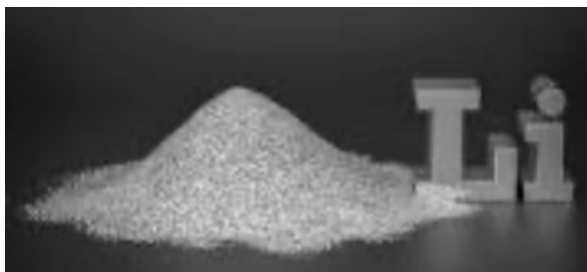




THE PARTICLE TECHNOLOGY FORUM (PTF) NEWSLETTER

An American Institute of Chemical Engineers (AIChE) Forum

Message From The Chair



Hope you and your families are enjoying the remaining summer season. It is now time to register for the AIChE Annual Meeting in San Diego, CA! We will be having PTF Awards Dinner on Wednesday evening at San Diego Wine & Culinary, social interactions during our poster session and planning meetings, and invited talks by some of our awards winners. A hearty congratulations to all of our award winners! You can read about them in the Fall issue and hear about their research at the conference in person. I will have much more to say about this year's winners at our PTF Awards Dinner.

These are exciting times for particle technology members playing a pivotal role in both the old and the new energy sectors. I am looking for an exciting speaker for the next webinar in the emerging technologies area. If you have recommendations, please reach out to me. PTF technical programs reflect the emphasis on low carbon solutions, new battery materials, etc.

Based on input from the PTF community, we have launched several new initiatives including increasing diversity, equity, and inclusion efforts.

My gratitude to this newsletter's editor, Dr. Shrikant Dhodapkar, for creating informative newsletter, Dr. Ben Freireich for planning all PTF sessions, and all members of the executive committee who keep programming and events running smoothly. We have one special session with invited speakers. Thanks to Prof. Maria Tomassone, Vice-Chair, who has been taking care of the PTF awards.

We are entering the period where we nominate and elect new leadership for the Particle Technology Forum Executive Committee. We need to elect two industrial and two academic positions on the EC. If you have interest or questions, please contact me or any of the EC members. Nominations are welcome.

A Peek At The Contents



- ◆ [PTF Executive Committee Elections](#)
- ◆ [Fluidization for Sustainability and Decarbonization Applications](#)
- ◆ [Atomic Layer Deposition on Particles to Make Better Electrocatalysts](#)
- ◆ [Redox-Activated Mixed Oxide Sorbent Particles Enabling](#)
- ◆ [Carbon-Negative Hydrogen Production](#)
- ◆ [Challenges With Handling Plastic Post-Consumer Waste](#)
- ◆ [Job Postings](#)
- ◆ [PTF Organization](#)

2024 / AIChE ANNUAL MEETING

October 27, 2024
to October 31, 2024

San Diego Convention
Center, Hilton San Diego
Bayfront

Registration Is Open

Hope to see you in person at AIChE Annual Meeting - October 27-31, 2024, Sand Diego Convention Center, Hilton San Diego Bayfront, USA. Remember to purchase PTF dinner tickets as part of the registration.

S.B. Reddy Karri, PhD, President &. CEO, PSRI
Chair, The Particle Technology Forum of AIChE
reddy.kari@psri.org



FROM THE EDITOR'S DESK

In our ongoing efforts to bring awareness and enhance engagement of the PTF community on the topic of **Emerging and Transformative Technologies for Decarbonization and Circularity**, this issue is an excellent starting point. Please reach out to me (sdhodapkar@dow.com) if you are interested in sharing your research or perspective on this topic.

Shrikant Dhodapkar, PhD
Senior R&D Fellow, AIChE Fellow
The Dow Chemical Company



AIChE PTF Executive Committee Elections

Deadline for nominations is **September 11, 2024**.

The election will begin on September 16, 2024 and will close on October 4, 2024.

The AIChE Particle Technology Forum (PTF) Executive Committee, according to the AIChE PTF by-laws, has equal representation between academics and individuals working in industry and other sectors that interface with the field of particle technology. The Executive Committee members act as liaisons to the PTF and play an important role in improving PTF by discussing and voting on PTF policy, working on PTF Events (such as judging posters at the annual meetings), recruiting new members/officers, and helping with PTF standing committees.

We are soliciting nominees for two (2) open positions as Academic Member Representative to the PTF Executive Committee and two (2) open positions for the Industrial Member Representative to the PTF Executive Committee. Interested candidates must be members of AIChE and the AIChE PTF, be willing to commit to a four (4) year term beginning in 2025, and lastly provide a short (one paragraph) biography for the ballot, which will be released as part of the upcoming Fall newsletter. This year's election will be held between **September 16** and **October 4, 2024**.

Interested individuals should reach out to - shankali.pradhan@merck.com and mkashyap@sabic.com.

Shankali Pradhan and Mayank Kashyap

Executive Committee - Industrial Member Representatives

Fluidization for Sustainability and Decarbonization Applications: The Parallel Evolving Roles of Processes and Computational Tools

Peter Blaser and Niraj Mehta, CPFD Software

Fluidization is a cornerstone of particle technology. Fluidized beds and other fluid-particle systems comprise critical parts in processes across a wide range of energy and energy-intensive industries, including refining, chemicals, and materials. In the 21st century, industries such as these are undergoing an energy transition, marked by sustainability and decarbonization aspirations. The need and desire to reduce an industry's environmental footprint has driven companies, research institutions, and governments to pursue innovative solutions and novel technologies. As the more promising technologies reach a scale-up and commercialization phase, many of these are utilizing fluidized bed platforms to achieve their ambitious goals.

This article examines the current trends in fluidization that have come about due to the newfound focus on sustainable applications, and how the role of computation tools used by those pursuing the applications is changing as well. From traditional industries driven by risk reduction motivators resulting in incremental process changes to the swift technological advancements in cutting-edge spaces driven by environmental and commercial urgency, we present a series of examples that illustrate the changing nature of fluidization in industrial processes and the parallel evolution of the role of computational tools used for such sustainability applications.

Trends in Fluidization

To begin, we briefly discuss recent trends and novel applications in the world of fluidization. Fluidized beds have been in commercial use for nearly a century, since the introduction of the Winkler coal gasification process in the 1920s. In the remainder of the 20th century, fluidization technology spread to multiple industrial application areas including refining, polyolefin polymerization, acrylonitrile synthesis, oxychlorination for vinyl chloride, dehydrogenation processes, cement calcination, and coal combustion, to name a few. However, while the applications were broad, much of the technology development was marked by small, incremental changes to a proven process, and conservative scale-up stages [1]. One exception to the last century's conservative scale-up trend is the rapid development of fluidized catalytic cracking technology in support of the Allied Powers during World War II [2].

In recent years, the number of applications using or exploring fluidized bed technologies has expanded rapidly, driven by the need for scalable approaches to material synthesis and energy for sustainability technologies. For example, gasification (or other thermochemical conversion processes such as pyrolysis) of biomass or of waste matter is largely accomplished using fluidized beds. These technologies represent important avenues for recycling and decarbonization pathways. Pyrolysis of waste plastic lets carbon rich matter that is not readily recyclable via mechanical means to be put to use, rather than collecting in landfills. Meanwhile, biomass gasification is a carbon neutral process, as biomass production removes exactly as much carbon dioxide from the atmosphere as combustion of biofuel-derived syngas produces.

For another example, electrification trends mean extensive green electricity production and storage requirements. Such systems rely on multiple materials which are most scalably produced using fluidized bed platforms. Examples include lithium, graphite, graphene, carbon nanotubes, polycrystalline silicon, nickel, and other electrode materials [3]. As the planet continues to increase adoption of renewable energy sources to meet power demands, and as transportation increasingly shifts from petrochemical fuels to electricity powered machines, the demand for efficient, affordable, scalable, and mass producible batteries and other electric components has never been higher.

The Shifting Role of Computational Tools

The application space of fluidization technology has expanded over recent history, and, in concert with this paradigm shift, the role of computational tools in the buildout and maintenance of fluidized processes has likewise transformed. Traditionally, computational tools were used to complement and augment existing engineering processes, which were primarily focused on incremental changes. Operations commonly relied on CAE software to troubleshoot unexpected behavior in order to reduce the frequency of interventions, increase the time between turnarounds, and generally maintain reliability. Additionally, plant operators would seek optimization changes targeted at ameliorating efficiency and increasing conversion and yield, with marginal economic improvement defining success. Changes to existing processes were only welcomed when the downside risk of such changes was considered minimal. As such,

computational tools were primarily used to understand the root cause of underperformance, minimize the risk of changes via virtual testing, and pursue optimization in a narrow sense only. This was digitalization, not digital transformation [4].

Nowadays, however, for those involved in the research, development and rapid commercialization of new application domains, such as the sustainability and decarbonization technologies mentioned above, computational tools align with a much broader corporate risk tolerance profile, and thus are used throughout the design, development, and deployment phases of chemical reactor engineering and scale-up. Owing in large part to the prodigious software and hardware advancements made over the last quarter century, computational power can tackle numerically taxing problems with relative ease. This has afforded research engineers the ability to virtually explore a broad parameter space, allowing for experimentation across an extensive range of ideas.

Furthermore, increased virtual testing capacity reduces the time and costs required for physical testing, which additionally reduces developmental risk. To be clear, physical testing – including cold-flow, pilot, and process demonstration scales – is still generally undertaken (and best-practice in the view of the authors), but the wider use of computational tools earlier in the R&D process generally means the physical testing can be significantly more targeted and detailed than would otherwise be possible without use of such tools. The newfound capability for comprehensive digital simulation and testing accelerates the scale-up from lab scale to pilot scale to industrial scale, thereby shortening the path to commercialization while also reducing scale-up risk. At the same time, companies developing nascent technology in bleeding edge spaces are simultaneously leveraging the computational results to effectively communicate the unique merits of their technology to customers, partners, and investors, and even in support of intellectual property protections.

The parallel evolving role of the fluidization-based technologies and the role of computational tools used for those technologies is demonstrated via three examples.

Traditional Industry and Computational Use Case - Oil Refining

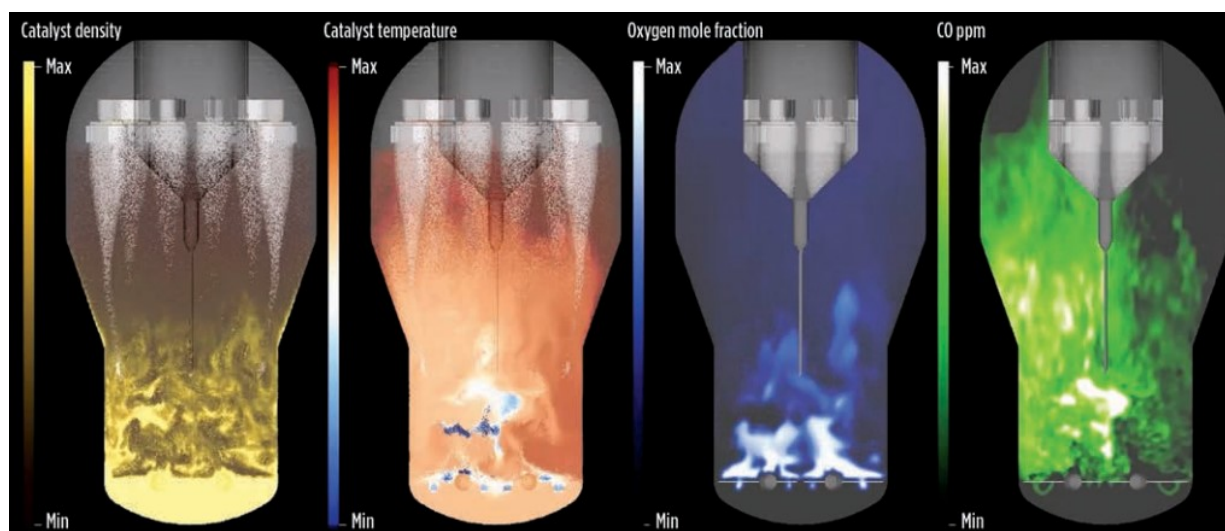


Figure 1. Hydrodynamics, Temperature, and Gas Composition in an FCC Regenerator

Our first example (Figure 1) illustrates the classic utilization of computational tools in the world of fluidization. This example, the Geelong Refinery operated by Viva Energy in Australia, is not only from a traditional industry – oil refining –, but also represents a traditional use case: risk reduction and reliability. The refinery had encountered issues with their FCCU that affected throughput, ultimately costing “tens of thousands of dollars per day” [5]. Engineers used CFD technology to identify the root cause of the problem. Potential changes and combinations thereof were tested virtually, with the most viable and efficient solution emerging. After implementation of the proposed change during a scheduled turnaround, the refinery saw greatly improved performance with lower afterburn, 4% increased maximum throughput, and a 75% reduction in panel operator intervention [6]. This example is typical of software use for well-established industries and applications, with the role of computational tools mirroring the risk-averse nature of the industry itself. Significant outcomes are still often obtained, but typically only via incremental changes.

Sustainability Application in a Traditional Industry - Cement



Figure 2. Novel cement calciner retrofit for decarbonization. Image courtesy aixergee.

Next, we look at an example from Germany, the Lengerich cement plant operated by Dyckerhoff, that demonstrates the transitional phase between traditional industries and typical computational tool usage and modern software techniques applied to novel processes. While the process is a well-known application of fluidization, cement calcination, the work is much more contemporary, using computational tools to assist in making dramatic changes for the sake of sustainability. The plant operators wanted to reduce both carbon monoxide emissions and overall carbon footprint by replacing fossil fuels with refuse-derived alternatives. Using CFD software, a novel retrofit was proposed, and its viability was verified virtually (Figure 2). Armed with the confidence to proceed with the change, the plant implemented the first-of-a-kind modified calciner geometry during a scheduled shutdown. Carbon monoxide emissions were reduced by 70% while the plant increased its thermal substitution rate by 22%. Notably, the ROI for the project was net positive within 6 months [7]. The success of this low-cost type of solution, and the role of the computational tool in acceptance of the change, serves as a template for traditional industries exploring non-incremental improvements for sustainability purposes.

Technology Development for Emerging Technologies



Figure 3 Computational tools integrated throughout technology development process. Image courtesy Molten Industries.

Finally, we enter the world of hydrogen. The past few years have seen a proliferation of research and development exploring decarbonization routes involving hydrogen as a fuel. Hydrogen production via methane pyrolysis is often accomplished either in a fluidized bed or by using other fluid-particle processes for the gas/particle separation and

handling. While the fundamental process is pyrolysis, the implementation pathways are broad, spanning molten metal reactors, microwave systems, and technologies with integrated carbon capture, to name a few. For example, Molten Industries, in collaboration with United States Steel Corporation, is leading a project funded by a U.S. Department of Energy grant to develop a pilot-scale system aimed at eliminating carbon emissions from iron reduction (Figure 3). This project integrates methane pyrolysis-driven hydrogen production with a pilot direct reduced iron (DRI) shaft furnace, leveraging renewable electricity to break down methane into hydrogen gas and solid graphite. The use of CFD models in conjunction with HPC technology has been integrated throughout the project. So far, this has proven crucial in accelerating the scale-up and commercialization of Molten's innovative technology, which has the potential to significantly reduce energy intensity, carbon emissions, and costs in steel production. Rapid development of novel fluidized bed technologies leads to pivotal strides towards critical goals of the sustainable economy, such as reducing the energy consumption and achieving carbon-neutrality in steel manufacturing [8].

Concluding Thoughts

While leveraging models in scale-up is not new, the urgency of scale-up and broad use of computational tools is unprecedented. Hydrogen, carbon capture, direct air capture, waste-to-fuels, biofuels, plastic recycling, battery materials, solar materials, electric vehicle components, and who-knows-what-else are all urgently required, being developed, and leveraging the latest computational tools to get to market as fast as possible. The organizations who are bringing these technologies to market are not afraid of risk – many will likely fail commercially – but instead must avoid the controllable risks associated with costly mis-steps and delays. And the latest computational tools are positioned better than ever to meet the challenge via GPU computing [9], cloud computing, machine learning, reduced order models, digital twins, AI, and more [10].

To conclude, the newfound focus on sustainability across the globe has opened up new paths in one of the most exciting applications of particle technology: fluidization. The potential for fluidization technology to tackle some of the planet's greatest obstacles has caused researchers and engineers the world over to think outside of the box and discover new ways to accelerate the development of novel processes. The evolution in the role of computational tools showcases the metamorphosis of approach.

As we look to the future nearly anything is possible. In the near term the trends highlighted herein are likely to continue. Or they may not. What is certain is that all linear extrapolations of non-linear phenomena eventually break down; city streets are not overrun with horse refuse, the 1920s stock market did not reach a permanently high plateau, we did not run out of oil in the late 20th century, and Moore's law no longer predicts CPU performance over time (GPUs on the other hand are the future... or are they?). What we can confidently assert, however, is that regardless of which sustainability and decarbonization technologies ultimately flourish, and which show less viability, fluidized bed technology remains a robust particle technology platform regardless of the application, and computational tools are adapting alongside the processes they simulate.

References

1. Jia Wei Chew, W. Casey Q. LaMarche, Ray A. Cocco. *100 years of scaling up fluidized bed and circulating fluidized bed reactors*. Powder Technology, Volume 409, 2022.
2. American Chemical Society National Historic Chemical Landmarks. *The Houdry Process for Catalytic Cracking*. <http://www.acs.org/content/acs/en/education/whatischemistry/landmarks/houdry.html>.
3. Karri, S. B. R. (2024, June). *Fluidization's Role in the Scale-Up and Commercialization of Sustainability and Decarbonization Technologies*. 2024 Barracuda Virtual Reactor Users' Conference. Chicago; Illinois.
4. Blaser, Peter & Barua, Rajat. (2019, April). *Digitally Transforming Refineries*. Hydrocarbon Engineering.
5. Blaser, Peter, Pendergrass, J., Gabites, J., & Brooke, A. (2018, September). *Viva energy's Geelong refinery reduces FCCU turnaround risk*. Hydrocarbon Processing.
6. Ibid.
7. Weng, Martin. (2022, June). *A First-Ever Innovative Brown-Field Modification in Conservative Cement Industry – De-Risked by Smart Simulation*. 2022 Barracuda Virtual Reactor Users' Conference. Chicago; Illinois.
8. *Molten Industries Leads Strategic Partnership With U. S. Steel and CFPD Software to Pioneer Carbon-Neutral Steel Production*. (2024, July 23). Business Wire.
9. Blaser, Peter, Larson, A., Parker, J., Akhavan, A., & Mehta, N. (2022). *The Role of GPU Computing in the Commercialization and Scale-Up of Fluidized Bed Conversion Processes*. Fluidized Bed Conversion Conference 2022.

10. In the opinion of the authors, some of the tools listed in the preceding sentence are proven technologies while others are emerging and show potential. All computational tools must be used well and combined with sound engineering judgement. An overview of various tools and applicability is beyond the scope of this article.

About Authors



Peter Blaser is Vice President of Operations at CFPD Software with 25 years' experience developing and applying specialized computational fluid dynamics (CFD) technologies. Peter is passionate about removing the guesswork surrounding the design, scale-up, and operations of industrial fluid-particle processes through intelligent use of digitalization technology.



Niraj Mehta is a Solutions Engineer at CFPD Software. Originally working on the Barracuda Virtual Reactor development team as a Software Engineer, Niraj now works in account management and business development. Niraj is keen on leveraging the intersection of high-performance computing and computational fluid dynamics to provide innovative solutions.

Atomic Layer Deposition on Particles to Make Better Electrocatalysts

J. Ruud van Ommen

Department of Chemical Engineering, Delft University of Technology, the Netherlands

Electrification of the process industry

The energy transition requires that the process industry moves away from fossil fuels. Instead, molecules such as carbon dioxide, water and nitrogen should be used as feedstock. Energy will, in the future, be mostly supplied as electricity. Using electrocatalysts, this electricity can be deployed to make valuable chemicals. At Delft University of Technology, the novel technology required for this transition is investigated in the framework of the e-Refinery (<https://www.tudelft.nl/e-refinery/>).

Electrocatalysts will play a vital role in those novel processes. However, electrocatalyst are not yet equally mature compared to regular catalysts currently applied in thermocatalytic processes. They still have limited lifetimes, e.g. due to sintering, leaching and poisoning. For large-scale industrial deployment, these points should be drastically improved. My group investigates atomic layer deposition on particles as a means to achieve this [1].

Atomic Layer Deposition (ALD) On Particles

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

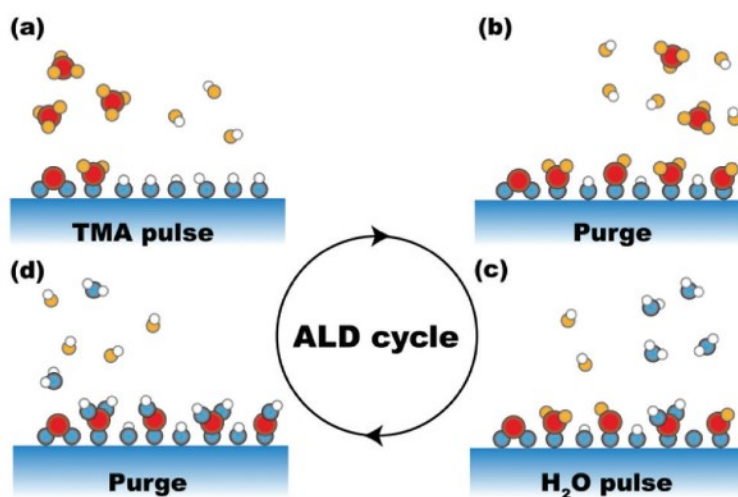


Fig. 1. Schematic representation of an ALD reaction: Al_2O_3 ALD based on trimethylaluminum (TMA, Reactant A) and H_2O (Reactant B): (a) exposure of the substrate surface to TMA and reactions between TMA and surface active sites (e.g., $-\text{OH}$ and oxygen bridges); (b) purging of excess TMA and reaction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

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

We apply ALD to particle substrates typically by fluidizing the particles. We fill a column with the powder we aim to

coat, and blow an upward flow of nitrogen through it to fluidize the powder. Then, we add the reactants A and B alternately to the nitrogen flow. We found that in this way, we can coat the surface of all particles in a very homogeneous way.

Example Applications For Electrocatalysts

Here, we employ atomic layer deposition to coat the surface of carbon black supported metal nanoparticles with an ultrathin layer of silicon dioxide (SiO_2) to prevent catalyst degradation. We will illustrate this approach with three examples:

1. Making nanoparticles containing both platinum and palladium for the conversion of CO_2 into formate;
2. Protecting platinum nanoparticles for the hydrogen evolution reaction against detachment and aggregation;
3. Protecting silver nanoparticles for conversion of CO_2 into CO against SO_2 impurities in the feed stream.

For example 1, we synthesized core-shell and alloy catalysts by ALD on the surface of fluidized carbon black particles. Supported Pt-Pd bimetallic catalysts are made and used for electrochemical CO_2 reduction. It is shown that the Pt-Pd alloy catalyst displays a 46 % faradaic efficiency toward formic acid, outperforming Pt@Pd and Pd@Pt core-shell structures that show faradaic efficiencies of 22 % and 11 %, respectively [3]. Moreover, both core-shell bimetallic catalysts (Pd@Pt and Pt@Pd) are not stable under electroreduction conditions. These catalysts restructure to more thermodynamically stable structures, such as segregated clusters or alloy particles, during the electrochemical reduction reaction, altering the catalytic selectivity (see Figure 2).

For example 2, we coated platinum nanoparticles with silica using ALD to prevent them from sintering and leaching during deployment as an electrocatalyst. Subsequently, we studied the current density before and after an accelerated durability test (ADT) at -0.2 V versus a reversible hydrogen electrode (RHE) in an H-cell setup. The current density of the unprotected catalyst was reduced by 34%. By contrast, for the catalyst protected with 2 SiO_2 ALD cycles, the current density was reduced by just 7%, whereas for 5 SiO_2 ALD cycles, the current density was reduced by only 2% (see Figure 3). The coating led to a factor five decrease in the Pt concentration in the electrolyte after the ADT [4].

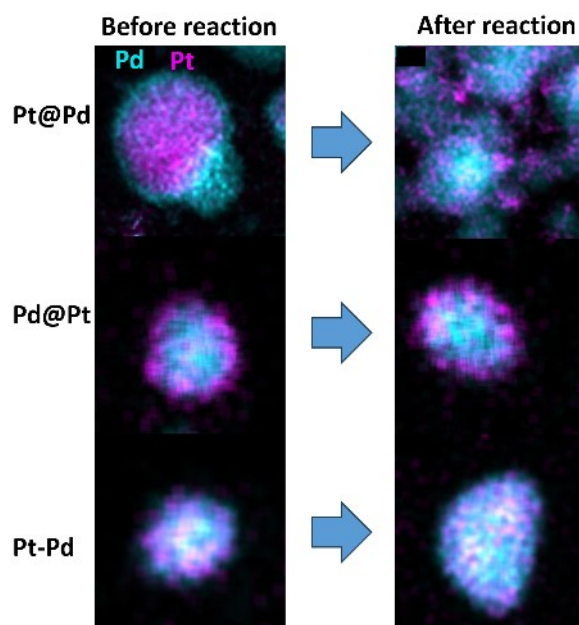


Figure 2. STEM-EDX elemental mapping of the core-shell (top and middle) and alloy particles, before and after the reaction.

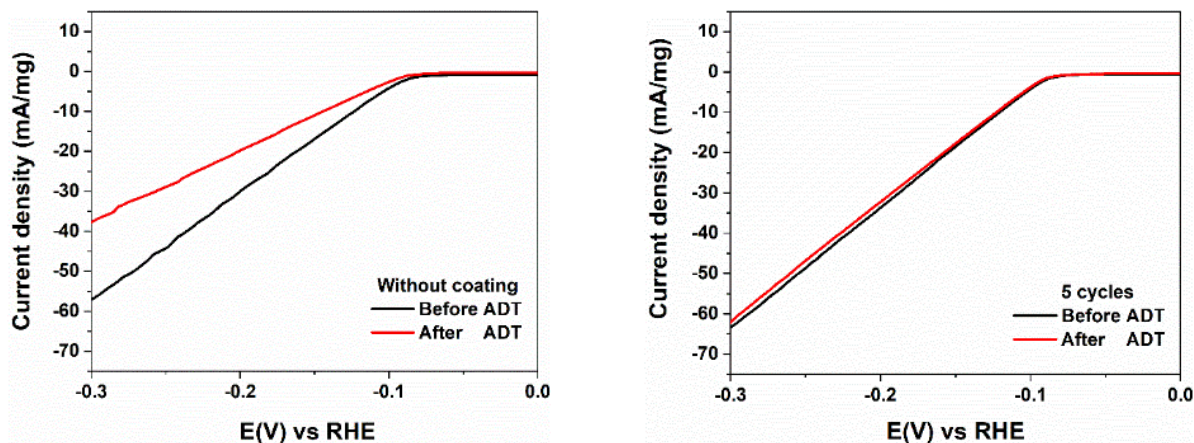


Figure 3. Hydrogen evolution on a platinum catalyst before and after an accelerated durability test (ADT). The left figure shows the performance without a protective coating, and the right figure shows the performance when the platinum nanoparticles are provided with a sub-nm coating of SiO_2 using 5 cycles of ALD.

For example 3, we coated silver nanoparticles with silica using ALD to protect them from poisoning. We studied the effect of SO_2 impurities (various concentrations, up to 1000 ppm) in the CO_2 feed to an electrochemical setup (H-cell), operated at various potentials. We observed that the silver catalyst stayed stable for 20 hours when fed with pure CO_2 . However, after only 1 hour of operation with 1000 ppm SO_2 added, the faradaic efficiency for CO already dropped from 70% to 46% at -1.0V versus RHE. For catalysts protected with 4 or 8 ALD cycles SiO_2 , the faradaic efficiency remained relatively constant (see Figure 4) [5]. This is likely due to the SO_2 and CO_2 permeating differently through the nano-coatings.

All three examples clearly show the strength of applying ALD to electrocatalyst particles in order to tailor their nanostructure and consequently boost their performance.

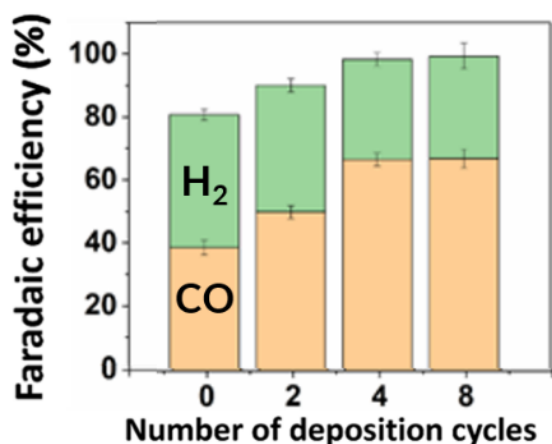


Figure 4. Faradaic efficiency of the Ag/CB catalyst with different thicknesses of SiO_2 coating (indicated by the number of deposition cycles) during 1h H-cell CA testing in a 0.1 M KHCO_3 electrolyte at -0.8V using CO_2 gas feed with 1000ppm SO_2 .

References

- [1] J. R. van Ommen, A. Goulas, *Mater. Today Chem.* 2019, **14**, 100183.
- [2] H. Van Bui, F. Grillo, J. R. van Ommen, *Chem. Comm.* 2017, **53**, 45.
- [3] M. Li, S. Fu, S. Saedy, A. Rajendrakumar, F.D. Tichelaar, R. Kortlever, J.R. van Ommen, *ChemCatChem*, 2022, **14**, e202200949.
- [4] M. Li, S. Saedy, S. Fu, T. Stellema, R. Kortlever, J.R. van Ommen, *Cat. Sci. Technol.* 2022, **14**, 1328.
- [5] M. Li, R. Kortlever, J.R. van Ommen, in preparation.

About Author



Prof. Ruud van Ommen is a full professor in the Chemical Engineering department at Delft University of Technology. His expertise spans a wide range of areas, including multiphase reactors, nanostructured materials, and particle technology. He has led numerous research projects, both fundamental and industry-collaborative. <https://www.tudelft.nl/tnw/over-faculteit/afdelingen/chemical-engineering/principal-investigators/ruud-van-ommen>

Email: j.r.vanommen@tudelft.nl



PTF Membership



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

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

Become a PTF only member (Annually \$15, Lifetime \$150)

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

You can also contact AIChE customer service at 800-242-4363 (US); 203-702-7660 (Outside the US); or email customerservice@aiche.org for membership questions and help.

PTF Membership Committee

Redox-Activated Mixed Oxide Sorbent Particles Enabling Carbon-Negative Hydrogen Production

Fanxing Li and Runxia Cai

Chemical and Biomolecular Engineering Department, North Carolina State University

The pressing global need for sustainable and clean energy sources has spotlighted hydrogen as a clean and versatile energy carrier and a critical component in achieving carbon neutrality. However, more than 99% of the hydrogen worldwide is still produced from fossil fuels (2022 data).[1] Therefore, new technologies that can generate carbon-free, cost-competitive hydrogen from renewable sources such as biomass and biogas are highly desirable. This article reports a new class of redox-activated sorbent particles we recently developed, which can significantly improve the efficiency for hydrogen production through an isothermal sorption-enhanced reforming and gasification (iSERG) processes. The process intensification enabled by iSERG offers the potential to produce carbon-negative hydrogen from biogenic feedstocks with a greatly simplified process scheme, high efficiency, and low cost. In the following sections, we will first explain the challenges facing conventional hydrogen production processes. This is followed by the introduction of the iSERG concept and the design principles of the sorbent particles, which are supported by computational and experimental data. Finally, the reactor design aspects and the path forward are discussed. Given that the iSERG sorbent concept builds upon a unique and synergistic combination of redox-based chemical looping, carbonate looping, and catalytic hydrocarbon (methane/tar) conversion, we hope that this article provides the readers a different perspective in designing reactive particles in the context of sustainable energy conversion and process intensification.

The Challenges for Conventional Hydrogen Production

Hydrogen production traditionally relies on methods like coal gasification and steam methane reforming (SMR), which, while cost-effective, result in substantial CO₂ emissions.[2] Moreover, these processes are highly complex, resulting in limited overall efficiency and a strong dependence on economies of scale. As a result, these commercial technologies are not suitable for direct application in biomass and biogas conversion because of the dispersed nature of their sources. Moreover, biomass gasification is inherently more challenging than coal due to its high volatile and moisture contents, lower heating values, and challenging flow properties.[3] Therefore, novel processes that can greatly simplify the conversion of these distributed biogenic feedstocks are required for cost-competitive production of green hydrogen.[4]

Sorption-enhanced reforming and gasification (SERG) has been investigated as a promising approach to intensify hydrogen production from biomass and biogas.[5] This method integrates gasification/reforming, the water-gas-shift reaction, and CO₂ capture into a single cyclic process. The two-step operation involves a reforming/gasification phase, where CO₂ is captured *in situ* to produce hydrogen-rich syngas, followed by a decarbonation step to regenerate the sorbent. However, conventional SERG requires substantial temperature swings ($\geq 100^\circ\text{C}$) to facilitate the efficient adsorption and desorption of CO₂ for practical applications. These thermal swings lead to high energy consumption ($\Delta H = 167.6 \text{ kJ/mol}$ for CaCO₃ at 800°C) and increase operational costs. Additionally, commonly used CaO-based sorbents often lose 50-80% of their initial CO₂ sorption capacity after just a few dozen cycles.[6] While steam re-activation at a lower temperature can regenerate CaO sorbents, it adds further complexity and cost to the process. [7] Another critical limitation to CaO-based SERG is related to CO₂-sorption thermodynamics: carbonate formation is thermodynamically unfavorable at high temperatures (e.g. $>750^\circ\text{C}$). Such an upper limit in the reforming/gasification reactor temperature results in slow reaction kinetics and high tar content from biomass-derived syngas.

Redox-Activated Isothermal Sorbents

To address these challenges, we set out to identify new sorbent materials that: (i) function at higher temperatures (e.g. 850°C); (ii) do not require temperature swings for CO₂-desorption; (iii) exhibit high stability under repeated CO₂ capture and release cycles.[8] If successful, these sorbents can minimize the energy requirements for CO₂ capture and release, simplifying the overall process to achieve high efficiency and low cost.

It turned out that the oxygen partial pressure changes inherent to typical gasification – regeneration cycles can be used as an effective trigger to enable isothermal CO₂ sorption and desorption. Our idea is simple: if we design a mixed oxide

that is stable under an oxidizing condition *and* contains (a) a highly basic cation such as Sr and Ba, and (b) a redox-active cation such as Mn or Fe, then the reducing environment in the reformer or gasifier would likely trigger the reduction of reducible cation to facilitate the decomposition of the oxide phase, leading to spontaneous carbonation of the basic cation. On the other hand, a regeneration environment with O₂ or air would lead to spontaneous re-oxidation of the redox-active cation, triggering CO₂ desorption and regeneration of the original mixed oxide phase (Figure 1).

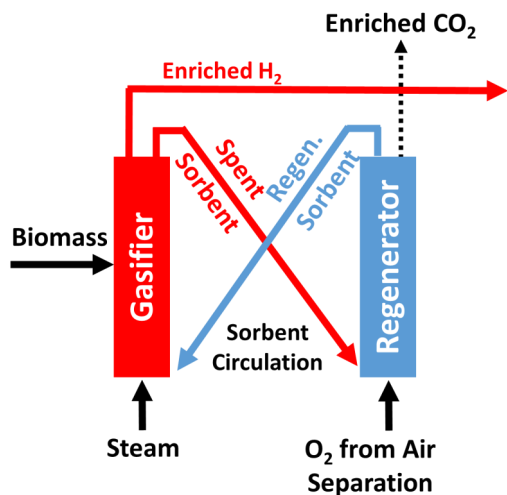


Figure 1. iSERG for H₂ generation with *in-situ* CO₂ capture. BaMnO₃ is used as a sample sorbent.

Gasification (overall rxn): BaMnO_{2.5} + Fuel + H₂O → BaCO₃ + MnO + 2H₂ + CO; (reduction of SrMnO₃ triggers carbonation, the syngas also contains minor CO₂ and CH₄)

Regenerator: BaCO₃ + MnO + 1/4 O₂ → BaMnO_{2.5} + CO₂ (≤0.25 mol O₂/mole CO₂ is used).

In fact, perovskite-structured (ABO₃) materials, which flexibly accommodate alkali earth cations in their A-site and transition metal cations in their B-site, represent one of many potential mixed oxides options that fit the abovementioned requirements. Perovskites are known for their excellent thermal stability and ability to undergo redox reactions, making them ideal for applications in high-temperature processes such as hydrogen production. By carefully tuning the composition and structure of these materials, we created sorbents with adjustable reaction enthalpies, allowing them to maintain stable, isothermal operation during the sorption-enhanced reforming/gasification process (Figure 2) [9].

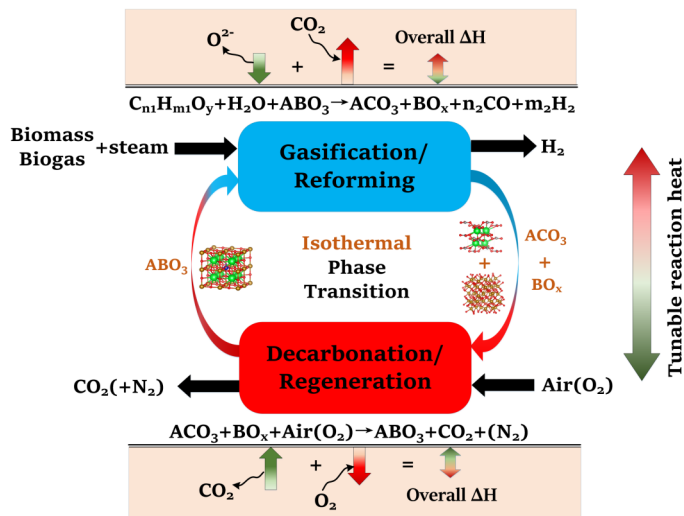
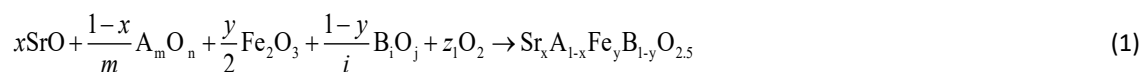


Figure 2. Schematic of the isothermal sorption-enhanced reforming and gasification (iSERG) concept utilizing perovskite-structured isothermal sorbents.[9]

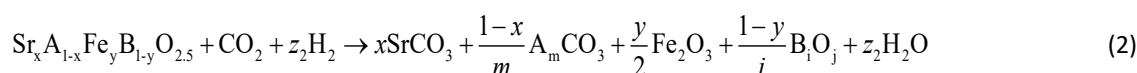
Sorbent Design and Screening

Using doped SrFeO₃ as the basis, i.e., Sr_xA_{1-x}Fe_yB_{1-y}O_{3-δ} (A = Ca, K, or Ba and B = Mn, Ti, Co, Cu, Ni, or Mg), our density functional theory (DFT) calculation-based sorbent design and screening process relies on thermodynamic feasibility of the following solid-state reactions:

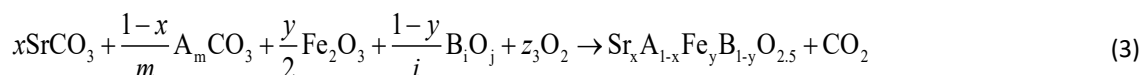
Synthesizability:



Sorption Reaction:



Desorption Reaction:



Following a general procedure outlined in Figure 3, we evaluated 1,225 perovskite structures for their ability to reversibly absorb and desorb CO₂, focusing on their thermodynamic properties and stability. The goal was to identify materials that could maintain high CO₂ sorption capacity while avoiding the thermal swing that is necessary for traditional sorbents.

From this screening, SrMnO_{3-δ} and related materials emerged as promising candidates. These materials demonstrated the ability to achieve a CO₂ sorption capacity of up to 78% through TGA experiments, far exceeding the required capacity for practical applications. Their uniquely flexible structure allows for the reversible incorporation and release of oxygen atoms, which is crucial for maintaining the redox cycle necessary for CO₂ capture and release. Our screening work also led to a useful correlation between thermodynamic parameters and sorption capacity, facilitating efficient sorbent optimization.

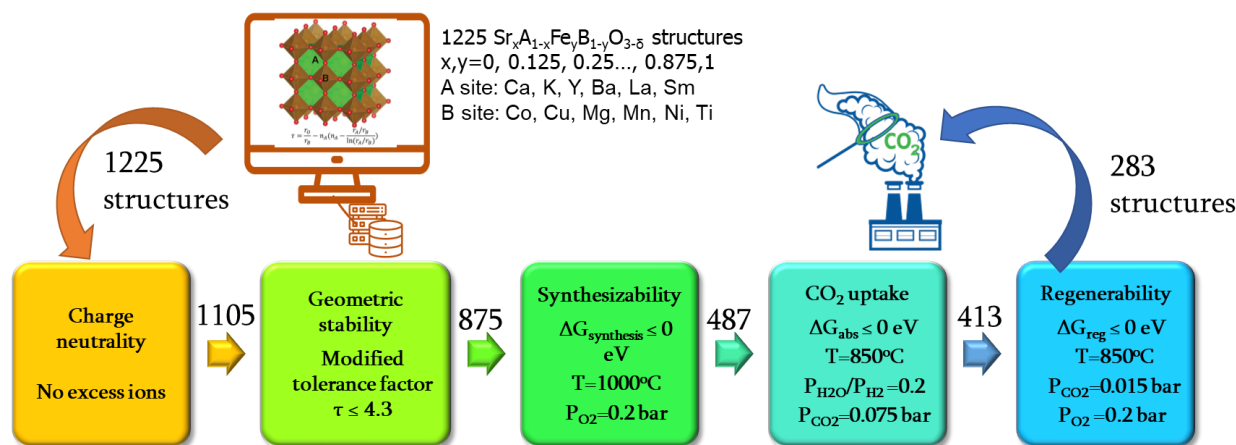


Figure 3. Computational screening workflow for iSERG sorbents. The values above each arrow represent the count of perovskite structures that successfully passed the preceding screening step.[9]

Experimental Validation for iSERG

To validate the practical applicability of the sorbents, we conducted a series of experimental to use the SrMnO₃ sorbent for reforming and gasification of methane, simulated biogas, woody biomass, as well as woody construction and demolition wastes in both lab-scale packed bed reactors and a small bubbling fluidized bed. Except for creosote treated wood (railroad ties), the sorbent was active to convert most, if not all the tar component in biomass, resulting in a clean, hydrogen rich syngas product. The results confirm the effectiveness of the sorbent and the feasibility of iSERG process (Figure 4). These tests also confirmed that the SrMnO_{3-δ} sorbents maintained high activity for CO₂

capture and release, even after repeated redox cycles. The results showed no significant degradation of the sorbents, indicating their potential for long-term use in industrial applications.

A key advancement of our research is the ability to achieve isothermal operation for CO₂ capture and hydrogen production. Traditional methods often suffer from the need to alternate between high and low temperatures, which increases energy consumption and can lead to sorbent degradation. In contrast, the redox-activated isothermal sorbents we developed operate effectively at a constant temperature.

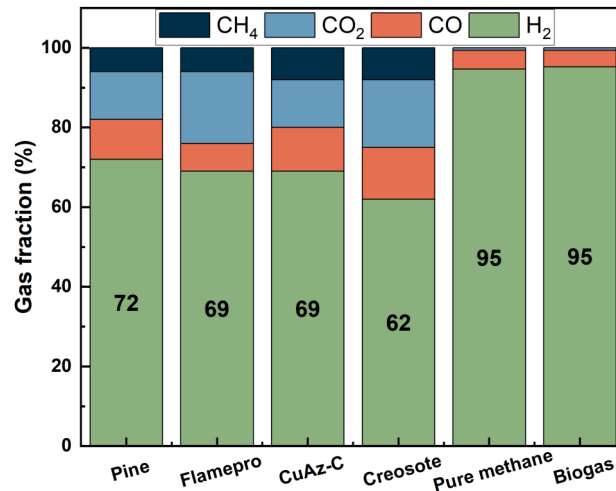


Figure 4. Hydrogen concentration produced from various biogenic feedstocks and methane.

The ability to maintain isothermal conditions is primarily due to the unique properties of the SrMnO_{3-δ} material. The perovskite structure allows for the controlled release and incorporation of oxygen atoms, facilitating the redox cycle necessary for CO₂ capture and release. This process is energetically favorable and helps maintain the structural integrity of the sorbent, even under continuous operation. Moreover, the sorbent can be regenerated with a small amount of pure O₂ to release near pure CO₂, facilitating in-situ CO₂ capture and carbon negative hydrogen from a life cycle analysis standpoint (Figure 5).

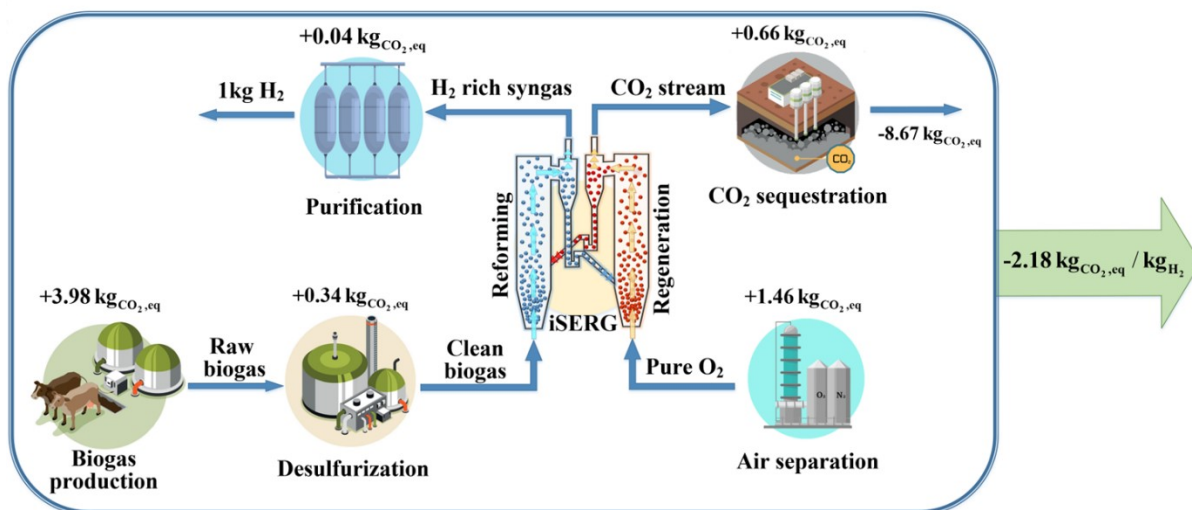


Figure 5. Schematic of the life-cycle analysis (LCA) for hydrogen production via the iSERG process. The global warming potential (GWP) was calculated based on a per kg H₂ basis. Recycle of the tail gas from the hydrogen purification step is not shown in this simplified schematic.[9]

The sorbents are also being characterized using advanced *in-situ* characterization techniques to map out the reaction

pathway, the rate limiting step, and optimization strategy for enhanced sorption kinetics. Our team is also working on kinetic modeling of complex sorbent reactions.

Scale-up Efforts and Future Directions

The development of redox-activated isothermal sorbents represents a step forward in biomass/biogas conversion and hydrogen production. By enabling efficient CO₂ capture under isothermal conditions, these sorbents offer a promising solution to the challenges of conventional hydrogen production methods. The reduced energy consumption and increased stability of the sorbents make them an attractive option for industrial applications, where cost-effectiveness and reliability are critical. While our experimental studies have been conducted at a lab scale to date, we are undertaking scale-up efforts in collaboration with PSRI (cold model study) and SEIN (hot unit), as shown in Figure 6. The cold model consisted of a gasification reactor and an air reactor (regenerator), both of which were operated under the bubbling fluidization regime for extended solid residence time (in minutes). An overflow structure was adopted to minimize the unreacted biomass char escaping from the gasifier to the air reactor. The solids were recirculated from the gasifier to the air reactor via a riser operated under the dilute phase pneumatic transport regime. The residence time of sorbents and biomass as well as the circulation rate all met the design requirements. The hot unit is currently under construction and is expected to be completed before the end of the year (Figure 6b). Scale-up synthesis of the sorbent particles is also currently underway.

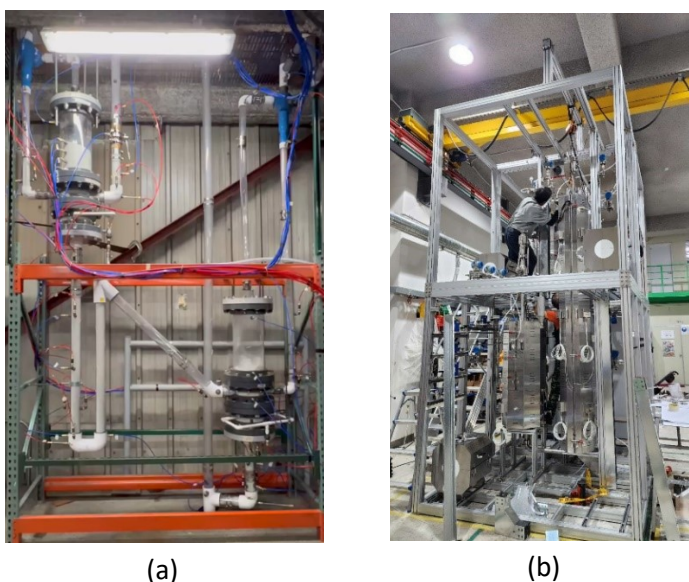


Figure 6 (a) The pilot-scale cold flow model for iSERG (in collaboration with PSRI); (b) the corresponding hot unit (under construction at SEIN).

We aim to use this article to showcase a potential application of particle technology combined with material design, optimization, and process intensification. Specifically, the iSERG approach leverages oxygen chemical potential as an additional degree of freedom to control CO₂ sorption and desorption more effectively than traditional temperature swings, particularly in reforming and gasification contexts. The sorbent also integrates air or CO₂ separation capabilities and offers the potential to control the overall heat of reaction and heat distribution between the gasification/reforming and regeneration steps. By tuning the surface properties of the sorbent, we can enhance its activity for tar conversion, resulting in a highly intensified process. The flexibility of perovskite (and other mixed oxide) structures provides a vast design space for the iSERG sorbent, making it an intriguing area for high-throughput screening, data-driven materials discovery and optimization, and self-driven labs.

From a practical standpoint, implementing iSERG at a relevant scale would require a well-designed circulating bed system. Additionally, the sorbent particles must be robust enough for fluidized bed operations, as indicated by our

lab-scale bubbling bed study. Thus, particle science and technology are crucial enablers for the success of this technology, as they are in many existing and emerging energy and chemical conversion technologies.

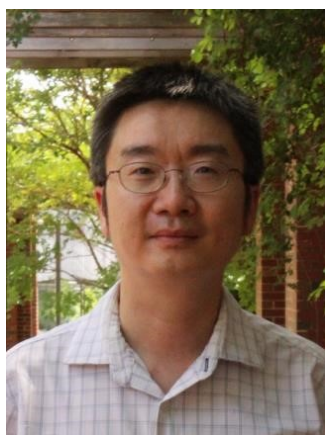
Acknowledgements

This work was supported by the U.S. Department of Energy Office of Energy Efficiency & Renewable Energy (no. EE0008809) and the US National Science Foundation (CBET-1923468). Other key contributors to the technical aspects of this work include my current and former group members at NC State: Dr. Kunran Yang, Dr. Xijun Wang, Ms. Mahe Rukh, and Mr. Leo Brody.

References

1. International Energy Agency, Global hydrogen review 2022, Paris, <https://www.iea.org/reports/global-hydrogen-review-2022>. (Access. Aug. 26th, 2024); 2022.
2. F. Dawood, M. Anda, G. M. Shafiullah, Int. J. Hydrogen Energy 2020, 45 (7), 3847-3869.
3. X. Zhao, H. Zhou, V. S. Sikarwar, M. Zhao, A.-H. A. Park, P. S. Fennell, L. Shen, L.-S. Fan, Energy Environ. Sci. 2017, 10 (9), 1885-1910.
4. L. Zeng, Z. Cheng, J. A. Fan, L.-S. Fan, J. Gong, Nat. Rev. Chem 2018, 2, 349.
5. A. M. Parvez, S. Hafner, M. Hornberger, M. Schmid, G. Scheffknecht, Renew. Sust. Energ. Rev. 2021, 141, 110756.
6. M. T. Dunstan, F. Donat, A. H. Bork, C. P. Grey, C. R. Muller, Chem Rev 2021, 121, 12681.
7. V. Manovic, E. J. Anthony, Environ. Sci. Technol. 2007, 41 (4), 1420-1425.
8. F. Li, R. Cai, M. Rukh, L. Brody, K. Yang, U.S. Patent, 63/503,508, 2024-05-17.
9. R. Cai, K. Yang, X. Wang, M. Rukh, A. S. Bosari, E. Giavedoni, A. Pierce, L. Brody, W. Tang, P. R. Westmoreland, F. Li, Energy Environ. Sci. 2024. (doi.org/10.1039/D4EE02119C)

About Authors:



Dr. Fanxing Li

Thomas M. Clausi Distinguished Professor in Chemical Engineering
Chemical and Biomolecular Engineering Department,
NC State University

Key Expertise Areas: Chemical reaction engineering, particle technology, chemical looping, catalysis, and chemical process intensification.

Dr. Runxia Cai

Tenure-track associate professor, School of Mechanical Engineering, Shanghai Jiao Tong University, 800 Dongchuan Road, Minhang District, Shanghai, 200240, PRC

Key expertise areas: My key expertise areas encompass various particle technologies, such as fluidized bed combustion, chemical looping gasification, thermochemical energy storage, as well as the design and numerical simulation of associated gas-solid reaction systems.

The work presented in this article was completed exclusively during Dr. Runxia Cai's postdoctoral research at NC State University before Oct. 2023.

Challenges With Handling Plastic Post-Consumer Waste (PCW)

Hans Schneider, Zeppelin Systems GmbH, Friedrichshafen, Germany

Harald Wilms, Wilms-ITC, Bremen, Germany

Introduction

The lifespan of plastic in various applications can be very short (e.g. single use drinking straws, bottles, packaging) or decades as in utility pipes and cables. Economy, ecology and public opinion are requiring industry to develop plastic PCW into a resource for new polymer, i.e. closing the loop to circularity. Thus, the recycling of plastic waste recently has become a growing industry which has to deal with many different and difficult to handle materials. This relates to the waste handling operations of bales from collection, sorting and washing of curb-side collected plastic but also to the handling and processing within plants for mechanical and chemical or advanced recycling.

Process Steps in Plastic Recycling

There is a vast number of recycling processes either in operation or under development which include a wide range of solids handling and processing operations – not all in the same sequence. The most economical recycling is mechanical recycling where cleaned and sorted waste is re-pelletized and can be used again in manufacturing of consumer goods. Multi-polymer, mixtures and blends may be preferably recycled through Advanced or chemical recycling where different physical, chemical and thermal processes are applied to produce chemical building blocks to be used for repeated polymerisation. Figure 1 gives a broad survey of all these operations. Of course, all process steps are connected by conveying operations and intermediate storage vessels to enable continuous operation.

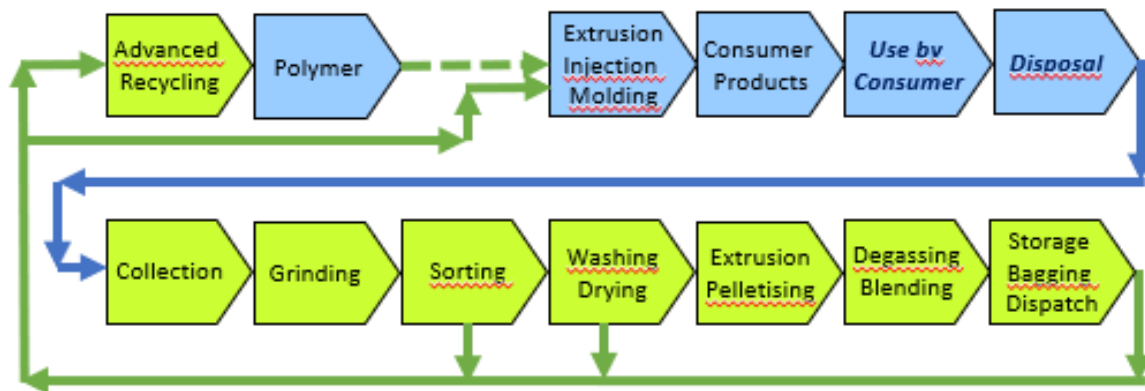


Figure 1: Overview of process steps in plastic recycling

The process steps are very versatile and meant to change the mechanical properties of the recycle plastic – either the composition, shape, size, or density. Therefore, the material along the recycling value chain is not uniform and not consistent and therefore difficult to describe.

Characterisation of Plastic Recycle

The difficulty in handling of plastic recycles results from certain properties which can best be described verbally like light, fluffy, flaky, soft, compressible, interlocking, irregular, brittle, spongy, elastic, compressed, agglomerated and so on. This variance of descriptions for the bulk material applies also for the individual particles which may range from flat to spherical, from square to elongated, from dense to light, from rigid to flexible, from hard to soft, from fibrous to curly – to name a few. The nightmare for process and equipment design engineers is the inconsistency of these properties what makes it impossible to apply specific design rules known from handling of 'ordinary' bulk solids. Due to the inconsistency and unpredictability the handling and processing equipment needs to allow for a broad distribution of all these properties – leading from expensive overdesign to malperformance. One common goal in many processing steps thus is to create a more uniform particle morphology for more easy and reliable handling.

Handling Behavior of Recycle Plastic

The low bulk density reduces the gravity effect on flowability. In general, the inconsistent and frequently poor flowability of plastic recycle require larger cross-sections of hopper openings to prevent arching. Mechanical means like screws to initiate and maintain flow are frequently used techniques. Belt conveyors, especially for sorting and Z-shaped elevation are suitable means of transportation. Dilute-phase conveying with low solids-to-air-ratio is an option

provided reliable feeding into the conveying line is possible - but may lead to further degradation with associated problems. Dense-phase conveying typically is no option due to the irregular shape and packing of the recycle plastic which does not allow stable and reproducible gas flow through the packed slugs in a conveying line thus preventing development of stable operating conditions.

The handling characteristics of various plastic waste depends on the source of waste and subsequent processing operations – as outlined in Figure 1. For instance, the regrind from plastic containers, bottles and other thick-walled, ‘massive’ plastic goods (e.g. window profiles, automotive parts, toys, household goods) – mainly produced from polyolefins and engineering plastics and their compounds - are the recycling materials most easy in handling (Figure 2). Their particle size is close to plastic pellets and the rough shape of irregular particles does not tend to interlocking. Arching is a minor problem, unless humidity or residual liquids generate a substantial cohesion or time consolidation. Pneumatic dilute-phase conveying generates a significant amount of fines and streamers. Flow from silos and hoppers does not require very large outlets.



Figure 2: Typical washed plastic regrind

Flakes from thin-walled ground PET bottles after washing are usually hard and stable with little fines and fibers (Figure 3). Due to the compressibility these particles tend to form arches in converging hoppers. To prevent arching, these flakes shall be subjected to only low compressive forces or low levels of fill in dosing equipment or hoppers. Mechanical discharge devices like screws and ploughs are suitable for reliable discharge and flow. Pneumatic dilute-phase conveying is possible, but will generate increasing fines level. The larger the particles become, the poorer the flowability will get due to interlocking and layering of particles into domes.



Figure 3: Typical washed PET bottle regrind

Handling of plastic film scrap like from shopping bags, packaging or agricultural film, becomes a challenge whenever the particle size gets fibrous or elongated, especially if the fill is still containing residual liquids or other contaminants (Figure 4). Handling becomes difficult and force is needed to move the packages of shredded and intertwined stripes or sheets of film. Mechanical conveying by belt conveyors is best means of transportation or very large screw feeders. Hoppers need extracting discharge devices and should serve more like a chute than a silo. Starve-feeding is recommended.



Figure 4: Typical shredded film

The low bulk density of shredded film, foam and lightweight packaging results in low gravitational forces – also to destroy arches in hoppers due to their own weight. Thus, densification or compaction is one means to improve the handling behavior – besides reducing the required volume for storage and transport. Typical means of compaction are friction agglomerators. The resulting agglomerates are dry due to the heat generated by friction of the plastic waste being squeezed through a set of rotating discs. The resulting particle size is typically in the range of several millimeters (Figure 5). The particles are rather stable and brittle. With increased heat, the surface may become smooth from melting and solidifying. The disadvantage is that this compaction step is energy-intensive. Storage, flow and pneumatic conveying are rather simple as long as the conveying distances are not too long and attrition turning the agglomerates into some sort of a light powder which can cause arching and discharge issues.



Figure 5: Typical recycle friction agglomerates

Another method of turning plastic waste into more easy to handle pellets is using a roller press (Figure 6). This process produces cylindrical pellets. Depending on the throughput, level of densification and temperature, these pressed pellets will gain a different level of strength. Typically, the outer cylindrical surfaces become strong and consolidated while the center remains in a softer state. Depending on the achieved hardness, these pellets can be pneumatically conveyed, but impacts may break the cylinders and then result in a light fluffy material with poor handling characteristics.



Figure 6: Typical pellets from a roller press

A very obvious example for the requirement of compaction or densification is foam from various packaging of insulation or cushioning applications (Figure 7). This foam may come very irregular shapes and sizes.



Figure 7: Typical shredded polyurethane and polystyrene foam

Technical applications frequently require reinforcement of polymers with glass or carbon fibers (Figure 8). Regrind of these materials contain a large amount of free and broken fibers which result in increased wear on the equipment. Segregation processes, e.g. in silos, may result in accumulation and agglomeration of light fibers into nests which are difficult to discharge from feeding hoppers.



Figure 8: Typical regrind with carbon and glass fiber reinforcement

Another type of very fluffy recyclates is residue from fibers and textiles as depicted in Figure 9. They have no longer any distinct geometry or size except their long fibrous shape and their intertwined nature. These products are very difficult to handle – maybe comparable to agglomerates from streamers or birds' nests. They can hardly be disintegrated again except by chopping.



Figure 9: Typical residue from woven and non-woven fibers and textiles

Special attention has to be given to multi-material waste, e.g. aluminum-laminated film or multi-layer plastics. Since these materials are difficult or impossible to sort for mechanical recycling of sorted plastics, they may be best recycled in advanced recycling processes. These processes also need a continuous and reliable feed of well-defined particles and thus should preferably use press agglomeration for pre-processing.

Testing of flowability and conveying behavior, especially attrition and particle breakage, are mandatory for successful equipment design. Flowability tests are certainly approaching their limit with many recycle materials, especially with bulk solids deviating strongly from 'normal'. No standard test equipment exists yet, but development is being pushed (see section on Research Requirements below)

Since characterisation by established means of powder mechanics may become difficult to impossible, it definitely is important to characterise products at least by a minimum set of data (particle and bulk density, particle hardness, compressibility, wall friction, humidity, chemical composition, ...) plus photos demonstrating particle shape. The listing of properties as given in FEM 2581 may serve as an initial guideline for communication purposes between equipment supplier and client, but can be altered or extended to fit special purposes.

The variability of particle sizes and shapes as well of bulk density is very wide, making characterisation very difficult. The following table gives a survey of widely accepted definitions and properties of plastic recycle materials. This can serve as an indication for description of respective materials – and what to expect. Handling problems may also result from contamination of the plastic waste. Residue of aluminum lids, e.g., can block rotary valves feeding a conveying system.

Table 1: Survey of typical plastic recycle materials characteristics

Typical Characteristics of Plastic Recycle Materials					
Type of Recycle	Particle Size, mm	Particle Thickness, mm	Shape	Bulk Density, kg/m ³	Origin
Plastic Regrind	2 - 5	1 - 4	irregural, chunky	250 - 500	Household, PE Bottles
Bottle Regrind / Flakes	3 - 8	0,2 - 1	flat	250 - 350	PET Bottles
Shreddered Film	2 - 100	0,05 - 0,2	flat, twisted, intertwined	150 - 250	Packaging & Agricultural Film
Friction Agglomerate	2 - 8	2 - 8	irregular, chunky	250 - 350	Compactor, Agglomerator
Press Agglomerate	3 - 12	5 - 25	cylindrical	300 - 350	Roller Press
Shreddered PU foam	any	any	any, irregular, fluffy	30 - 150	Insulation, Cushoning
Shreddered PS Foam	5 - 300	5 - 200	any, irregular, lengthy	30 - 150	Packaging
Fiber Reinforced Plastic	5 - 100	2 - 15	any, irregular, lengthy	300 - 600	Vessels, Sport, Automotive, Blades
Non-woven & woven Fibers	any	any	any, knoted, coiled, intertwined	250 - 650	Clothing, Yarn, Fishing & Marine

Challenges in Handling Recycle Materials

The description and especially the photos above already indicate challenges for any system or equipment design engineer – or even more for purchasing agents in engineering or operating companies. The biggest challenge is the heterogeneity of the materials and the wide range of properties, as also can be seen from the above Table. This heterogeneity makes it extremely important, but also extremely difficult to get representative samples. Samples taken from one bale may be different in chemical and mechanical properties from another bale, truck load, shredder or collection area or sampling period. Also, seasonal fluctuations may occur. Getting ‘a’ sample already is difficult – getting a representative sample from a heterogeneous material such as plastic recycle is even more difficult and often a real challenge. Sampling, with all its statistical parameters and relevance, is a science [1] frequently ignored. Referencing specific samples for specific design and performance requirements becomes mandatory for each supplier.

Materials somewhat similar to plastic recycle are biomass or fibrous materials, which also may be interlocking, moist and inconsistent or heterogeneous. Thus, tensile testers as under development for fibrous materials [2] may also be useful for plastic recycle, especially for recycling of trim residue from extrusion and calendaring [3].

Characteristics of Material Handling Equipment

The difficulty in handling does not result from individual particles with odd properties, but from the aggregation of these particles in form of bulk solids, i.e. a continuum of particles interacting with each other and any kind of boundary set by any type of apparatus. The challenges thus result from the range of properties to be considered, especially since heterogeneity, different degrees of interlocking, compressibility and moisture content each will have a significant influence on design and performance.

Typically, the more fluffy materials [4] – think of shredded foam - are compressed the less they tend to move voluntarily without expanding into open space. Therefore, either preventing compaction or forcing movement out of a vessel by means of extraction have become two favored methods for gravity flow feeders: Horizontal compaction can be reduced in diverging hoppers with single or multiple screws at the bottom transporting the recycle materials horizontally [3] or rotating dischargers [5] forcing the material into an open space.

Metering and dosing become easy once the bulk material is no longer under compression or compaction. If the interparticle contacts are minimized, then handling becomes less of a challenge. Thus, discharge and metering typically need to get separated into two steps. Feeding of metered amounts into reactor vessels, e.g. in chemical recycling or gasification can best be accomplished via lock hoppers which may even get rather small and operate at numerous short cycles ('batches') to allow an almost continuous feeding.

Giving room for expansion has also resulted in the successful application of gravity blenders with a central pipe and multiple lateral intake openings allowing horizontal flow into the central pipe due to baffles above the intake openings. Conventional bin design and shear testing principles may help – especially for measuring wall friction -, but also reach their limits if the recycle materials gets too fluffy, too interlocking, too compressible – in short: too difficult. Then only tests in pilot-scale facilities can help [3].

Research & Development Requirements

This illustrated survey of plastic recycle demonstrates the difficulty and complexity to characterise these products and to describe their handling behavior, flowability and conveyability. The existing methodology and models for characterization of bulk solids e.g. with shear cells cannot be applied for this group of materials. To overcome this situation, the WPMP (Working Party on the Mechanics of Particulate Solids) of the EFCE (European Federation of Chemical Engineering) is setting up research activities to investigate testing methods and determine relevant properties. The projects in this joint research approach are also meant to serve as an education platform for ESRs (Early Stage Researchers). Ideas of research projects and applications are currently collected.

Since industry and market development resulting from public interest cannot wait until these important research activities are completed, characterisation methods are being developed by industry. The methods are based on measuring some sort of resistance to compression and reconstitution after a previous pressure is reduced – a typical example of anisotropy. Figure 10 demonstrates how fluffy or elastic recycle materials may react to compression and release of pressure - also by reducing the weight of the material above. The packed recycle materials do not recover complete elastically from compression, but also retain a plastic deformation and change in packing structure influencing their flow behavior. These effects may also depend on time, i.e. the reconstitution may take not only a free volume to expand into, but also time.

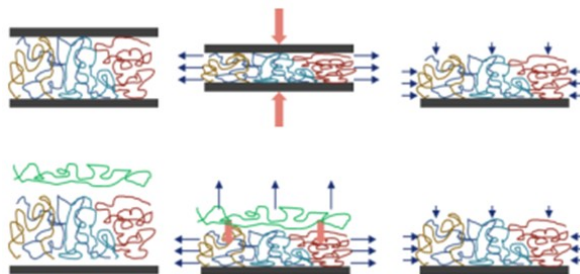


Figure 10: Reaction of elastic/irregular/fibrous materials to compression – theoretical model

Respective tests can be carried out in a compression tester as shown in Fig. 11. The fluffy material is placed in a transparent cylinder and then is loaded vertically before releasing the vertical pressure.

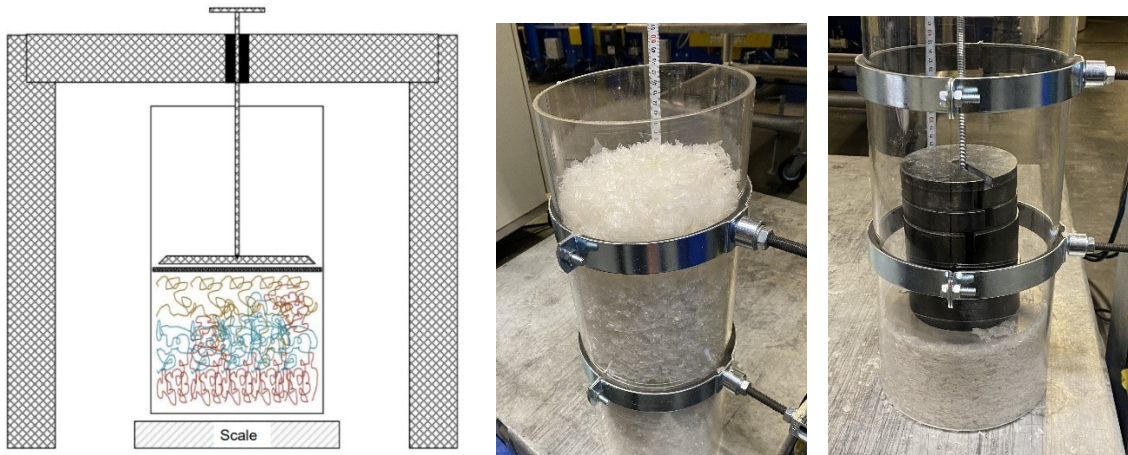


Figure 11: Testing the compression behavior of elastic/irregular/fibrous materials

In order to investigate, quantify and understand these effects, Zeppelin has recently developed and built a special transparent test silo with total flexibility in geometry. The width of the rectangular bin and the lower walls can be adjusted in inclination and outlet width to study the development of flow and the formation of bridges for any specific material in question. This allows to investigate and visualize the flow behavior of fluffy materials. Figure 12 shows the variability of the test silo geometry and an example of flow development. The ultimate goal will be a prediction of flow behavior in large silos based on lab scale tests.

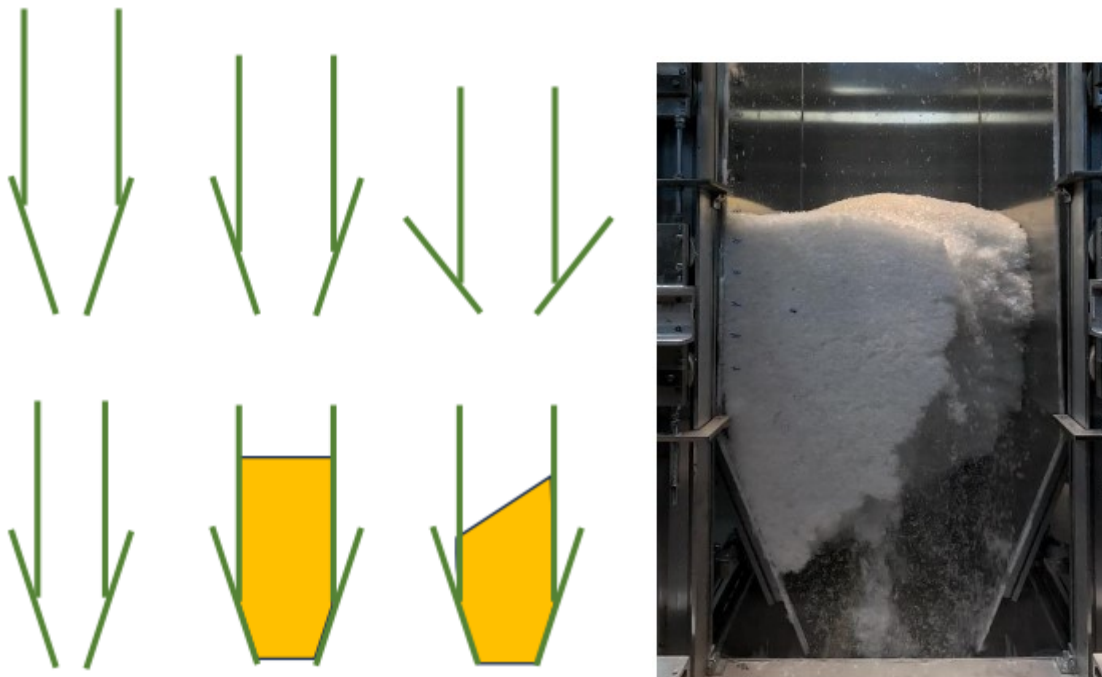


Figure 12: Variability of test silo geometry and flow propagation of fluffy material

Conclusion and Outlook

The complexity in bulk solid characteristics and behavior is significantly increased in the recycling industry. New methods of testing need to and are being developed in industry and academia. This will result in more reliable solids handling equipment design. Until then, testing and comparison with experience and expertise are the most relevant contributors to successful plant design and operation. Of course, one major element is also maintaining a product as consistent as possible with the least variability. This also can be supported by stable pre-processing steps.

References

- [1] Sommer, K., Sampling of powders and bulk materials, Springer, Berlin, 1986
- [2] Beitz, S. et al., Development and validation of an analytical method for tensile strength determination of fibrous bulk solids, Advanced Powder Technology 32(4), October 2021
- [3] Schneider, H., Case Study: Silo and System Design for Fibrous Recycling Materials, Abstract, CHoPS 2022
- [4] Beitz, S., Fluff-TEC – Zeppelins Weg zum Handling von Recyclingmaterialien, LIAN- Symposium 2024, Hochschule Zwickau
- [5] Wilms, H. Examples for Handling of Post-Consumer Plastic Waste, Abstract, CHoPS 2022

About Authors:



Dipl.-Ing. Hans Schneider (hans.schneider@zeppelin.com) studied mechanical engineering and process technology at the TU Kaiserslautern with focus on solids handling and modelling of gravity blenders. For more than 25 years he is working in process technology and R&D at Zeppelin Systems. During his career he was actively working on process solutions in silos, developing models and industrial solutions for silo blending, fixed and moving bed silo technologies. Further activities are in the field of pneumatic and hydraulic conveying of solids and related equipment. Currently he holds the position of Vice President Technology & Innovation. He is a member of numerous bulk solids handling working parties.



Dr.-Ing. Harald Wilms (harald@wilms-itc.com) studied mechanical engineering and process technology at the TU Braunschweig, where he also received his Ph.D. for his research on loads in silos. He worked for more than 30 years in development, technology, project management, sales, and business development in plant engineering for bulk solids handling. Since 2018 he works as an independent consultant for bulk solids handling and training. He is the author of more than 150 technical papers and a member of several bulk solids handling working parties.

Job Posting

Solids Processing Research Scientist

Dow's Plastics & Hydrocarbons R&D organization has an exciting opportunity for a talented & motivated **Research Scientist** with expertise in Solids Processing and Handling (particle technology) in our New Process Technology Development organization. This organization is responsible for process research & development, technology implementation, and troubleshooting across all technology platforms and global assets aligned to our Plastics & Hydrocarbons businesses. As a member of this team, you will work closely with capital project & engineering teams as well as our technology centers to conceptualize, innovate, and design new processes. While the group has a global presence, the current position will be located in **Lake Jackson, TX** at our Texas Innovation Center – a premier work environment with modern offices & laboratories equipped with the latest technology.

The key responsibilities for this role will be to provide technical expertise in the areas of solid particle conveying (pneumatic and mechanical), silo storage, fluidization & fluidized bed processes, drying, coating, feeding/dosing, classification, separation technologies (solid-solid, gas-solid, solid-liquid), mixing/blending, particle engineering, sustainability, and plastics circularity. The ideal candidate will bring in-depth expertise and practical knowledge across a breadth of these solids processing technology areas, and apply scientific principles for innovation, troubleshooting and problem solving.

Key Responsibilities / Duties:

- As the subject matter expert (SME) on solids handling & processing, support R&D and manufacturing organizations for product development, process innovation and troubleshooting.
- Support solids processing aspects of sustainability project in plastics & hydrocarbons.
Coach and mentor junior scientists and technologists.

Required Qualifications:

A minimum of a Master's degree in Chemical Engineering, Mechanical Engineering, or Process Engineering is required; emphasis on solids processing & handling (particle technology) strongly preferred

Minimum of 5 years of relevant experience specifically in the field of solids processing after graduation with the highest degree

Preferred Qualifications:

- PhD with emphasis in solids processing / particle technology
- Prior industrial experience in pilot plant or manufacturing plant operations, ideally involving design and troubleshooting real world problems and developing innovative & practical solutions
- Proven track record of high performance and ability to convert complex technical issues into straight-forward value propositions
- Ability to generate and interpret data to make statistically relevant conclusions that will be used for process development and design

Note: Domestic relocation assistance is available for this role and may be provided based on eligibility.

Dow Offers:

- A robust total rewards program, including: competitive base pay, variable pay that rewards individual, team, and Company performance, and comprehensive benefits
- On-going learning opportunities within a diverse, inclusive and rewarding work environment
- Career experiences that can span different Dow businesses and functions with opportunities for personal and professional growth
- The chance to work within a global company and interact with colleagues from around the world
- Opportunities that spark your imagination and ignite your passion to help others

Please contact Dr. Shrikant Dhodapkar (sdhodapkar@dow.com) to apply for the position.

PTF Awards and Dinner Sponsors



**Sponsor of the
Lifetime Achievement
Award**

ELSEVIER



Shell Global Solutions
**Sponsor of the
Thomas Baron Award**



The Dow Chemical Co.
**Sponsor of the
Particle Processing Award**



**Sponsor of the Lectureship in
Fluidization Award**



**Sponsor of the
Young Professional Award**



University of Pittsburgh
University of Pittsburgh Alumni
**Sponsor of the
George Klinzing Best PhD Award**



**Sponsor of
PTF Service Award**



Sponsor of PTF Awards Dinner



**Sponsor of Student Poster Competition
Award**



Particle Technology Forum Organization

PTF OFFICERS

CHAIR
 Dr. S.B. Reddy Karri
reddy.karri@psri.org



CO-CHAIR
 Dr. Maria Silvina Tomassone
silvina@soe.rutgers.edu



TREASURER
 Dr. Heather Emady
Heather.emady@asu.edu



PAST CHAIR
 Dr. Jim Gilchrist
gilchrist@lehigh.edu

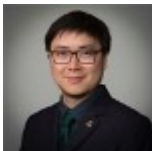


PTF EXECUTIVE COMMITTEE (INDUSTRY)

◆ Dr. Wyatt Casey LaMarche
casey.lamarche@gmail.com



◆ Dr. Yi Fan
yfan5@dow.com



◆ Dr. Mayank Kashyap
mkashyap@sabic.com



◆ Dr. Shankali Pradhan
shankali.pradhan@merck.com



PTF EXECUTIVE COMMITTEE (ACADEMIC)

◆ Dr. Bodhi Chaudhuri
bodi.chaudhuri@uconn.edu



◆ Dr. Maria Silvina Tomassone
silvina@soe.rutgers.edu



◆ Dr. Alexandra Teleki
alexandra.teleki@scilifelab.uu.se



◆ Dr. Sheena Reeves
smreeves@pvamu.edu





LIAISONS AND COMMITTEE CHAIRS

CTOC Liaison	Dr. Ah-Hyung (Alissa) Park	ap2622@columbia.edu
Nominating Committee Chair	Dr. Maria Silvina Tomassone	silvina@soe.rutgers.edu
PTF Newsletter Editor	Dr. Shrikant Dhodapkar	Sdhodapkar@dow.com
PTF Webmaster	Dr. Yi Fan	yfan5@dow.com
PTF Student Workshop Chair	Dr. Ben Freireich Dr. Aaron J. Moment	bfreireich@originmaterials.com ajm2293@columbia.edu
PTF Programming Chair	Dr. Ben Freireich	freireib@gmail.com
PTF Dinner Sponsorship	Dr. Maria Silvina Tomassone	silvina@soe.rutgers.edu
PTF Awards Sponsorship	Dr. S.B. Reddy Karri	reddy.karri@psri.org
PTF Education Committee Chair	Dr. James Gilchrist	gilchrist@lehigh.edu
Staff Liaison	Mr. Todd Caparizzo	toddc@aiche.org
Staff Liaison	Ms. Mike Livsey	tinam@aiche.org
Accounting	Ms. Leila Mendoza	leilm@aiche.org

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.