_0), where β_0 is the minimum magnetic strength to induce flow, and their shear rate, $\dot{\gamma}$. Their apparent negative angle of repose follows the Mohr-Coulomb yield criterion when cohesion, c , is a linear function of the magnetic force.

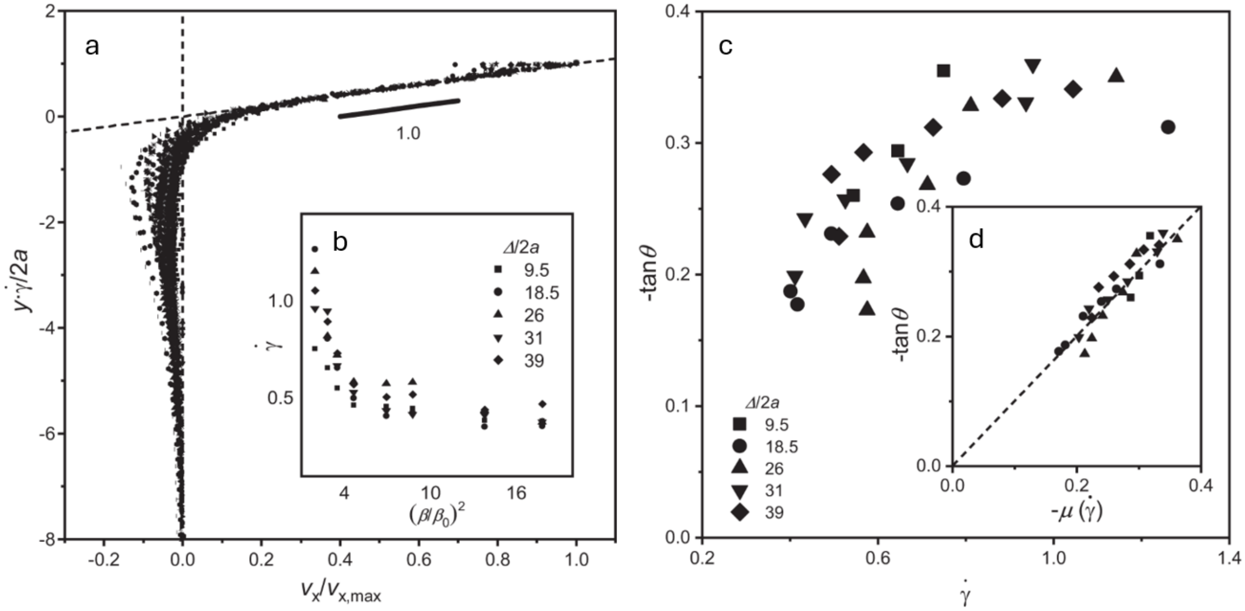

Fig. 2 (adapted from prior work[5]): a) The velocity profile of Janus particles flow under the influence of gravity scales with its shear rate and maximum velocity. b) The shear rate is a function of magnetic force, attenuated by the distance of the rotating magnetic field in multiple experiments varying the depth of the granular bed, Δ . c) The measured angle of repose, θ , depends on the shear rate and d) collapses when related to the coefficient of friction, μ (Υ) , using the Mohr-Coulomb yield criterion.

More details can be found in our original paper[5], however the question that remains is, "*What is the larger implications of designing granular media having magnetically responsive flow?*" This breaks the paradigm of controlling granular flows through their boundary conditions in chutes, funnels, rotating drums, screw conveyors, vibration, and through fluidization. Yet, as demonstrated above, the rules of granular physics remain in responsive granular flows. Several examples are easily demonstrated in classic and non-classic driven systems:

Funnel flow (Fig. 3a): An hourglass is a universal timekeeping device, delivering material at a constant flow rate unless jamming occurs. Gravity-driven flow in funnels and chutes are the primary modes of powder transport and delivery in industry. Below, we demonstrate three modes of flow in a simple funnel. The left image is passive flow of the granular media, demonstrating the formation of a rat hole where most material remains relatively undisturbed at the edges of the orifice. The center and right images show the impact of imparting torque on the particles, either directing them to roll toward the center or all roll to the right. In the same amount of time, flow directed toward the center has completely emptied the funnel and flow directed to the right shows clear anisotropy to how the funnel empties, also resulting in imperfect flow delivery. The local particle-induced fluidization empties material at a faster rate than the simple gravity flow. Various protocols can be added, such as directing alternating rolling directions during funnel flow to enhance mixing and altering local residence times through the orifice.

Climbing stairs (Fig. 3b): As demonstrated in Fig. 1b, heaping flow uphill results from the applied torque. This flow will move uphill as long as the boundary underneath it at an angle lower than the resulting negative dynamic angle of repose. Similarly, experiments have demonstrated transport up staircases to use less material to heap and transport to desired heights. The particles pile locally against each step boundary and overcome the steps when sufficient material has been delivered to the step. This ability to overcome obstacles is useful for delivery in complicated geometries with less material than filling a larger cavity, yet it remains limited by the material angle of repose.

Segregation (Fig. 3c): It is well-known that granular media spontaneously segregates when flowing[3,12]. The interplay between the flow kinematics and segregation are nontrivial. Janus particles (black) mixed with non-responsive and slightly less dense particles (white) flow, partially mix, and undergo segregation. These flows also demonstrate signatures of instabilities similar to Kelvin-Helmholtz waves that occur when fluids having density gradients undergo sheer.

Swarming (Fig. 3d): With the goal of utilizing collective granular dynamics of micro-rollers for robotic systems of drug delivery or transport[13], directing collective motion of particles proves to be relatively straightforward once the principles of granular flow are applied. Janus particles are readily concentrated into localized swarms by designing rotating magnetic field have locally stable eigenvalues that act as local sinks. The concentrated particles move collectively faster than a single roller and can be re-swarmed to new locations, moved unidirectionally, or combined with more complex architecture, such as 3D printed walls or vasculature where they collectively move along the wall. Understanding the rules of the road of these systems is only possible with an understanding of granular kinematics. Machine learning and phenomenological models readily capture their behavior.

In summary, there are deeper levels of understanding still necessary in the prototypical systems of passive granular systems, including how stress is dissipated and how constitutive equations can be developed to capture segregation, intermittency, and structural heterogeneity. Yet, this system provides a new perspective that not only will have its own applications in robotics and microscale transport for a wide variety of applications but also give new insights into passive systems and how to design new approaches to manipulate granular matter. Our community can use systems like these to push our understanding of particulate matter, train the next generation of students, and find new and exciting applications that inherently use our common understanding of granular dynamics. I openly invite collaborations with those who may have ideas of new applications, new ways of using these particles for fundamental studies, or simply wish to have samples of these particles to manipulate for your own studies.

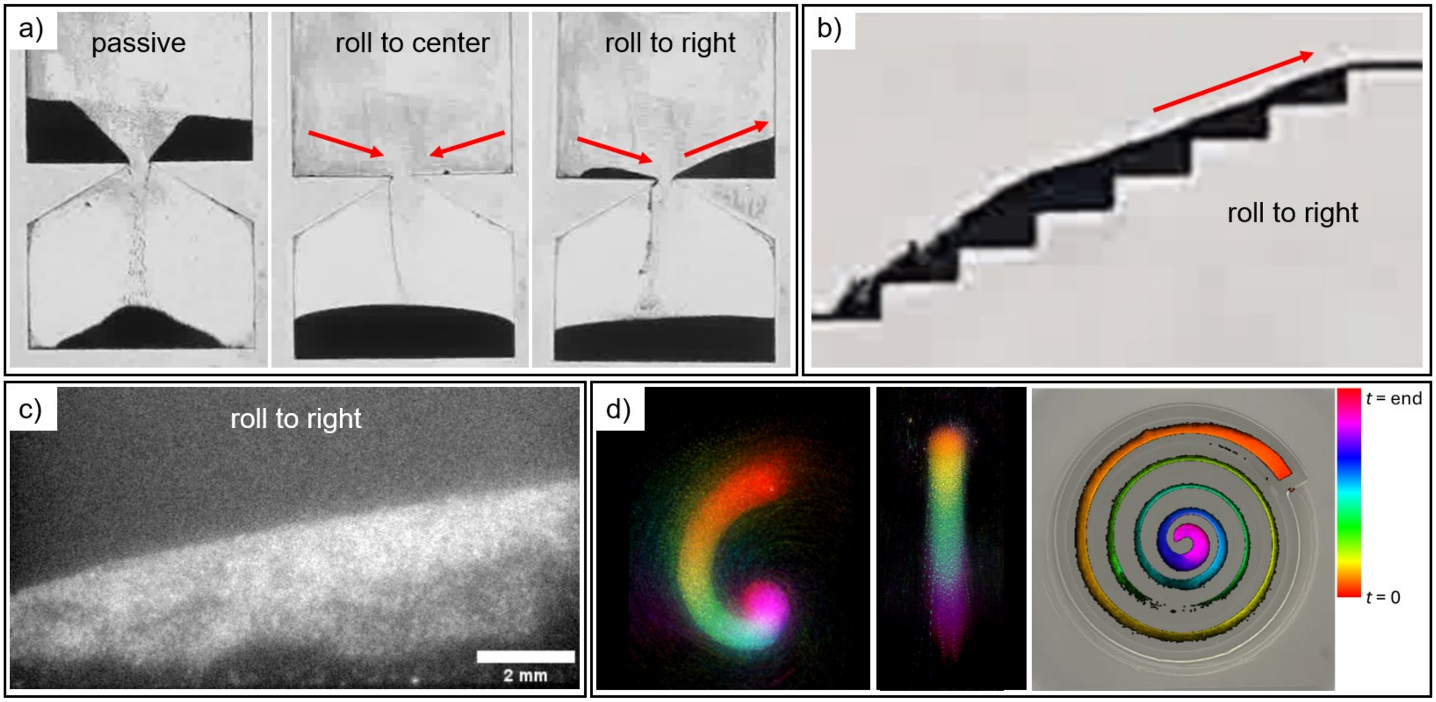

Fig. 3: a) The gravity-driven flow through an orifice results in stagnant material common in granular systems unless the microrollers are magnetically actuated to roll toward the orifice. b) Uphill flow of microrollers is aided by climbing stairs, leaving material behind that helped convey material to the upper levels. c) Passive, unfunctionalized particles (white) spontaneously undergo mixing and segregation with microrollers (black) of the same core material. A mixing layer forms where the black, more dense particles driving the flow create greater degrees of mixing with stronger friction imparted through magnetic attractions. d) Swarms of particles form when the field has a local sink. These swarms are more readily transported to different locations through swarming, unidirectional flow, and can be manipulated by walls architected to take advantage of the microroller field-directed flow (color is time from the initial condition to the final condition).

Acknowledgements

The landscape of science and engineering has changed greatly since receiving this award. All research herein was discovered by, inspired by, and performed by the students and early career researchers supported by federal funds. We are grateful to prior funding from the National Science Foundation and the Johns Hopkins Applied Physics Laboratories supporting this science, education, and discovery. Original work on responsive granular flows[5] was performed by Dr. Samuel Wilson-Whitford, Dr. Jinghui Gao, and Dr. Maria Chiara Roffin. The undergraduates in my lab that have contributed to creative demonstrations and applications of this system include W. Buckley, D. Kramer, M. Sisca, B. Sauder, C. Cui, M. Enan, A. Oh, G. Powell, J. Riffle, T. Richarson, O. Percaccio, K. Weis, E. Kore, A. Donnelly, G. McKinley, and N. Tobin, primarily supported through Lehigh University's Mountaintop Summer Experience. Special thanks to Julio Ottino, Richard Lueptow, Jennifer Lewis, Devang Khakhar, and Hugo Caram who have been incredible mentors in my academic career.

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Key Research Areas: Particle Technology, Fluid Mechanics, Suspensions, Complex Fluids, Rheology, Granular Media, Coatings, Mixing, Convective Deposition

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PTF Award Winners 2024

Shell Thomas Baron Award In Fluid-Particle Systems

Dr. Carlos M. Rinaldi-Ramos

Department of Chemical Engineering and J. Crayton
Pruitt Family Department of Biomedical Engineering,
University of Florida, Gainesville, FL 32611
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Citation: For outstanding contributions in ferrohydrodynamics, nanoparticle characterization, thermal cancer therapy using magnetic nanoparticles, and magnetic particle imaging, advancing particle technology with groundbreaking research and mentoring.

Dr. Carlos M. Rinaldi-Ramos is the Chair and Dean's Leadership Professor in the Department of Chemical Engineering and a Professor in the J. Crayton Pruitt Family Department of Biomedical Engineering at the University of Florida. He was born and raised in Puerto Rico, receiving his Bachelor of Science degree in Chemical Engineering from the University of Puerto Rico, Mayagüez in 1998. He completed degrees in Master of Science in Chemical Engineering (2001), Master of Science in Chemical Engineering Practice (2001), and Doctor of Philosophy (2002) in Chemical Engineering at the Massachusetts Institute of Technology. Prior to the University of Florida, Dr. Rinaldi-Ramos was a Professor in the Department of Chemical Engineering at the University of Puerto Rico, Mayagüez from 2002 to 2012.

Dr. Rinaldi-Ramos is a leading scientist in the areas of fluid dynamics and colloidal hydrodynamics of magnetic nanoparticle suspensions (ferrofluids) and biomedical applications of magnetic nanoparticles. His research spans theory and simulation of magnetic nanoparticle response to dynamic magnetic fields, nanoparticle synthesis, and surface modification, characterization of nanoparticle interactions with biological environments, and studies to advance their biomedical applications. In the field of ferrofluids, Dr. Rinaldi-Ramos has made fundamental contributions to the understanding of suspension-scale flows of magnetic nanoparticles in time-varying and rotating magnetic fields. Through a combination of theoretical and experimental work, his group demonstrated that the description of ferrofluid flows in rotating magnetic fields requires consideration of internal angular momentum transport through the so-called couple stress and spin viscosity which are unique features in the description of flows of structured continua. In the field of nanomedicine, Dr. Rinaldi-Ramos has made outstanding contributions to harnessing localized nanoscale heating for magnetic nanoparticle thermal cancer therapy. Dr. Rinaldi-Ramos has pioneered the development and application of new methods to evaluate nanoparticle stability and diffusion in complex and biological fluids. Based on non-invasive monitoring of nanoparticle response to oscillating magnetic fields, these methods permit quantitative measurements of nanoparticle aggregation state, hydrodynamic size, and diffusion in complex environments such as polymer melts, polymer solutions, highly concentrated protein solutions, whole blood, and tissues. More recently, Dr. Rinaldi-Ramos has contributed to understanding the physics of magnetic nanoparticle response to alternating magnetic fields, enabling rational design of high-sensitivity and high-resolution tracers for magnetic particle imaging, an emerging biomedical imaging technology.

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Thomas Baron Award

A Magnetic Journey from Ferrofluids to Biomedical Imaging

Carlos M. Rinaldi-Ramos
Dean's Leadership Professor and Chair of Chemical Engineering and
Professor of Biomedical Engineering at the University of Florida

I was humbled and honored to receive the Shell Thomas Baron Award in Fluid Particle Systems at the 2024 Annual Meeting of the American Institute of Chemical Engineers. However, I had a very difficult time writing this perspective article. I don't usually spend time dwelling on my past work, so to find inspiration for this short article I read perspectives from past distinguished recipients. I truly resonated with past awardee Mark Swihart, who stated that "[t] his award is the result of the creative efforts of dozens of students … who have carried out the work that was recognized." That sentiment deeply aligns with my own experience. As an academic and educator, I believe that guiding students to become independent researchers is a profound privilege. Although I enjoy the thrill of scientific discovery, I find it even more rewarding when it is part of helping trainees learn and grow. . In addition to mentoring students, I see my role as a steward of public investment in science and technology, especially through Federal grants that support university research aimed at advancing knowledge and addressing societal needs. I therefore feel truly grateful and privileged to share some of the work I've conducted with many wonderful students, postdocs, and collaborators over the past 26 years thanks to generous Federal support from the National Science Foundation (NSF) and the National Institutes of Health (NIH), among other funding sources.

Foundations in Ferrofluids

Ferrofluids are stable suspensions of superparamagnetic nanoparticles. Despite containing 1-10% by volume of magnetic material, these fluids remain liquid and responsive to magnetic fields. This responsiveness manifests in visually arresting ways, such as the well-known normal field, or "spiking", instability governed by the interplay between surface tension and magnetic forces.[1] My introduction to ferrofluids came as a first-year graduate student at MIT, inspired by a talk from Alan Hatton on using suspensions of magnetic nanoparticles for contaminant separation. In it, he showed how magnets could be used to drive the motion of ferrofluids while controlling interfacial area for contaminant transport. I eventually joined the lab of Howard Brenner, whose theoretical interest in polarizable materials led me to explore structured continua and rotational flows induced in ferrofluids by rotating magnetic fields. My first and only paper published with Howard explored the potential physical consequences of replacing volumetric electromagnetic forces using the so-called Maxwell stress tensor and argued that such replacement, while convenient mathematically, could lead to erroneous calculations of rates of work and energy dissipation in polarized continua.[2] This was followed by work with Markus Zahn, who taught me continuum electromechanics, which led to applying perturbation methods to understand so-called spin-up flows in ferrofluids that arise due to transfer of internal angular momentum of the sub-continuum particles to bulk rotational motion.[3, 4] As a graduate student I enjoyed using analytical and approximation techniques to solve problems combining linear and internal angular momentum with Maxwell's equations in the magnetoquasistatic limit. However, as I approached graduation I increasingly wondered whether these models held any relation to physical reality. Howard once told me that to be a good theoretician, one must understand experiments. This motivated me to spend time in Alan Hatton's lab learning about ferrofluid synthesis and experiments from friends and colleagues, including Lino Gonzalez, Geoff Moeser, and Seyda Bucak.

Bridging Theory and Experiment with Ferrofluids

Upon starting my faculty career at the University of Puerto Rico at Mayagüez (UPRM), I found it difficult to recruit students to continue theoretical in ferrohydrodynamics. My first talk to new graduate students had 15 slides – a title slide, 13 slides full of equations, and one slide with cartoons depicting potential applications in magnetically targeted drug delivery, magnetic nano-biosensors, and magnetic hyperthermia treatment, all of which could be explained using the equations in the preceding slides. Days later, two graduate students approached me about joining my group, however, neither was interested in theoretical work. Instead, they wanted to work on the applications I described in my last slide. I am glad I listened to these two students and took the risk of pivoting from theoretical work to bridging theory and experiment. I am also grateful these two students, Adriana Herrera-Barros and Victoria Calero-Diaz del Castillo, took the risk of becoming my first two graduate students.

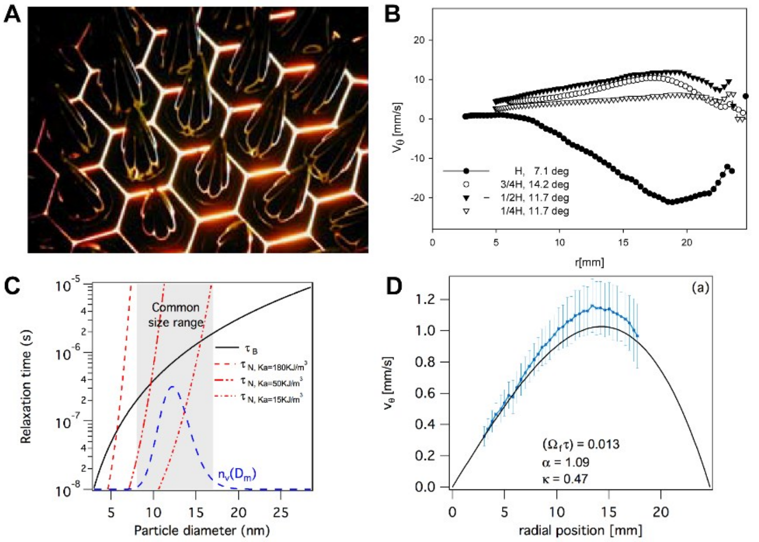

Figure 1. A. Normal field ("spiking") instability in a ferrofluid.[1] **B.** Bulk velocity measurements at various height in a ferrofluid cylinder subjected to a rotating magnetic field.[7] The positive flow direction qualitatively agrees with spin-up flow model. Flow at the top of the cylinder, near the free surface (H) is counter rotating with the applied magnetic field. **C.** Dependence of Brownian (τ_B) and Neel (τ_N) relaxation times on particle size for nanoparticles with different magnetocrystalline anisotropy constants (K_a), and illustration of typical size distribution in a ferrofluid.[10] **D.** Quantitative agreement between spin-up flow model and experiments for a cobalt ferrite ferrofluid.[10]

Being at a primarily undergraduate institution with relatively low research activity and a chemical engineering PhD program that had just started the year before, our research focused on fundamental understanding of the response of suspensions of magnetic nanoparticles to dynamic, time-varying magnetic fields, as this understanding was critical to emerging applications. Our initial goal was to synthesize iron oxide magnetic nanoparticles of controlled size with which to test basic models of their behavior. This was 2002 and there was already a deep literature on the synthesis of magnetic nanoparticles. Naively, we thought this should be the easy part of our work. However, there was only one transmission electron microscope and there were no dynamic light scattering instruments or magnetometers in Puerto Rico at the time. Additionally, UPRM did not offer startup packages, and we could barely purchase the chemicals needed to synthesize nanoparticles, much less have the means to characterize them! Fortunately, in 2003 I secured a NSF grant to acquire the first superconducting quantum interference device (SQUID) magnetometer in Puerto Rico. This was followed by seed funding through the Puerto Rico NSF Experimental Program to Stimulate Competitive Research (EPSCoR), two small grants from the NSF and one from the American Chemical Society Petroleum Research Fund (ACS PRF) to study ferrofluid flows, and eventually the NSF CAREER award in 2006. With this funding, I was able to acquire key instrumentation and recruit additional students to study ferrofluid flows in uniform and non-uniform rotating magnetic fields, theoretically and experimentally. This work demonstrated that the description of ferrofluid flows in rotating magnetic fields requires consideration of the transport of internal angular momentum through the so-called couple stress and associated spin viscosity, carried out with Arlex Chaves Guerrero[5-9] and Isaac Torres Diaz.[10-14] Initially, we could only achieve qualitative agreement between theory and experiment, and this is where our initial focus on nanoparticle synthesis and characterization[15-21] paid off. We realized that only a small fraction of the iron oxide nanoparticles in typical commercial ferrofluids responded to the rotating magnetic fields by particle rotation, instead of internal dipole rotation, a pre-requisite to driving bulk rotational flow in a rotating magnetic field. This led Isaac to formulate cobalt ferrite ferrofluids, wherein all nanoparticles respond to rotating magnetic fields by particle rotation which resulted in quantitative agreement between theory and experiments.[14] With Darlene Santiago, we extended this work to study the magnetorheology of magnetic nanoparticles suspended in liquid crystals and other surfactant solutions.[22-24] Additionally, after a summer in Juan J. de Pablo's group at the University of Wisconsin at Madison, Jorge H. Sanchez and Denisse Soto Aquino used Brownian dynamics simulations to further explore the colloidal hydrodynamics of spherical and non-spherical nanoparticles in time-varying magnetic fields.[25-32]

Toward Biomedical Applications

Although my PhD work focused on theoretical transport phenomena, I had always been fascinated by the interface between engineering, biology and medicine. The superparamagnetic nature of iron oxide nanoparticles, resulting in exceptionally high magnetic susceptibility and nonlinear dynamic response at technically feasible magnetic field amplitudes, enables imaging and actuation capabilities not possible with other materials. This unique response, coupled with their biocompatibility, has opened the door to a variety of diagnostic and therapeutic technologies, including magnetic resonance imaging contrast agents, immunomagnetic separations, magnetically controlled drug carriers, and magnetic hyperthermia. With additional support from the NSF and from the NIH, and with my long-time friend and collaborator Madeline Torres-Lugo, we pursued research in biomedical applications that rely on magnetic nanoparticle response to time-varying magnetic fields. With Adriana Herrera Barros, Carola Barrera Cuadro, Lenibel Santiago Rodriguez, and others, we formulated nanoparticles with exceptional colloidal stability in biological environments and that can transform the energy of alternating magnetic fields into heat,[15, 18-20, 33-39] which Mar Creixell Turon and Angelie Rivera-Rodriguez from my group, as well as others from Madeline's group (Hector Luis Rodriguez Luccioni, Merlis Alvarez Berrios), leveraged to study hyperthermia cancer treatment.[40-47] Of note, Mar demonstrated how receptor mediated uptake of targeted magnetic nanoparticles could be leveraged to kill >99% of cancer cells through intracellular heating and without a perceptible temperature rise[43] and Maribella Domenech showed that this phenomenon arises from disruption of nanoparticle-loaded lysosomes, activating lysosomal death pathways that are upregulated in many cancer cells.[48] Further evidence of nanoscale heating phenomena was provided by Liliana Polo Corrales, who demonstrated thermal transitions of thermosensitive polymers grafted on the surface of magnetic nanoparticles in response to alternating magnetic fields while the bulk temperature remained below the polymer's transition temperature.[49]

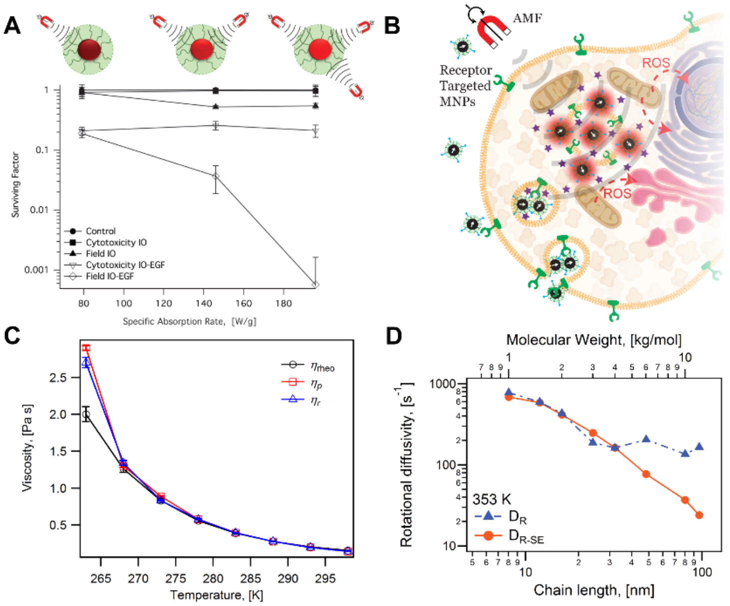

Figure 2. A. Cancer cell killing, expressed as surviving factor, induced by nanoscale heat dissipation by magnetic nanoparticles.[43] The condition Fild IO-EGF corresponds to receptor targeted nanoparticles that dissipate heat in the presence of an applied magnetic field. No bulk temperature rise was observed. **B.** Putative mechanism of cell death via lysosomal membrane permeabilization by internalized nanoparticles. **C.** Quantitative agreement between nanoscale viscosity (η_p and η_r) estimated from DMS measurements of cobalt ferrite nanoparticles suspended in mineral oil and viscosity determined from bulk rheology (η_{rheo}).[62] **D.** Deviation between experimental rotational diffusivities determined from DMS measurements (D_R) and the predictions based on the Stokes-Einstein equation (D_{R-SE}) for cobalt ferrite nanoparticles in PEG melts.[68]

Additional synthesis and formulation work was carried out by Roberto Olayo Valles, Melissa Cruz Acuña, and Eric Fuller, who developed magnetically controlled nanoparticle drug and nucleic acid carriers,[50-54] Andrew Garcia, Ishita Singh and Victor Rivera-Llabres, who formulated magnetic alginate microparticles to produce tissue engineering scaffolds through magnetic templating,[55-57] and by Andreina Chiu Lam, who formulated nanoparticles with exceptional colloidal stability in cryopreservation agents suitable for long-term cryobanking and rapid nanowarming of cryopreserved organs.[58] John A. Medford and Jeremiah Hubbard extended our hyperthermia work to non-biomedical applications in magnetothermal repair and curing of polymer nanocomposites.[59, 60] Further, with the ability to synthesize magnetic nanoparticles with controllable relaxation mechanisms and exceptional stability in complex and biological fluids, coupled with our understanding of their colloidal hydrodynamics in alternating magnetic fields, and with additional support from the NSF, we leveraged dynamic magnetic susceptibility (DMS) measurements to study nanoparticle stability and diffusivity in complex and biological fluids. The intracellular environment can be described as crowded, complex, and confined, wherein biomacromolecules with characteristic dimensions of 1-10's of nm are present at high concentration, and where membranes, organelles, and filamentous matrices restrict motion. Although important in designing nanoparticles for biomedical applications, understanding of the transport of nanoparticles in such environments remains limited. Early work by Victoria, Adriana and Carola had already demonstrated how DMS measurements of cobalt ferrite nanoparticles could be used to monitor nanoparticle stability and measure viscosity at the nanoscale,[61-63] laying the groundwork for future studies in other complex and biological fluids. Edwin de la Cruz and Sergio Sierra studied synthesis and nanoparticle dispersion and stability in polymer composites,[64-67] while Lorena Maldonado studied nanoparticle rotational diffusion in polymer solutions and melts,[68, 69] Rishit Merchant studied nanoparticle rotational diffusion in emulsions,[70] and Ana C. Bohorquez and Mythreyi Unni studied nanoparticle diffusion and stability in concentrated protein solutions, whole blood, and in tissues *ex vivo*.[71-74] Of note, Lorena demonstrated that nanoparticle rotational diffusion is faster than expected from the Stokes-Einstein equation when nanoparticle hydrodynamic radius is smaller than the radius of gyration of free polymer in polymer solutions and when it is smaller than the chain length of free polymers in melt,[68, 69] while Mythreyi demonstrated that nanoparticle rotational and translational diffusion in hyaluronic acid solutions and in whole synovial fluid are orders of magnitude faster than expected from the Stokes-Einstein equation.[74]

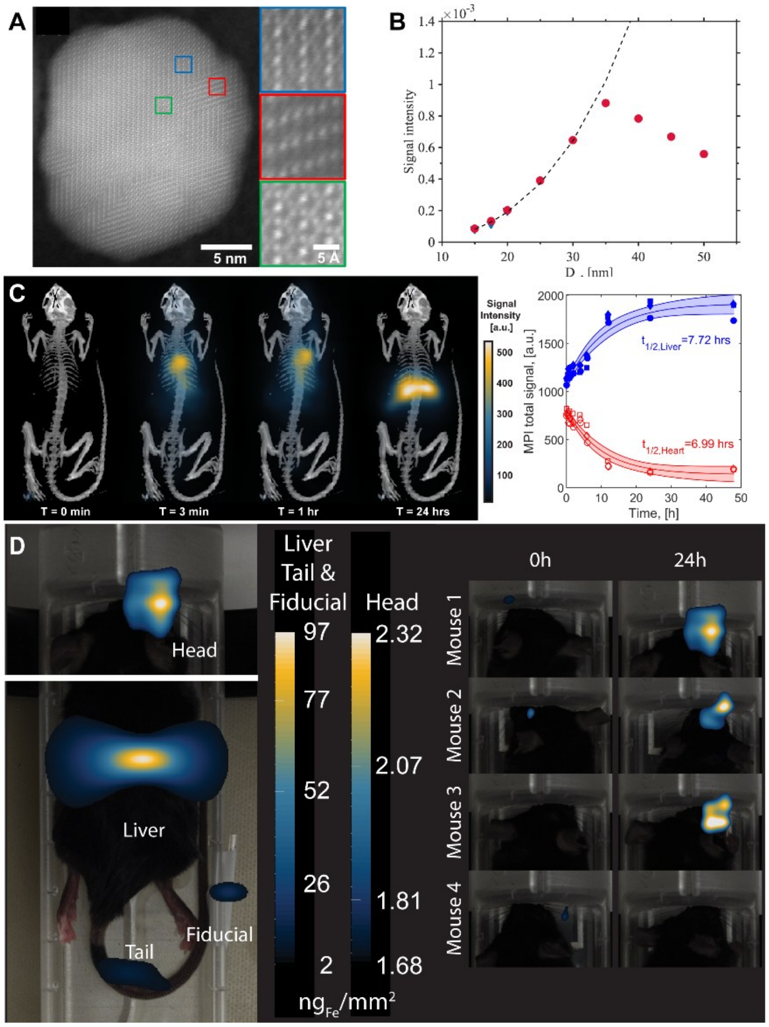

Figure 3. A. Neatly defect free iron oxide nanoparticles synthesized via thermal decomposition in the presence of molecular oxygen.[82] **B.** Computational predictions, based on the Landau-Lifshitz-Gilbert mode, of particle size dependence of MPI signal intensity.[79] **C.** Monitoring nanoparticle blood circulation and tumor accumulation using MPI.[86] **D.** Tracking adoptive T cell transfer brain cancer immunotherapy using MPI.[85]

Engineering Better Tracers

My lab is currently focused on advancing tracers for and developing applications of magnetic particle imaging (MPI), an emerging molecular imaging modality that enables non-invasive, tomographic, unambiguous, sensitive, and quantitative imaging of the distribution of magnetic nanoparticles in living subjects. MPI signal is not attenuated by tissue and arises solely from exogenous iron oxide nanoparticles that are biocompatible and biodegradable. While MPI is relatively new, rapid progress towards clinical translation is taking place and there is much excitement over applications in blood pool and molecular imaging. Initially, without access to MPI scanners, NIH and NSF supported computational work by Rohan Dhavalikar and Zhiyuan Zhao, who used Brownian dynamics and the stochastic Landau-Lifshitz-Gilbert equation to evaluate the effects of particle size, magnetocrystalline anisotropy, relaxation mechanism and rate, and particle-particle interactions on their MPI performance.[75-81] In collaboration with MPI pioneers Steven Conolly and Patrick Goodwill at the University of California Berkeley, we tested these theoretical predictions against MPI measurements.[75] Mythreyi Unni developed new tracer synthesis techniques that yielded nearly defect free nanoparticles with enhanced MPI performance and magnetic heating capabilities.[82] Also, in collaboration with Conolly and his PhD student Zhi Wei Tay, we demonstrated the use of MPI in combination with heat release from magnetic nanoparticles to achieve image-guided and spatially selective cancer thermal therapy, using particles synthesized by Andreina Chiu Lam.[83] Then, also in collaboration with Conolly and Zhi Wei, we demonstrated that strong particle-particle magnetic interactions within nanoparticle chains allow unprecedented high resolution MPI, using nanoparticles synthesized by Shehaab Savliwala.[84]

While this work was exciting to us, the lack of MPI hardware at the University of Florida was limiting our ability to work. This changed in 2019, when we acquired one of the first MOMENTUM™ MPI scanners from Magnetic Insight, Inc., thanks to support from the Herbert Wertheim College of Engineering and the J. Crayton Pruitt Family Department of Biomedical Engineering. With it, Angelie Rivera-Rodriguez was the first to demonstrate the potential of MPI for in vivo quantitative tracking of adoptive T cell transfer cancer immunotherapy,[85] work that eventually led to my first R01 from the NIH, aimed at developing novel tracers for highly sensitive tracking of T cell cancer immunotherapies, in collaboration with Duane Mitchell at UF. This was followed by work by PhD students Sitong Liu, Andreina, and Angelie, who demonstrated how our high-performing MPI tracers could be formulated as long-circulating blood pool imaging agents.[86] Further work explored a variety of MPI tracers. Nathanne C. Rost evaluated magnetoliposomes as MPI tracers,[87] Eric Fuller formulated theragnostic nanocarriers combining high drug loading and MPI signal,[52] Sitong Liu produced dual-imaging agents combining MPI signal and computed tomography (CT) contrast,[88] Victor Rivera-Llabres formulated microparticle MPI tracers,[89] and current PhD candidate Ambar C. Velazquez-Albino explored the influence and reproducibility of post-synthesis treatments to enhance MPI performance.[90] As we learned to use the MPI scanner we became interested in robust approaches to signal analysis and tracer quantification. Nicole Sarna, Leyda M. Marrero, and Ryan deGroff led the development and testing of 3D-printed mouse phantoms with anatomically correct cavities and that allowed us to test MPI measures of tracer mass against ground truth.[91] In collaboration with Paula Foster and her PhD student Olivia Sehl, Hayden Good conducted an inter-user and inter-laboratory comparison of MPI quantification approaches, demonstrating comparable quantification accuracy when well documented acquisition and analysis protocols were followed.[92] Hayden later reported the first comprehensive study of the effect of object size on MPI signal distribution, and its analogy to the partial volume effect (PVE) observed in nuclear imaging.[93] More recently, Eric Daniel Imhoff has reported a comparative study of commercially available MPI tracers, with associated comprehensive magnetic and MPI performance characterization with the goal of providing benchmarking data for others in the field.[94] Finally, soon we expect to report on studies demonstrating sensitive and quantitative *in vivo* tracking of T cells, by Angelie Rivera-Rodriguez, and of dendritic cells, by Bo Yu, imaging of brain bleeds due to traumatic brain injury, by Hayden Good, and longitudinal quantitative tracking of nanoparticle lymph node transport, by Esteban Bermudez-Berrios.

Looking Ahead

With significant institutional strengths in engineering, chemical and physical sciences, pharmacy, veterinary medicine, and medicine, UF offers a unique environment supporting research at the interface between engineering and medicine. I am excited to work with trainees and collaborators at UF and beyond to achieve the tremendous potential of biomedical applications of magnetic nanoparticles. MPI related research at UF is highly interdisciplinary. For example, we are leveraging MPI to track adoptive cell transfer cancer immunotherapies Duane Mitchell (Neurosurgery),[85] we are evaluating the use of MPI to track clearance of intraarticular drug carriers with Blanka Sharma and Kyle Allen (Biomedical Engineering),[95-97] we are using MPI to assess traumatic brain injury with Lakiesha Williams (Biomedical Engineering) and Marcelo Febo (Neuroscience), and we are exploring other applications in the treatment of cancer and neurodegenerative diseases with Elias Sayour (Neurosurgery), Leighton Elliott (Hematology & Oncology), and Vinata Vedam-Mai (Neurology). This activity puts UF at the forefront of formulating MPI tracers optimized for sensitivity and resolution, multi-modal imaging, cell tracking, and theragnostics. I consider myself extremely lucky because these exciting applications are enabled by the unique response of magnetic nanoparticles in alternating magnetic field, a topic that has fascinated me since my days as a PhD student.

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PTF Award Winners 2024

SABIC Young Professional Award

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Citation: Aerosol reactor design and nanoparticle multiscale simulation, for optimization of particle synthesis and scale-up for applications in catalysis, and energy storage.

Dr. Eirini Goudeli is a Senior Lecturer (Assistant Professor) in the Department of Chemical Engineering and leads the Laboratory of Aerosol and Particle Technology at The University of Melbourne. She received her PhD from ETH Zurich, Switzerland (2016) and carried out postdoctoral research at The University of Minnesota (2017-2018) before joining The University of Melbourne.

Her research program focuses on the design of nanoparticles during aerosol synthesis for catalysis and energy applications integrating detailed multiscale modeling of particle formation and growth in aerosol reactors. She has published 48 papers in leading scientific journals and has received funding from both government and industry. Her contribution in aerosol science and nanoparticle technology has been recognized by numerous prestigious awards, including the 2020 Selby Research Award, the 2018 Inaugural GAeF (German Association for Aerosol Research) Award for Outstanding PhD in Aerosol Science and the 2016 ETH Medal for Outstanding PhD Thesis.

She has served as the Chair and Co-Chair of the Nanoparticle Division (Area 3D) of the Particle Technology Forum. She is Executive Editor of the *Aerosol Research* journal and an early-career editorial board member of the *Journal of Aerosol Science*.

Sponsor of the
Young Professional Award

Aerosol reactor design and nanoparticle multiscale simulation, for optimization of particle synthesis and scale-up for applications in catalysis, and energy storage

Eirini Goudeli
Department of Chemical Engineering, The University of Melbourne, Australia

Nanoparticles are synthesized globally at millions of tons annually in high-temperature, gas-phase flame reactors, serving a range of applications—from tire reinforcements to cosmetics and catalysts. As the nanotechnology industry approaches a projected market size of $289 billion by 2030, engineered nanomaterials have emerged as its backbone, constituting 80% of the industry's revenue. Innovations in aerosol synthesis and other synthetic processes have significantly enhanced our understanding of nanoparticle properties. This knowledge has spurred the development of materials with specific functionalities, enhancing their utility and performance across various applications. The rise of startups and spinoffs like HeiQ, TurboBeads AG, Hemotune AG, and Alivion AG, showcases the transition from innovative aerosol synthesis techniques to high-market value products, highlighting the critical role of nanoparticle quality in scaling production and integrating new products.

Understanding nanoparticle properties through advancements in aerosol synthesis has led to optimized material functionalities, enhancing performance across various applications. The process complexity of nanoparticle production spans a vast range of length/time scales, from atomic-level interactions to macroscopic phenomena, demanding a multiscale approach to model these systems. Integrating models across different scales, from density functional theory (DFT) and molecular dynamics (MD) to mesoscale simulations (e.g., discrete element method, DEM) and continuum models (e.g., computational fluid dynamics, CFD), lays a solid foundation for establishing detailed structure-property relationships essential for material innovation (Figure 1a).

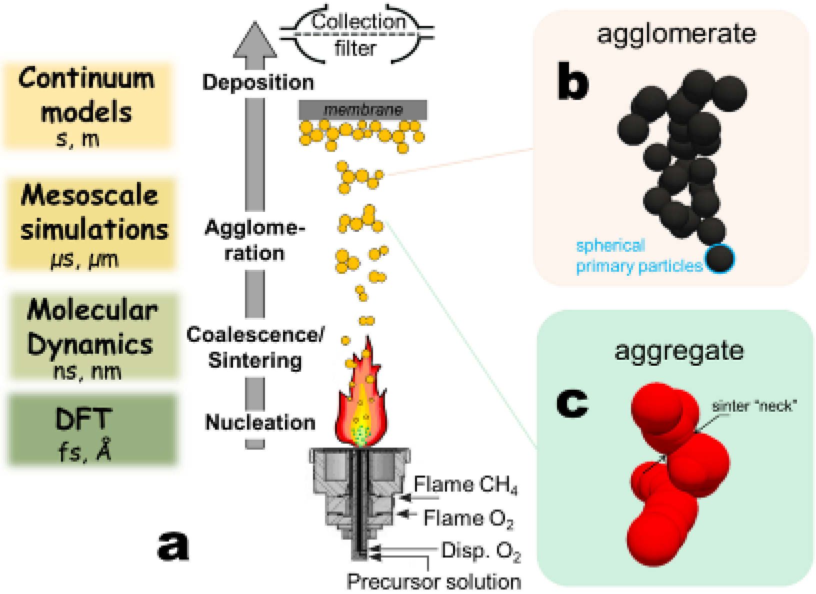


Figure 1. (a) Schematic representation of nanoparticle production by flame spray pyrolysis. The mechanisms at different stages of nanoparticle growth can be modeled by hierarchical modeling, encompassing quantum mechanics calculations (e.g., DFT), molecular dynamics, mesoscale simulations, and continuum models. (b, c) Fractal-like particles of different structures are formed in flames depending on process conditions.

Aerosol reactor design by multiscale modeling

Different stages of aerosol synthesis involve distinct particle growth mechanisms. Early on, gas-to-particle conversion, a kinetically unfavorable process, takes place where clusters form by nucleation of vapor molecules and/or condensation of monomers and decompose by evaporation (Figure 1a). Once particles exceed a critical size surmounting the nucleation barrier, stable nuclei form and grow by condensation, surface growth or sintering. These growth mechanisms are encountered at high temperatures (e.g., in early particle formation in flames, hot wall or laser reactors) and result in chemically bonded nanoparticles, the so-called aggregates (Figure 1c). Further downstream in the process, coagulation of aggregates leads to physically bonded fractal-like particles, the so-called agglomerates (Figure 1b).

The intricacies of nucleation and early particle growth, occurring at nanosecond scale, pose significant challenges for both the experimental investigation and the precise control of particle characteristics at the nanometer scale[1]. Accurate analysis requires a combination of in-situ non-intrusive optical diagnostics and ex-situ measurements[2]. Atomistic molecular dynamics (MD) simulations play a pivotal role at this juncture, offering atomic and femtosecond resolution, enhancing our understanding of material properties at the atomistic level. These simulations effectively complement experimental techniques like High-Resolution Transmission Electron Microscopy (HRTEM) and X-Ray Diffraction (XRD), bridging the gap between detailed atomic interactions and macroscopic experimental observations.

Engineering the nanocrystallinity of particles by closely monitoring synthesis process parameters is crucial for optimizing their morphology, electronic, catalytic, and nanomechanical properties. For instance, defect-free single gold crystals are highly sought after for their use in electronic devices due to their enhanced electrical properties. On the other hand, polycrystalline structures, such as nanodecahedra, are preferred in photonic and sensing applications due to their superior light interaction capabilities.

The crystallization temperature significantly affects the crystal size of the end particle. If crystallization from an amorphous state occurs by cooling the nanoparticles near their solidifying temperature, a few large crystal domains are formed (Figure 2, top). At these temperatures, nucleation by accretion is the dominant mechanism[3]. Crystallization well below the solidifying temperature takes place by explosive nucleation, which promotes the formation of multiple supercritical nuclei that grow into each other resulting in many small crystal domains (Figure 2, bottom). These intricate processes are detailed through MD simulations, which enable tracking the atomic trajectories and elucidating crystallinity dynamics at the nanoscale[3]. The differences in the crystallinity of gold nanoparticles can be quantified by XRD spectra calculations obtained by MD, which can be directly compared to XRD patterns obtained by experiments. In nucleation by accretion, the XRD patterns exhibit four distinct peaks corresponding to the (111), (200), (220), and (311) facet orientations (Figure 2: orange XRD pattern). The (111) facet is the most dominant peak, corresponding to the most stable plane. In explosive nucleation, these peaks are broader, reflecting the presence of smaller crystal domains (Figure 2: blue XRD pattern). This effect is particularly evident in the weaker reflection of the (200) peak compared to that observed in nucleation by accretion.

Such atomistic insights from MD simulations and simulated XRD spectra can also help differentiate the morphology of multicomponent NPs, such as alloyed vs. segregated Ag-Au bimetallics. For instance, alloyed Ag-Au nanoparticles exhibit less distinct (200) crystalline plane reflections and attain smaller, highly polycrystalline structures, compared to the sharper and more defined peaks seen in segregated nanoparticles[4]. The transient evolution of the crystallinity can also influence nanoparticle growth dynamics in the high-temperature environments of the flame. For example, initially amorphous 4 nm nanoparticles coalesce ~100 times more rapidly than crystalline ones at isothermal conditions of 800 K.[5]

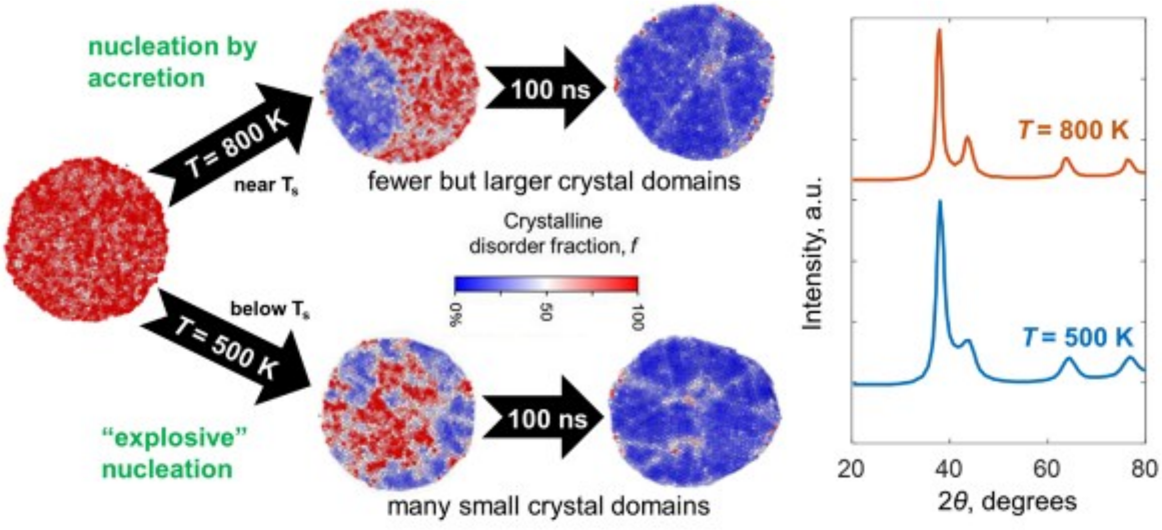
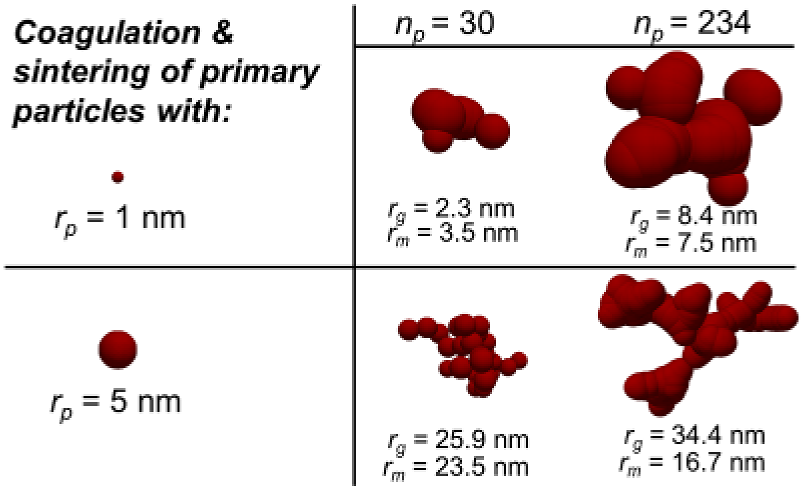


Figure 2. Crystallization of a 10 nm gold nanoparticle at 800 (top) and 500 K (bottom). The crystallization temperature affects the mechanism of crystal nucleation and end particle crystallinity.[4]

The sintering rates and crystallinity information obtained from MD simulations can be utilized in mesoscale particle dynamics models in a hierarchical modelling approach. Mesoscale models, such as discrete element method, simulate the dynamics of particle growth, allowing for the prediction of collision rates of monodisperse[6] and polydisperse particles[7] during agglomeration in the gas-phase, and the evolution of their morphological and size characteristics. By incorporating, concurrently with agglomeration, sintering[8] or surface growth rates[9] obtained either by phenomenological models or from MD simulations, mesoscale models can elucidate the effect of these mechanisms on the morphology, size distribution, and coagulation rate of the resulting fractal-like aggregates and agglomerates (e.g., Table 1). For example, discrete element method simulations have revealed that increasing the polydispersity of the constituent primary particles in aerosol agglomerates, delays the attainment of their asymptotic fractal dimension and geometric standard deviation of their size distribution. This delay complicates the correlation of the agglomerate mobility diameter with mass by universal power laws.



Coagulation & sintering of primary particles with:	$n_p = 30$	$n_p = 234$
$r_p = 1$ nm	$r_g = 2.3$ nm $r_m = 3.5$ nm	$r_g = 8.4$ nm $r_m = 7.5$ nm
$r_p = 5$ nm	$r_g = 25.9$ nm $r_m = 23.5$ nm	$r_g = 34.4$ nm $r_m = 16.7$ nm

Table 1. Snapshots of aggregates formed during coagulation and sintering of primary particles with radius, r_p, of 1 (top) and 5 nm (bottom) at 2000 K.[8]

Such detailed modelling is crucial for the on-line characterization of aerosol-made materials with *in-situ* measurements by power laws, as they demonstrated that accounting for the evolution of agglomerate structure hardly impacts the characteristics of product particles while their coalescence rate has far more impact, requiring its accurate knowledge[10]. These results greatly facilitate the design of aerosol synthesis of materials and the use of simplified aerosol dynamics in reactor fluid mechanics for systematic design of aerosol processes and industrial scale-up.

Nanoparticle synthesis for methanol conversion

The detailed characteristics of fractal-like aggregates and agglomerates formed in flames (e.g., Figure 1b-c), as revealed by multiscale simulations, are crucial for optimizing nanoparticle performance and functionality. These characteristics influence key properties such as conductivity, gas sensor sensitivity, mechanical strength in nanocomposites, and fuel cell performance. Also, depending on their structure, nanoparticles find different applications. For example, aggregates (Figure 1c) find applications in catalysis, insulators or electroceramic devices, while weakly-interacting agglomerates (Figure 1b) are attractive in pigments and nanocomposites.

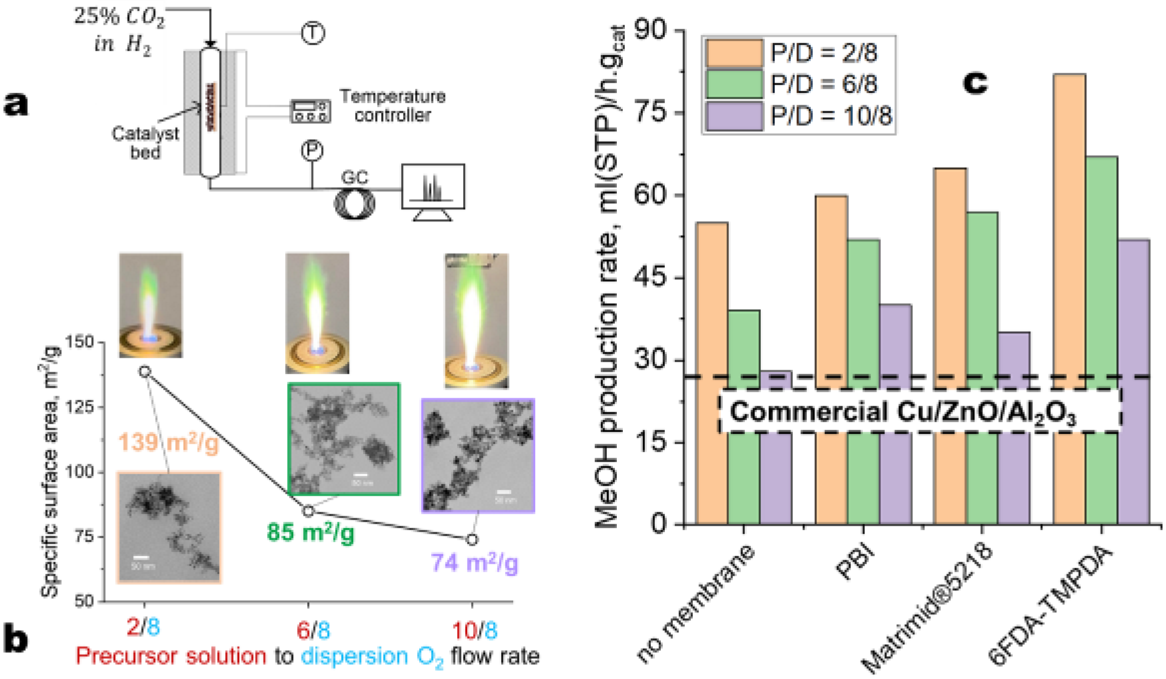


Figure 3. (a) Experimental setup for methanol production by CO_2 hydrogenation using hybrid nanocatalyst-membrane reactors. (b) Specific surface area of nanocatalysts as function of the precursor solution (P, mL/min) to dispersion oxygen (O, L/min) during flame synthesis. (c) Methanol production rate for different P/D ratios of standalone or membrane-embedded flame-made nanocatalysts.

Flame spray pyrolysis synthesis routes allow for precise control over the nanoparticle characteristics by adjusting process conditions. Decreasing the precursor flow rate, for example, leads to smaller primary particles that result in the formation of agglomerates with more open, filamentary structure and higher specific surface area, compared to aggregates formed at a lower precursor flow rate (Figure 3b). Such structural variations can have a dramatic effect on nanoparticle performance. This is exemplified by flame-made CuO/ZrO_2 nanocatalysts embedded in polymeric membranes[11] used for methanol production by CO_2 hydrogenation (Figure 3a). Methanol is a highly efficient carrier for hydrogen due to its impressive energy density, and a crucial precursor in various industrial applications. Traditional methanol synthesis relies predominantly on natural gas, releasing CO_2 as a byproduct contributing to greenhouse gas emissions. Direct CO_2 hydrogenation offers a greener alternative.

Flame-made CuO/ZrO_2 nanoparticles have demonstrated significantly higher methanol yields via CO_2 hydrogenation compared to commercial $Cu/ZnO/Al_2O_3$ ones (Figure 3c). Once embedded in polymeric membranes[12] via direct aerosol deposition (Figure 1a), nanoparticles produced at a precursor flow rate of 10 mL/min can boost methanol production rate[11], achieving a remarkable ~70% increase compared to conventional catalytic fixed bed reactors at 200 °C and 20 bar. This performance can be enhanced further when reducing the precursor flow rate during aerosol synthesis to 2 mL/min, achieving a 106% increase in methanol yield at the same conditions (Figure 3c).

As synthesis and application of nanoparticles continue to drive advancements across various industries, multiscale modeling is critical in understanding and optimizing particle manufacturing, from their atomic structure to their integration into functional systems. In this endeavor, the synergy between experimental methods and simulation models will be crucial for navigating the complexities of nanoparticle engineering for future technological breakthroughs.

The strength of simulation models lies in their ability to decode nanoscale mechanisms, such as crystallinity dynamics and structural nuances at the atomistic level, that govern the performance of nanoparticles in applications like catalysis and gas sensing. This deep understanding is vital for linking process conditions to material performance and facilitating effective scale-up.

Acknowledgements

I am deeply honored to receive this prestigious award, and I would like to express my gratitude to PTF, as well as to my nominator, Prof. Sotiris Pratsinis, and the members of the award selection committee for this recognition. I would also like to acknowledge financial support from the Australian Research Council's Discovery Projects funding scheme (DP220103715) and The University of Melbourne.

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PTF Award Winners 2024

George Klinzing Best PhD Award

Dr. Anuj Joshi

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Email: ajoshi23@dow.com

Citation: The dissertation explores various particle design strategies, considering the reactor configuration and overall process, with the aim of establishing technologies through valorization of diverse feedstocks.

Anuj Joshi received his Bachelor in Chemical Engineering from the Institute of Chemical Technology India in 2018 and his Ph.D. in Chemical Engineering from The Ohio State University in 2023 under the supervision of Prof. Liang-Shih Fan. Anuj's research involved developing processes for valorizing different feedstocks such as stranded natural gas, waste biomass, and hydrogen sulfide. Specifically, he synthesized an iron-based catalyst for high-pressure dry and mixed methane reforming. He also devised a new moving bed chemical looping configuration for improved syngas yield from biomass and developed a chemical looping process for converting hydrogen sulfide to hydrogen using a nickel sulfide-based carrier. Anuj's knowledge of engineering particles to achieve enhanced reaction rates is also evident from his work on producing hydrogen from hydrogen sulfide. He synthesized a novel metal sulfide chemical looping carrier supported on another metal dioxide for this process. This metal dioxide support boasts a "bifunctional" role: it enhances the carrier's textural properties and it acts as a catalyst for hydrogen sulfide decomposition, significantly accelerating reaction rates. This support-material interaction offers valuable insights for researchers exploring diverse chemical processes. He has authored over 12 research articles, 3 book chapters, and holds 3 patents with over 150 citations.

Anuj is currently a Senior Research Specialist at The Dow Chemical Company in Texas working in their Industrial Solutions' Process and Catalyst R&D.

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Exploring Material and Process Design Strategies for the Production of Commodity Chemicals

Anuj Joshi
Senior Research Specialist
The Dow Chemical Company, TX

Introduction

The increasing population, along with a rise in the standard of living, has led to the demand for energy and chemicals reaching unprecedented levels. To fulfill the demand, fossil fuels are being utilized, causing enormous CO_2 emissions and resulting in the climate change problem faced by humanity today. Although the past couple of decades have witnessed growth in sustainable renewable energy sources, fossil fuels are still projected to remain the dominant contributor to the energy production scenario [1]. It is important to understand that fossil fuels are not only limited to power and electricity generation, but they also serve as feedstocks for the production of several specialty and commodity chemicals. The commodity chemical industry, which includes the manufacture of syngas, hydrogen, methanol, ammonia, etc., accounts for more than a third of total industrial energy consumption [2]. The current processes for the generation of these chemicals suffer from drawbacks such as high endothermic heat requirement, use of energy-intensive unit operations, coke deposition on the catalyst, and reliance on the economics of scale for feasibility [3]. Despite their limitations, these processes are critical to the world, and advancements are underway to improve their overall efficiency. However, to mitigate dependence on fossil fuels, considering the need for decarbonization, new technologies that can efficiently utilize sources such as biomass, hydrogen sulfide gas, stranded natural gas, and waste plastics for the production of commodity chemicals are required [4–6]. Furthermore, technologies that achieve process intensification to enhance product yields and efficiencies or render safer operations are also essential, even if, in some cases, the complete elimination of fossil fuels cannot be achieved. Chemical looping is a promising technology that can effectively utilize various sources for the sustainable and economical production of chemicals. It involves splitting the desired reaction into multiple sub-steps, facilitated by solid chemical looping carriers. Depending on the application, these carriers can be metal oxides, metal sulfides, metal nitrides, etc. Figure 1 shows a wide range of non-exhaustive chemical looping schemes that utilize different process configurations and looping carriers [3]. The chemical looping technology, with its wide range of applications, has the potential to achieve higher yields at better efficiencies and lower costs than conventional technologies [3]. This can be attributed to the various advantages [3,7–9] offered by the chemical looping technology such as:

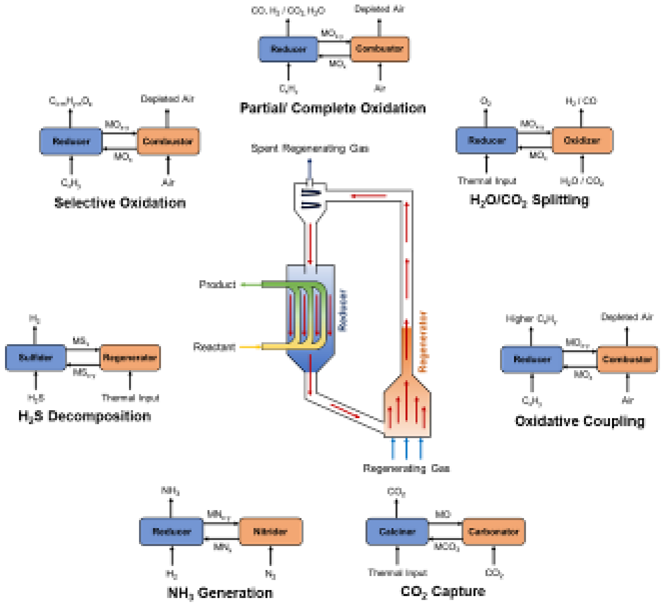

Figure 1: Various Chemical Looping Schemes [3]

Product Separation: As the chemical looping process involves splitting the reaction into multiple sub-steps, inherent product separation is achieved, eliminating energy-intensive and expensive downstream separation steps.

Elimination of Feed Conditioning: The chemical looping system achieves inherent product separation as the products are obtained at different reactor outlets. By extension, feed conditioning, such as the requirement of an air separation unit to avoid downstream separation, is also eliminated as the inlets to the reaction and regeneration steps are different.

Flexibility in Operation: The chemical looping process offers more degrees of freedom to achieve improved performance than conventional processes. Each sub-step of the chemical looping scheme can be operated at different conditions (temperature, pressure, etc.). This results in optimum performance in each step, which improves the throughput and the overall product yield.

Perspective on Chemical Looping and Dissertation

The outlook on chemical Looping technology is very positive, as evidenced by its increasing adoption by the industry [10–12]. However, understanding the various aspects of this technology and the synergy between them is key for further development. At the heart of any chemical looping application is its carrier, and developing the carrier requires inputs from reaction engineering, particle science, and also reactor configuration and design [3] - which is often overlooked. Incorporation of reactor design for developing carriers is necessary (although not sufficient) as important details such as gas-solid flows and transport phenomena can affect the system's overall throughput. Moreover, process design, optimization, life-cycle analysis, and economic evaluation also need to occur in parallel with the development of the carriers and reactor design for the successful commercialization of the technology [3]. This section provides a brief perspective on the aspects of the chemical looping technology.

Chemical Looping Carrier

Unsurprisingly, most of the research around chemical looping technology, regardless of application, is on the development of carriers as it directly influences the product. An ideal carrier should have a high capacity to react, high attrition resistance from physical and chemical stresses, lower mass transfer resistance and good reactivity, and high heat-carrying capacity [7]. Cost-effective manufacturing of these carriers is also desirable. Some of these parameters, like the cost of carrier, depend on the product margin, but an in-depth knowledge of particle science is necessary for achieving target values for most of the parameters. A modified Ellingham diagram based on thermodynamic calculations can be generated to narrow the scope for active component selection [3]. However, the scope of such analysis is limited only to the availability of underlying thermodynamic data. Density Functional Theory calculations can also aid in some decisions, like the selection of active components and promoters [3], but they need to be followed by extensive testing and characterization to understand long-term performance and morphological changes. Moreover, adding supports can help increase surface area and attrition resistance [3]. However, experimental evaluation is necessary to confirm whether the supports do not interact with the active component and/or promoters. The effect of support on ionic mobility also needs to be tested, as it is known that some carriers tend to form core-shell structures after multiple redox cycles. Even synthesis techniques play an important role in the performance of the carrier [3]. While some methods are better than others, selecting the one that can be scaled at the commercial level is essential. Ideally, everyone wants a cheap carrier that can sustain infinite redox cycles without losing reactivity and strength. However, it is crucial to acknowledge that carrier life is limited, and ultimately, economics should guide decisions on active components and support selection.

Chemical Looping Reactor Configuration

As mentioned earlier, at the heart of any chemical looping application is its carrier, but the overall success of the technology also requires a well-designed reactor system [3]. Irrespective of the performance of the carrier, achieving thermodynamic yield is dependent on the gas-solid flows, and thus, understanding its effect is essential in cases where both the equilibrium product yield is desired (for example, carbonaceous feedstocks for syngas or power generation) and even where undesired (for instance, selective oxidations such as formaldehyde and ethylene oxide generation). Thus, developing a chemical looping reactor system requires a fundamental insight into the synergy between multi-phase flow hydrodynamics, its effect on thermodynamics, and reaction kinetics.

Conventionally, chemical looping reactor systems are designed in one of three ways: (i) Fixed Beds, (ii) Fluidized Beds, and (iii) Moving beds. Table 1 lists the key characteristics of each of these reactor systems.

Table 1: Key Characteristics of Various Reactor Systems [3,9,13]

Reactor Type	Key Characteristics
Fixed Bed	Offers a low rate of carrier attrition Requires multiple beds in parallel for continuous operation Susceptible to hot spot formation and high pressure drop Solid utilization may be limited
Fluidized Bed	Lowest risk of hot spot formation Established technology with a lot of know-how Best heat and mass transfer characteristics among the three reactor types Back mixing nature can limit solid utilization
Moving Bed	Offers precise control over solid residence time Thermodynamic limits of solid utilization can always be achieved Complex operation as solid flow control is not straightforward

Except for fixed beds, wherein the reaction and regeneration of the carriers occur in the same reactor, for both the fluidized bed system and the moving bed system, the regeneration of carriers usually occurs in a fluidized bed reactor, which is in fluid connection with the reaction section of the system [9]. Thus, the advantages and disadvantages listed in Table 1 for the fluidized bed and moving bed systems are relevant to the reaction section.

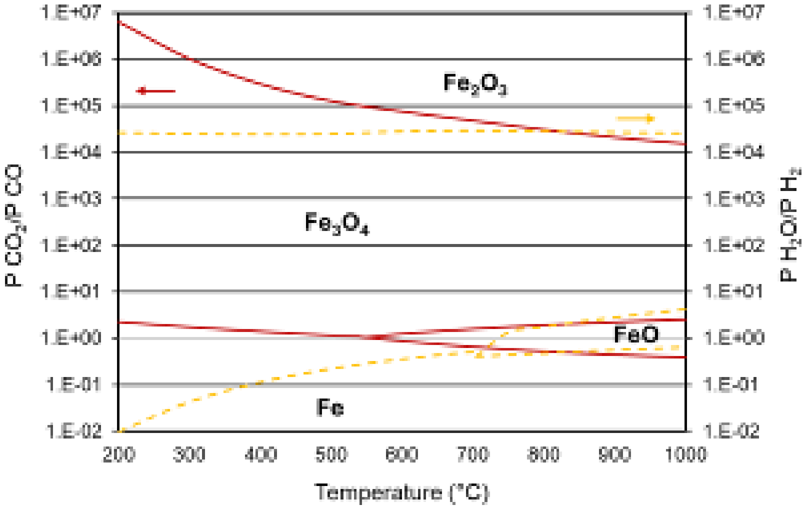

Figure 2: Phase Diagram of Iron Oxide as a Function of CO_2/CO and H_2O/H_2 Partial Pressure [9]

To elaborate on the importance of reactor configuration on the product, consider the case for iron-based carriers (iron oxide as the active component). Figure 2 displays the thermodynamic phase analysis for iron-based carriers against CO/CO_2 and H_2/H_2O partial pressures, which is particularly important for the conversion of any hydrocarbon (natural gas, coal, biomass, etc.) for syngas/power generation [9].

For a moving bed system using natural gas and an iron-based carrier, if the natural gas is sent in a co-current direction with the particle flow toward the exit of the reactor (both gas and solid exit), the Fe_2O_3 would be reduced to Fe/FeO, and concurrently the CO/CO_2 (and H_2/H_2O) concentration ratio in the gas phase would be high, indicating syngas generation. However, if the natural gas is sent in a counter-current direction with the particle flow, the gas at the reactor exit would be in equilibrium with Fe_2O_3, and thus, the CO/CO_2 (and H_2/H_2O) concentration ratio in the gas phase would be low, indicating complete combustion, required for power generation. Thus, with the same carrier, the gas-solid contacting pattern directly determines the selectivity of the product [7–9]. Moreover, for a fluidized bed with the same carrier, Fe_2O_3 cannot be reduced to the extent achieved in moving bed as the gas concentration ratios cannot be controlled due to the back mixing nature of fluidized beds [9]. Thus, the solid requirement to achieve the same reactant conversion increases for the fluidized bed compared to the moving bed for iron-based carriers.

It is essential to note that the difference between a moving bed and a fluidized bed explained above does not necessarily hold for all carriers, which further supports the importance of synergy between carriers and reactor design.

Furthermore, despite the disadvantages of each reactor system listed in Table 1, economics ultimately decides the commercial scale operation. For example, even though complete utilization of carrier might not be possible in a fixed bed reactor, it can still be preferred as the carrier attrition might be lower due to lower physical stress – lower carrier attrition means lower solid inventory, which in turn means lower operating costs.

The overarching conclusion of this section is that developing a chemical looping technology is not straightforward, and scale-up decisions depend on the application. In the dissertation [14] on which this article is based, an effort has been made to showcase the intricacies of various applications, such as biomass conversion to syngas, hydrogen sulfide decomposition to hydrogen and sulfur, and selective oxidation of methanol to formaldehyde. As it is not possible to explain each process, a discussion on the latest effort on biomass gasification is provided in the following section, as among the various processes part of the dissertation, this is at the forefront of commercialization.

Process Intensification of Biomass Gasification

Lignocellulosic biomass is an attractive feedstock that is increasingly looked at to be upgraded to valuable products due to its abundance, carbon neutrality, and low cost [15,16]. Several approaches, including a chemical looping approach by The Ohio State University (OSU), have been developed for biomass reforming [17–19]. The chemical looping technology of OSU, Biomass to Syngas (BTS), involves splitting the gasification into two steps – Reduction and Regeneration- and utilizes an iron-based oxygen carrier . The proprietary iron-based carrier has been shown to sustain multiple redox cycles.

The reducer (wherein the 'Reduction' step occurs) is a co-current moving bed reactor wherein the carriers donate their lattice oxygen to biomass to form syngas. Steam and/or CO_2 is also co-fed along with biomass to aid char gasification and improve syngas yield. The reduced carriers are then transported to a fluidized bed regenerator (for the 'Regeneration' step), where they regain their oxygen by reacting with air before being transferred back to the reducer. This system, portrayed in Figure 3(a), has shown the potential to address the challenges associated with other biomass gasification processes and is also demonstrated at the sub-pilot scale.

While developing the BTS technology, the focus was always on operating the unit autothermally, i.e., operating without any external heat input [19,20] - the exothermic regeneration of the carriers accounts for the endothermic biomass gasification. However, sustainable heat generation methods such as solar-powered electric heaters are expected to be available in the future, a question was posed to the BTS system - whether external heat could improve the syngas yield, and if so, how would it be achieved?

A new reactor configuration termed 'cross-current', as depicted in Figure 3 (b) [21], was devised to answer that question. It is similar to the co-current unit, except that the exit of the syngas stream is shifted to the middle of the reactor rather than near the solid exit. This allows for the exiting gas and solid streams to not be in equilibrium with each other. The steam and/or CO_2 is co-fed from the bottom of the reactor (where the syngas exit was in the co-current configuration).

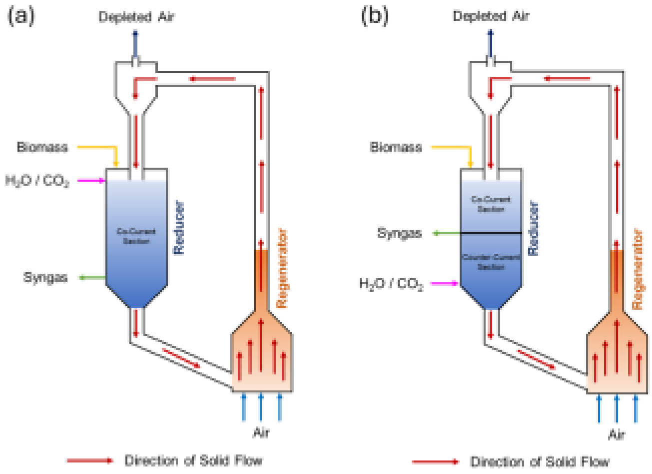

Figure 3: (a) Co-Current and (b) Cross-Current Reactor Configurations [21]

ASPEN simulations were conducted to understand the advantages of the cross-current system over the co-current system. Figure 4 [21] showcases the performance of both systems under the autothermal condition.

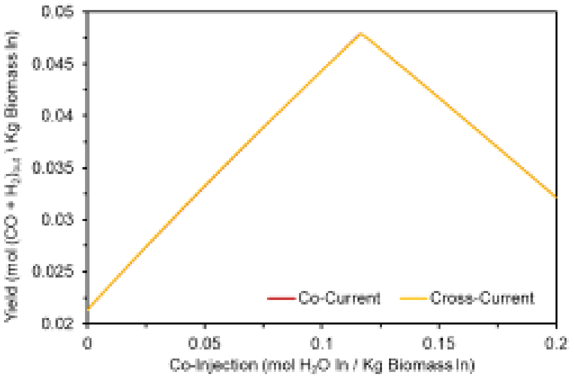

Figure 4: Comparative Performance of Both Configurations Under Autothermal Condition [21]

The results indicate that both systems have no difference, which might be puzzling to some readers. However, the key piece to solving this puzzle is understanding the effect of solid conversion (and, by extension, gas-solid thermodynamics). Even when there is no co-injection, the solid conversion does not exceed 33.33%, which means that Fe_2O_3 (0% solid conversion) is not reduced beyond FeO (33.33% solid conversion). This is because a high solid flow rate is required to maintain the autothermal condition, and at that flow rate, the biomass-to-carrier ratio is not high enough to achieve solid conversion beyond 33.33%. Any addition of co-injection further reduces the solid conversion, as the co-injection streams act as a heat sink. It is important to note that the carrier at this stage is highly optimized for strength and durability. Although it would be ideal to have more heat capacity of the carrier so that the biomass-to-carrier ratio can be improved, but that would come at the cost of other parameters. Again, the overarching point is that carriers can be optimized only to a certain extent, making optimization of process parameters equally important.

Figure 5 [21] shows the steam co-injection on solid conversion for different starting solid conversion values for both configurations. For all starting solid conversions at or below 33.33%, the effect of steam co-injection is the same, as evidenced by the autothermal condition. However, above 33.33%, the nature of the curve is different. There is a plateau region for the co-current configuration that is not present in the cross-current system and can be exploited.

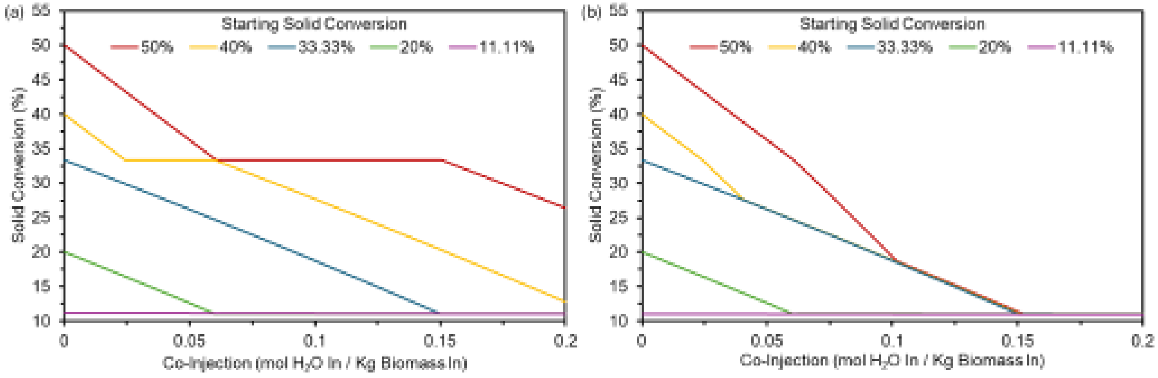

Figure 5: Solid Conversion for (a) Co-Current and (b)Cross-Current Reactor Configuration [21]

An isothermal operation would be necessary to obtain a condition where solid conversion exceeds 33.33% (presence of FeO and Fe), as an autothermal operation cannot achieve it. Thus, external heat input would be necessary. There are also other nuances of the carrier which put a ceiling on the solid conversion. Ideally, 100% solid conversion (complete reduction to Fe) is desired, but it might not be practical due to other constraints, and 40% solid conversion is not exceeded. The article on which this section is based delves into some of these nuances [21].

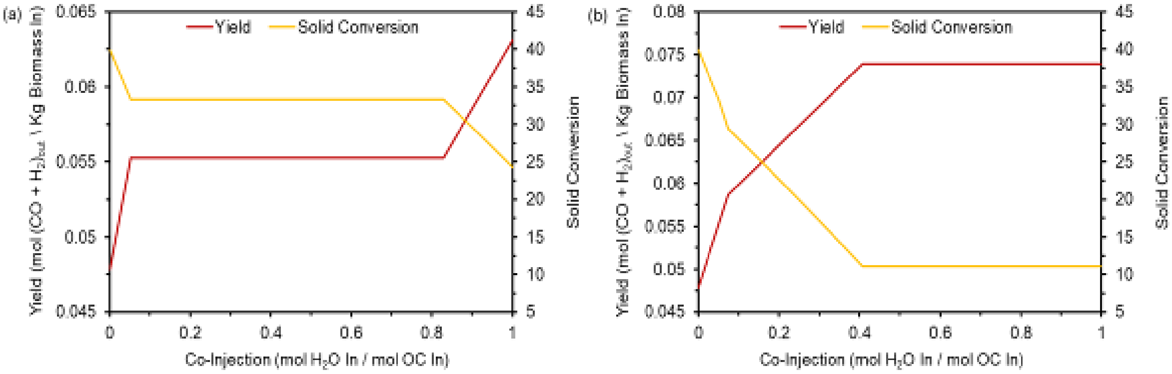

Figure 6: Performance of (a) Co-Current and (b)Cross-Current Reactor Configurations Under Isothermal Condition [21]

Figure 6 showcases the performance of both systems under the isothermal condition, under the constraint that at no co-injection, the biomass-to-carrier ratio is such that 40% solid conversion is achieved. It is quite evident from the figure that syngas yield for the cross-current system exceeds that of the co-current system at a lower co-injection requirement. The plateau region in the co-current system is due to exiting gas and solids being in equilibrium and H_2O/ H_2 and/or CO_2/CO gas concentration ratios not reaching high enough to oxidize the carrier. This goes back to the concept explained in Figure 2. However, as the exiting gas and solid streams are not in equilibrium for the cross-current system, the thermodynamic barrier does not exist, and a ~34% higher syngas yield is achieved at lower co-injection flow rates. It is important to note that co-current will eventually reach the same high syngas yield, albeit at higher co-injection flow rates.

This section shows that process intensification does not necessarily need a carrier redesign, and simple process changes can lead to huge gains. The cross-current system has the same solid residence time as the co-current system, so the char gasification rate remains unchanged, which is usually the rate-limiting step [21]. Thus, depending on heat availability, the unit can be operated in either the co-current or the cross-current configuration, as the design volume across the different configurations remains the same.

Conclusion

This article is written to apprise readers of the importance of chemical looping and briefly explain some of its key aspects. To develop a carrier, an iterative approach entailing carrier synthesis, thermodynamic and atomistic simulations, and long-term testing is required for carrier design. However, an optimized carrier formulation is not sufficient, although necessary, for the efficient performance of a chemical looping system. The reactor configuration also controls the product's throughput. The reactor design needs to consider the system's thermodynamics, desired gas-solid contact, formation of unwanted products, and the carrier's constraints. Process simulations are also necessary to understand the operating space of the process and expected product yield. Thus, conducting simulations is important prior to carrier design and reactor selection to understand the feasibility. Thus, all three aspects of the chemical looping system – carrier development, reactor configuration, and process simulations- must be studied to establish a technology.

The methodology described above is applied to various chemistries at different stages of development in the dissertation on which this article is based. In the dissertation, various material and process design strategies are explored for the utilization of two domestic and waste sources – biomass and hydrogen sulfide, toward syngas and hydrogen generation through the chemical looping route. In addition, a novel chemical looping-based process for the selective oxidation of methanol to formaldehyde is developed, eliminating the contact between methanol and oxygen. The dissertation [14] was written with the hope that apart from initiating some technologies, it would provide guidelines on technology development through material and process design.

Acknowledgments

I would like to express my sincere gratitude to the Particle Technology Forum for the award and for the opportunity to present the perspective of my dissertation in the newsletter. I would also like to thank my advisor, Prof. Liang-Shih Fan, and my colleagues at The Ohio State University for their support.

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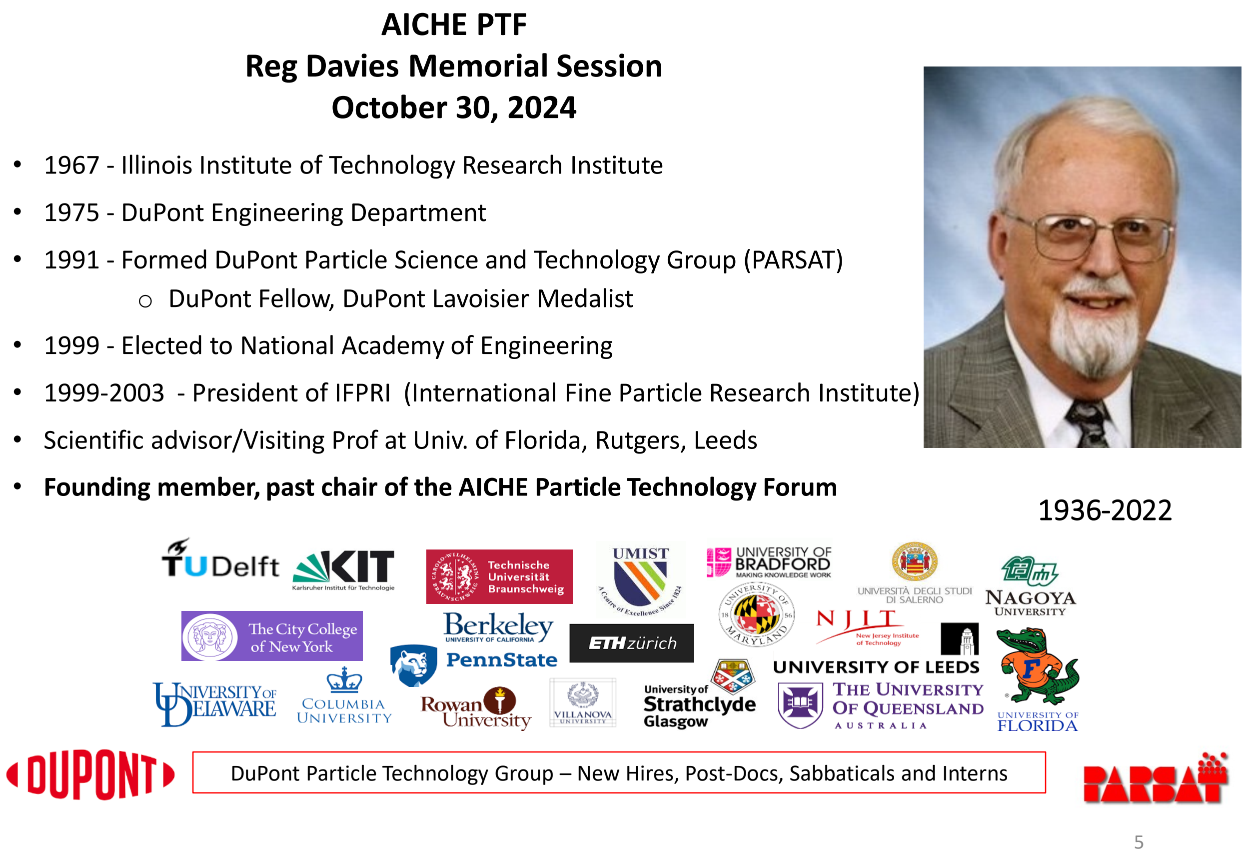


AICHE PTF
Reg Davies Memorial Session
October 30, 2024

- 1967 - Illinois Institute of Technology Research Institute
- 1975 - DuPont Engineering Department
- 1991 - Formed DuPont Particle Science and Technology Group (PARSAT)
    - DuPont Fellow, DuPont Lavoisier Medalist
- 1999 - Elected to National Academy of Engineering
- 1999-2003 - President of IFPRI (International Fine Particle Research Institute)
- Scientific advisor/Visiting Prof at Univ. of Florida, Rutgers, Leeds
- **Founding member, past chair of the AICHE Particle Technology Forum**

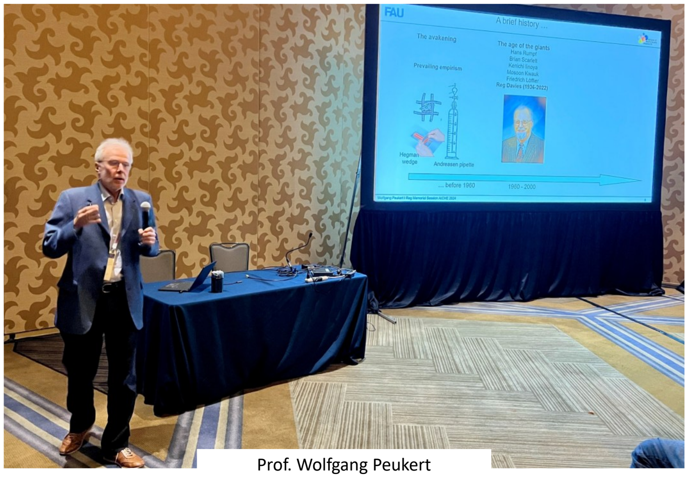
1936-2022

DuPont Particle Technology Group – New Hires, Post-Docs, Sabbaticals and Interns

5

Session organized and chaired by Tim Bell (DuPont, retired (pictured)) and Willie Hendrickson (Aveka, and President of IFPRI)

Reg Davies Memorial Session


FAU

A brief history …

The avakening

Prevailing empirism

The age of the giants
Hans Rumpf
Brian Scarlett
Kenichi Iinoya
Mosoon Kwauk
Friedrich Löffler
Reg Davies (1936-2022)

Wolfgang Peukert I Reg Memorial Session AIChE 2024

Prof. Wolfgang Peukert
Univ. of Erlangen-Nuremberg


Reg Davies
Particle Technology Champion

Unifier
- United particle technology across disciplines, organizations, industries
- Academic/industrial

Leader
- By example
- Created DuPont PARSAT – a leading industrial particle technology group
- Lead IFPRI

Mentor
- Passionate
- Inspiring

Dan Green
GlaxoSmithKline (GSK), former DuPont


70 YEARS OF SOLIDS SUSPENSION:
From Kneule to Giacomelli

Richard K. Grenville[1] & Jason J. Giacomelli[2]

1. RKGMixes LLC, Wilmington, DE
2. SPX Flow Mixing Solutions, Palmyra, PA

Honorary Session: Reg Davies Special Topics
AIChE Annual Meeting, San Diego, CA
30th October 2024

SPXFLOW

Richard Grenville
Retired from SPX, former DuPont


Ingredion
Be what's next.

2024 AIChE ANNUAL MEETING | October 27 – 31, 2024 San Diego Convention Center Hilton San Diego Bayfront

Solid-Liquid Separation – An Overview and the Challenges

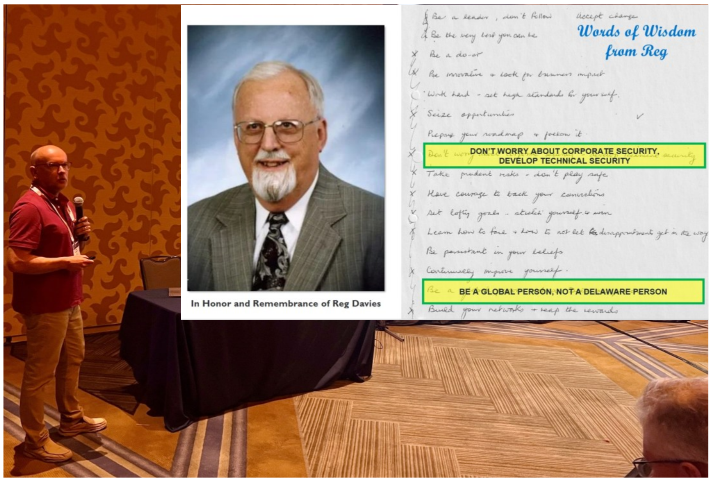
Dr. Karsten Keller
VP, Global Process Development and Digital Innovation
Bridgewater, NJ

October 30, 2024

In Honor and Remembrance of Reg Davies
"The Particle Man"

ONE INNOVATION

Karsten Keller
Ingredion, former DuPont


In Honor and Remembrance of Reg Davies

Words of Wisdom from Reg

Be a leader, don't follow accept change
Be the very best you can be
Be a do-er
Be innovative & look for business impact
Work hard - set high standards for yourself.
Seize opportunities
Prepare your roadmap & follow it
DON'T WORRY ABOUT CORPORATE SECURITY, DEVELOP TECHNICAL SECURITY
Take prudent risks - don't play safe
Have courage to back your convictions
Set lofty goals - stretch yourself & win
Learn how to fail + how to not let ~~the~~ disappointments get in the way
Be persistant in your beliefs
Continuously improve yourself.
BE A GLOBAL PERSON, NOT A DELAWARE PERSON
Build your networks + reap the rewards

Erik Gommeren
International Flavors and Fragrances, former DuPont


THE SOLIDS PROCESSING CAPABILITY AT DOW
THE PAST, PRESENT AND FUTURE

SHRIKANT DHODAPKAR, JÖRG THEUERKAUF
THE DOW CHEMICAL COMPANY

October 30, 2024

Jorg Theuerkauf
Dow Chemical, former DuPont intern

Professor Leonard Austin Memorial Session
Chaired By Dr. Ecevit Bilgili

The Human Prof. Austin

- Sofia will always remember Leonard as the sweetest husband, full of life and vitality: witty and with a great sense of humor.
- Leonard loved animals, especially his dogs, enjoyed traveling, was an avid reader and enjoyed listening to music
- Family and friends that meant the most to Len. He remembered his family, students, colleagues and friends around the world with such love.
- Witty and passionate

"Writing a paper with him was a learning experience: he was very particular on how graphs looked like, and did not accept anything but perfection.." (Prof. Luis Marcelo Tavares*)

"...He was short in stature but large in his knowledge and attention to the details. Grad students were pushed to work long hours ... with great satisfaction. I know I learned a lot from him..."

*Credit: https://min-eng.blogspot.com/2022/11/leonard-george-austin-1929-2022.html
https://www.statecollege.com/obituaries/leonard-g-len-austin/

3

CELEBRATING

THE INTELLECTUAL CONTIBUTIONS OF

LATE PROFESSOR LEONARD (LEN) G. AUSTIN

1929-
2022

To The Field of Comminution Processes

World Of Particle Technology—Student Workshop

Ben Freireich, PhD, PE
Vice President, Research & Development
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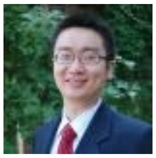

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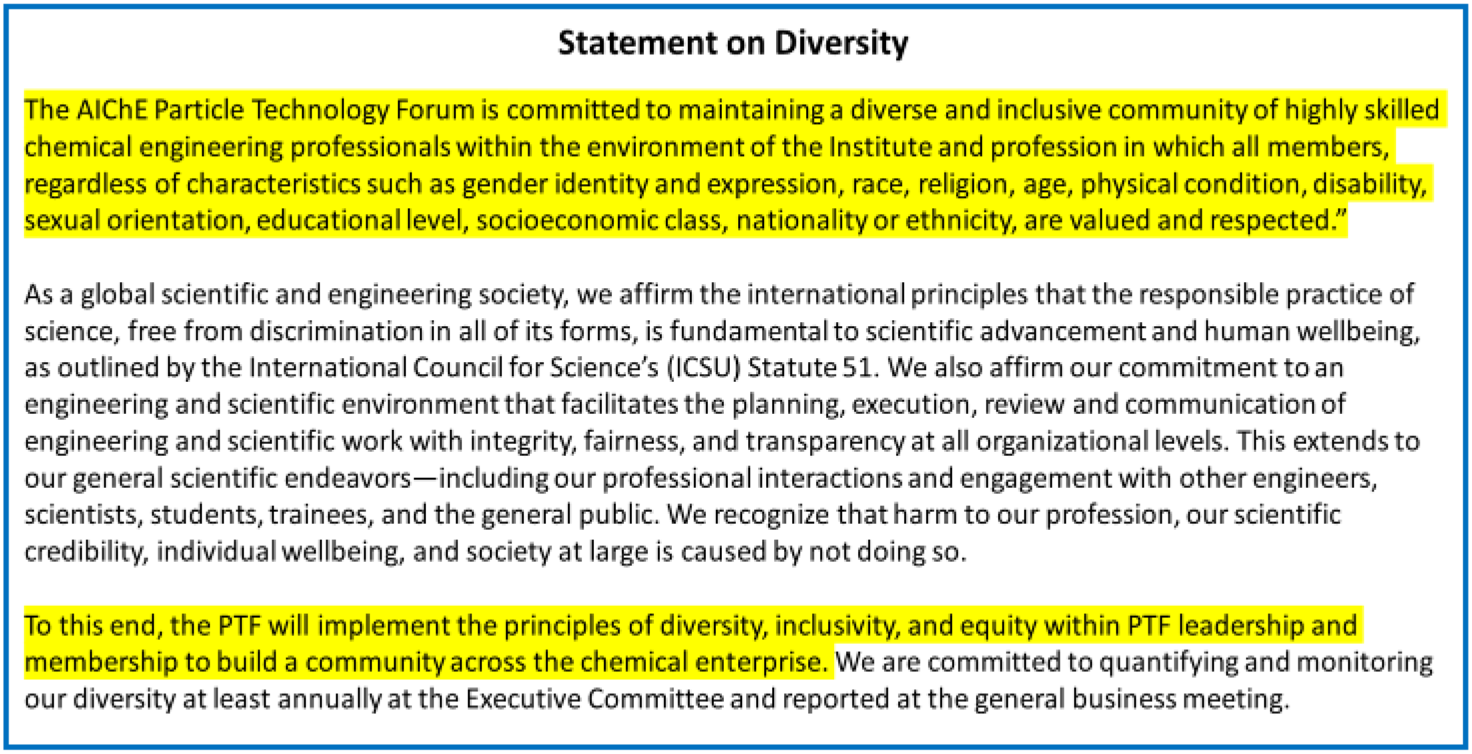

Statement on Diversity

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.