U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Advanced Manufacturing Office

Process Intensification Workshop

September 29-30, 2015
Alexandria, VA

The DOE Office of Energy Efficiency and Renewable Energy (EERE)'s Advanced Manufacturing Office partners with industry, small business, universities, and other stakeholders to identify and invest in emerging technologies with the potential to create high-quality domestic manufacturing jobs and enhance the global competitiveness of the United States.

This document was prepared for DOE/EERE's AMO as a collaborative effort between DOE AMO, Energetics Incorporated, Columbia, MD and New West Technologies.

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1. WORKSHOP EXECUTIVE SUMMARY

The Department of Energy's Advanced Manufacturing Office (AMO) held a workshop on Process Intensification (PI) to gather inputs from stakeholders on the vision of future opportunities and technical challenges facing development and scale-up of materials, process, and equipment that can make step-change improvements of PI system performance. Several themes, which emerged throughout the workshop, are interconnected and contribute toward the vision of rapidly deploying cost-effective, innovative new materials and technologies.

Key findings are:

- **Focused Institute Effort to Support Highly Diverse PI Applications**: An institute could provide small and medium manufacturers access to research and demonstration (R&D) capabilities and resources, and could assist smaller companies to drive innovation and allow for maturing of technologies. It could assist in the creation of user test beds where academia, laboratories, and industry can work and validate new materials/processes and aid in transferring technology to market. However, a successful PI institute will need an appropriately bounded scope of work. Given the diversity of potential PI applications and associated equipment and conditions, creating an institute capable to suit all industry needs is not feasible. Scope must be optimized to ensure as broad a reach as possible without overextending capabilities. A too-narrow focus might also limit the number of interested parties or artificially prevent innovative research.
- **Modular Applications**: As opposed to the traditional manufacturing models involving large centralized facilities, a new paradigm involving modularity and geographically scattered feedstocks was considered. New technologies should be easily added to existing processes using a plug-and-play development approach. Challenges to replacing current in-plant processes with new modular systems include reducing the risks and costs associated with downsizing manufacturing processes where adoptability is key. Also, modular capital planning versus economies of scale capital planning is a major barrier to implementing modular technologies.
- **Shared Knowledge**: Key to successful research into the PI of chemical reactors and reactions is access to a shared body of knowledge on this topic. Information in the PI field is not readily transparent, and any advances could likely affect or be applied to multiple facilities and companies.
- **Industrial Motivation and Value Proposition**: Ways to encourage and motivate industry toward PI were identified as key to developing and deploying technologies and reaping potential energy savings. A strong business case for new PI technologies is needed, including an assessment of the benefits of energy productivity and energy efficiency. Energy productivity needs to be coupled with a payback period and the return on investment. Technology development and economic analysis are needed to explain the cost-benefit of new PI methods. Studies are also needed to determine scaled-down and cost effective approaches for new PI technology.
- **Advanced Materials and Characterization**: Innovative materials and processing techniques have the ability to enable PI. These materials could lead to increased performance and/or decreased costs. For example, 3-D printing, low-cost sorbents, and metal organic frameworks are potential opportunities for advancement. Improved methodology is needed to characterize material properties (including thermos-physical and thermodynamic properties) and quantify property changes during operations in harsh environments. Graded materials are a potential area for development.
- **Technology to Market Considerations**: A better process is needed for transitioning breakthrough technologies to industry through an institute, center of excellence, or shared demonstration facilities. For example, test beds or pilot demonstrations where academia, laboratories, and industry can work together and validate new materials/processes would accelerate technology commercialization. In addition, an environment is needed for identifying,

evaluating, prioritizing and moving the most promising technologies from laboratory-scale to pilot-scale; this environment would include partners, expertise, and funding – and is required for effective technology transfer.

Background

Process intensification (PI) is a set of often radically innovative principles ("paradigm shift") in process science, chemistry and equipment design, which can bring significant (more than a factor of two) benefits in terms of process and chain efficiency, capital and operating expenses, quality, and waste reduction, and process safety.[1] PI enables the reduction of a manufacturing plant, processing facility or equipment size while achieving enhancement in capacity, productivity or other production and commercial profitability objective. This is accomplished by efficient plant, facility or apparatus/equipment design and/or introduction of alternate process methods, which in-turn enables dramatic decreases in consumption and requirement of energy and/or other resources, processing time, process waste, etc. Successful introduction of PI to a chemical, thermal or other manufacturing process – while controlling the precise required environment to flourish – results in better products and sustainable processes which are safer, cleaner, smaller, cheaper, and more energy efficient than current processes and equipment.

Creating more efficient and safer chemical processing systems will reduce chemical sector energy use and greenhouse gas emissions and be highly beneficial to the sector's current growth. DOE's 2006 Chemical Bandwidth Study[2] and the DOE's 2014 U.S. Chemical Industry Energy Bandwidth Study[3] comparing exergy consumption for current industry norms, best commercially available technologies, emerging new technologies and theoretical limits in manufacturing processes identified the top energy consuming chemicals produced in the United States[4]. Of the 19.24 quadrillion British thermal units (quads) used in the overall US manufacturing sector in 2010, these chemical production processes utilized 1.15 quads and accounted for 63% of the total onsite energy consumed in the chemicals manufacturing industry. The updated energy consumption figures project a total opportunity for628 trillion British thermal units (TBTU)/year energy savings for 12 chemicals resultant from the successful development and implementation of new PI technologies and practices. Using a simplified assumption of $13.09/ MMBtu[5] for industrial energy, this equates to a potential annual cost savings of $8.2 billion for these 12 chemicals.

Benefits

Traditional chemical conversion and separation processes are typically thermally and volume-conversion driven. PI is a paradigm shift in transitional processing by enabling a move from centralized to distributed processing. This shift would drive a new equipment-manufacturing industry and enable a larger market penetration of clean energy and energy efficient technologies. Key markets include fuels, fine chemicals,

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[1] National Science Foundation Workshop on Process Intensification, October 2014, www.processintensification.org, Adapted from European Roadmap of Process Intensification. 2007

[2] Chemical Bandwidth Study. Draft. Prepared by JVP International and Energetics, Inc. for U.S. Department of Energy, Industrial Technologies Program. 2006.

[3] Chemical Industry Energy Bandwidth Study. Prepared by Energetics, Inc. for U.S. Department of Energy, AMO. 2014.

[4] 12 chemicals (listed in descending order of energy consumption) are Ethylene, Ethanol, Chlorine/ Sodium Hydroxide, Ammonia, Nitrogen/Oxygen, Propylene, Terephthalic Acid, Carbon Black, Ethylene Oxide, Methanol, Hydrogen, Sulfuric Acid

[5] Based on a simplified value of $13.091 / MMBTU (calculated average of the industrial price of electricity and natural gas) EIA 2014: http://www.eia.gov/electricity/annual/html/epa_01_01.html and http://www.eia.gov/dnav/ng/hist/n3035us3m.htm

and specialty chemicals, where there is a particular opportunity in using distributed biomass, waste sources, and stranded natural gas. Another pertinent market is flow batteries for grid-scale energy storage. Moreover, next generation PI technologies will support the development of new processes to enable innovative business models and provide new opportunities to produce better products. PI technologies supplement the implementation of related manufacturing applications including just-in-time and distributed manufacturing, as well as modularization for scale-up and improved construction and integration.

Other benefits include

- Reducing upfront capital / risk to encourage investments in clean-energy technologies, enabling distributed processing that take advantage of regional economics and stranded energy assets (e.g., biomass, waste streams, wind, natural gas, and solar).
- On-site toxic and/or hazardous chemical production increasing safety due to reduced risks in transportation and storage.
- Reducing time to market for new investments, which can reduce the risk from market changes prior to a process coming on-line.
- Flattening the economy-of-scale curve for equipment and processes through novel concepts in process integration, small-scale unit operations, PI, and manufacturing approaches. Examples include micro-channel conversion and separation processes.
- Shifting equipment fabrication and assembly from on-site to factories with controlled environments, consistent highly-trained labor, better quality control, and more amenability to advanced manufacturing, automation, and control.
- Adopting advanced-manufacturing processes including those that reduce material waste such as selective laser melting (SLM) and incremental forming. This change is of particular importance when expensive materials are required, such as high-temperature alloys for steam reforming of natural gas.

Workshop Overview

The U.S. Department of Energy (DOE) held a Process Intensification Workshop on September 29-30, 2015. Representatives from industry, academia, DOE national laboratories, and non-governmental organizations gathered in Alexandria, Virginia to hear keynote addresses, expert panel discussion, and participate in workshop breakout sessions. Discussion topics focused on challenges and opportunities for PI technologies.

Manufacturing remains the essential core of U.S. innovation infrastructure and is critical to economic growth and national defense. Experts point to a gap in the innovation continuum that exists between R&D activities and the deployment of technological innovations in the domestic production of goods. Concerns have been raised that this gap could have long-term negative consequences for the economy and the defense industrial base. As global competition to manufacture advanced products intensifies, the performance of the country's innovation ecosystems must improve. Industry, academia, and government partners need to leverage existing resources, collaborate, and co-invest to nurture manufacturing innovation and accelerate commercialization.

The Advanced Manufacturing Office (AMO) within DOE's Office of Energy Efficiency & Renewable Energy (EERE) partners with private and public stakeholders to improve U.S. competitiveness, save energy, create high-quality domestic manufacturing jobs and ensure global leadership in advanced manufacturing and clean energy technologies. AMO invests in cost-shared research, development and demonstration (RD&D) of innovative, next generation manufacturing processes and production technologies that will improve efficiency and reduce emissions, industrial waste, and the life-cycle energy consumption of manufactured products. The results of these investments include having manufacturing energy efficiency harnessed as a competitive advantage, and cutting-edge clean energy products competitively manufactured in the United States. AMO is particularly interested in the challenges associated with advanced manufacturing technology that might be overcome by pre-competitive collaborations conducted via a Manufacturing Innovation Institute (MII).

The workshop builds on two prior AMO Requests for Information (RFI): the first RFI, issued in the spring of 2014, solicited industrial and academic input on a broad range of cross-cutting technologies that could benefit from investment in a MII; the second RFI, issued in late summer of 2014, was more narrowly focused[6]. Through these RFIs, AMO sought information about the challenges associated with advanced manufacturing technology that could potentially be overcome by pre-competitive collaboration as part of a potential new Institute.

Panel Discussions

Two panels of subject matter experts (SME) provided their insights on the capability needs and research trends on PI. The panel on the first day composed of SMEs from non-government organizations (NGO) while the panel on the second day drew from industry experts. Biographies of the SMEs can be found in Appendix D.

Highlights of the NGO SME panel include:

- Dr. John Marra, a Senior Technical Advisor with the U.S. Department of Energy and former President of the American Ceramic Society, discussed PI efforts that were led by the ceramics industry in conjunction with DOE. These collaborations focused on improving the efficiency of existing processes (such as high-efficiency gas burners) and developing new processes and technologies (such as low-temperature fabrication techniques).
- Dr. Darlene Schuster of the American Institute of Chemical Engineers called on the workshop attendees to view PI broadly, as PI is the nexus of many fundamental areas of chemical engineering (such as transport processes and separations) and impacts many industries, including pharmaceuticals and water treatment, in addition to traditional energy-intensive industries.
- Mr. David Turpin of the Agenda 2020 Technology Alliance provided his view of two PI opportunities in forest products. The first opportunity discussed was an increase in process water reuse to achieve a 50% reduction in fresh water use. The second opportunity discussed was reduced paper drying energy requirements.
- Mr. Phil Callihan from the National Center for Manufacturing Sciences emphasized the role of collaboration between industry, national laboratories, academia, and government, and discussed how this collaboration feeds innovative PI research and development across supply chains.
- Mr. Denis King of the Institute of Electrical and Electronics Engineers USA Energy Policy Committee reminded participants of the potential for PI technology advancements to address clean energy technology needs, with emphasis on energy storage devices and advanced power electronics, to facilitate connection of renewables to the electric distribution system.
- Dr. Brian Paul, a professor from Oregon State University, Director of the Microproducts Breakthrough Institute, and representing the American Society of Mechanical Engineers, described the breadth of industries impacted by PI, among them power generation, transportation, and healthcare. Dr. Paul also discussed opportunities for advancing PI technology specific to solar thermochemical reactions.

[6] The areas of interest in the second RFI included advanced materials manufacturing, advanced sensing, control, and platforms for manufacturing, high-efficiency modular chemical processes, and high value roll-to-roll manufacturing.

Highlights of the industry SME panel include:

- Dr. William Ayers, CTO of Ayers Group, LLC, highlighted the importance of incorporating end-user needs in PI technology design. He provided an example of how end-user needs in the semiconductor industry drove a de-centralized modular production technology to satisfy chemical purity standards while increasing customer safety and reducing insurance costs.
- Mr. Billy Bardin of the Dow Chemical Company discussed key areas of PI focus within Dow, including energy utilization, process design and process flowsheet optimization, chemical conversion, waste minimization, advanced control and optimization, and distributed manufacturing. He also proposed metrics to measure the impact of PI, such as capital intensity, waste intensity, and raw material efficiency.
- Mr. David Constable of the American Chemical Society Green Chemistry Institute described current efforts in achieving less energy intensive alternative separations in the pharmaceutical industry. He highlighted activities that are designed to create an innovation roadmap to advance the rational design and predictable, widespread industrial application of less energy-intensive separation processes. He also identified efforts to prioritize RD&D needs for technology initiatives.
- Ms. Michelle Pastel of Corning Incorporated provided an overview of glass and optical fiber fabrication and process innovations at Corning Incorporated.
- Dr. Dane Boysen of the Gas Technology Institute provided his perspective of the scalability challenge that manufacturing industries face. He challenged workshop participants to change the paradigm of how PI is viewed, to go from monolithic solutions more modular ones, and to seek new open business models rather than niche applications.
- Mr. Gary Luce of the Eastman Chemical Company highlighted key barriers that prevent a company in incorporating new PI technologies. For example, innovative process efficiency changes can come into conflict with operational or product quality requirements. Also, users may resist new PI technology due to unfamiliarity.

Workshop Discussions and Breakout Sessions

The workshop discussions provided AMO with further information on both cross-cutting and specific manufacturing challenges as well as a basic rationale for an innovation institute, consistent with the missions of the DOE. Federal presentations given at the workshop are available at http://energy.gov/eere/amo/downloads/process-intensification-workshop-september-29-30-2015. Six breakout sessions were conducted.

The breakout sessions were:

- **Chemical Reactions and Reactors:** Chemical processes are energy intensive and entail high capital costs for chemical processing. Operations are also inefficient when not at full capacity, leading to low energy productivity when at reduced capacity utilization. Advancements in chemical reactions and reactors could lead to a 20-50% energy efficiency improvement in bulk chemical and petrochemical production, and a 50% reduction in costs for specialty chemicals.
- **Thermal Intensification – High Temperature Processes:** Significant energy is lost in thermal process heating systems that do not contribute to the desired material/product transformation. Opportunities to utilize transformational technologies to enable a shift away from relatively inefficient traditional heating processes to much more efficient advanced processes that utilize selective heating; alternative low- or non-thermal processes; and improved heat recovery systems. Of the 7.2 quads of process heating energy used in manufacturing in 2010, an estimated 0.9 quads could be saved through advanced processes with many applications exceeding a 50% reduction in energy requirements.

- **Mixing and Mass Transfer:** Mixing and mass transfer are key to manufacturing operations. Improvements in mixing and mass transfer could achieve significant reductions for processing time and improve efficiencies. In some applications, time requirements for specific processing operations could be reduced by more than 50%.
- **Chemical Separations and Crosscutting Technologies:** Separation technologies are estimated to consume 22% of in-plant energy use in U.S. manufacturing, with particularly high usage in the chemical industry. Membranes and other advanced separation processes could reduce the required chemical separations energy by 20-45% for specific high volume chemicals.
- **Other Process Intensification Applications – Water, Food, and Energy:** Many manufacturing processes are not designed with full consideration of the life-cycle aspects of energy, materials, and water. PI approaches can be undertaken in areas such as food processing, water treatment, and energy transformation to significantly reduce operating costs. For example, industrial water treatment energy requirements could be reduced by more than 50%.
- **Environmental Management:** Opportunities abound to achieve more sustainable operations and reduce environmental impacts. Greater recovery and recycling of in-plant wastes and increased end-of-life recycling are just two opportunities. Over 200 TBTU of energy could be saved by increased by increased utilization of recycled material in five selected industries alone.

Participants in each breakout session answered a different set of questions that were appropriate for the topic. At the workshop, participants identified mid-Technology Readiness Level (TRL) R&D needs, market challenges, metrics and impacts, and technology advancement considerations for PI.

For each breakout, one focus question and two to four supplementary questions were prepared in advance for detailed discussion. Participants were encouraged to identify and discuss synergies and indirect impacts of targeted research on other sectors.

Individual participant’s views and responses were captured using a compression planning and brainstorming process, which draws on small groups to identify and/or analyze information in a compressed time period using the focus questions and story boards for real-time capture of ideas.

Highlights from the breakout group discussions and questions posed are outlined in the following chapters; full responses from each breakout are included in Appendix B. The Appendices also include the meeting agenda (Appendix A), a combined list of participants from all the breakout groups (Appendix C), and an acronym list (Appendix E).

2. SUMMARY OF RESULTS

Chemical Reactions and Reactors

Process intensification (PI) has been practiced in the chemicals manufacturing industry for decades. Broadly, it encapsulates a host of ideas on ways to reduce energy, waste, and costs to increase the competitiveness of manufacturing operations. This breakout group broadly covered the concepts and ideas most closely related to chemical reactions and reactors. Reactors are central to chemical manufacturing, allowing manufacturers to precisely control the formation and breaking of chemical bonds to produce value-added products. Highlights of discussions are outlined below; the full results of discussions are provided in Appendix B.

> ***Framing Statement:*** *Chemical processes are energy intensive and entail high capital. Operations are also inefficient when not at full capacity, leading to low energy productivity when at reduced capacity utilization. Advancements in chemical reactions and reactors could lead to a 20-50% energy efficiency improvement in bulk chemical and petrochemical production, and a 50% reduction in production costs for specialty chemicals.*

Discussion was not limited by existing operational definitions of PI; any concepts or technologies that represent an improvement over the industry standard were within scope. Note that many of the same operations and processes targeted by PI research in chemical manufacturing have analogues in other sectors (e.g., food manufacturing, mining).

BARRIERS/CHALLENGES FOR CHEMICAL REACTIONS/REACTORS

Shared Knowledge: Key to successful research into the PI of chemical reactors and reactions is access to a shared body of knowledge on the topic. Information on PI is not readily transparent, and any advances could likely impact or be applied to multiple facilities and companies, beyond a single system. How best to expediently develop a method to share information while protecting intellectual property is also a challenge.

Industrial Motivation and Value Proposition: Ways to encourage and motivate industry toward adopting PI were identified as key to developing and deploying technologies and reaping potential energy savings. A strong business case for new technologies is lacking. Given the present low cost of energy, this may require considering other metrics like production or operating cost, use of raw materials or other resources, etc. PI research (e.g., when close to commercial deployment) could be a competitive advantage in a market of commoditized goods. The pre-competitive space is fertile ground, but may not necessarily have the same level of engagement and funding interest from industry. This is a larger concern when considering the financial viability of a potential PI Institute.

R&D NEEDS FOR CHEMICAL REACTIONS/REACTORS

Petrochemical Applications: Petrochemicals were identified as an area of interest for PI R&D and high impact. These highly integrated facilities produce a wide range of chemicals (e.g., ethylene, benzene, vinyl chloride) and consume large quantities of energy. The unique opportunity for petrochemicals afforded by abundant supplies of shale gas was also discussed, particularly transforming undervalued methane and alkanes to higher value chemicals.

Modular Applications: As opposed to the traditional chemical manufacturing model involving large centralized facilities, a new paradigm involving modularity and geographically scattered feedstocks was considered. Within this same context, micro-reactors were often mentioned because of their potential to enable operations not predicated on large economies of scales.

METRICS FOR CHEMICAL REACTIONS/REACTORS

Suggested Targets

- Energy reduction of at least 20% over the current state of the art.
- CO_2 emissions reduction of at least 15% over the current state of the art.
- Life-cycle cost analysis indicative of return on investment ROI less than 3 years; ROI multiple after 3, 5, and 10 years.
- Operating and maintenance (O&M) and capital cost lower than existing processes by 50% at pre-pilot stage.
- O&M and capital cost lower than existing processes by 20 to 25% at technological readiness level (TRL) 5.
- Cost reduction (per unit mass of product); e.g., cost reduction of at least 15% over current state-of-the-art.

INSTITUTE CONSIDERATIONS

Defining PI Efforts for Highly Diverse Chemical Manufacturing: Given the diversity of potential chemical reactions and associated equipment and conditions, creating a single institute capable of handling all possible reactors and technical challenges is not feasible. Performing technology validation on multiple reactor scenarios could necessitate hundreds, if not thousands, of hours of operation. While it would be desirable to have a multifunctional catalyst, it could easily be outperformed by a series of highly specific ones. Institute scope must be optimized to ensure a broad reach without overextending capabilities. A too-narrow focus might also limit the number of interested parties or artificially prevent innovative research.

Thermal Intensification – High Temperature Processes

Thermal intensification operations, also known as process heating, transform materials like metal, plastic, rubber, concrete, glass, and ceramics into a wide variety of consumer and industrial products. Industrial process heating processes such as heating, drying, curing, and phase change operations account for about 70% of process energy in the U.S. manufacturing sector. Highlights of discussions are outlined below; the full results of discussions are provided in Appendix B.

> ***Framing Statement:*** *Significant energy is lost in thermal process heating systems that do not contribute to the desired material/product transformation. Opportunities exist to utilize transformational technologies to enable a shift away from relatively inefficient traditional heating processes to much more efficient advanced processes that utilize selective heating; alternative low- or non-thermal processes; and improved heat recovery systems. Of the 7.2 quads of energy used in manufacturing for process heating in 2010, an estimated 0.9 quads could be saved through advanced processes with many applications exceeding a 50% reduction in energy requirements.*

CHALLENGES/BARRIERS FOR THERMAL INTENSIFICATION

Alternative Processes: The manufacturing process that currently depends on thermal intensification needs to be well understood and re-evaluated. Entirely new manufacturing technologies may be needed.

Flexibility in Processing: The development of thermal intensification processes should address siting logistics and the tradeoff between capital expenditures and operational expenditures per unit of production. Manufacturing processes should be designed to enhance production flexibility without decreasing energy efficiency across a range of utilization capacities. Scalability, turndown, and de-centralization are key considerations.

Advanced Materials: There is a limited availability of corrosion-resistant and high-temperature materials for improving manufacturing processes. Materials with unique properties are lacking to meet the conditions in extreme environments (e.g., high temperature/extreme thermal gradients) without a loss of material strength or ductility.

R&D NEEDS FOR THERMAL INTENSIFICATION

Advanced Materials and Characterization: Improved methodology is needed to characterize material properties (including thermos-physical and thermodynamic properties) and quantify property changes. Conduction-convection materials, nano-materials, ceramic matrix composites, and high thermal conductivity materials are needed for thermal intensification applications. Novel materials that improve the heat transfer coefficient in heat exchanger design or provide robust energy/heat control containment (e.g., thermally insulating materials that are transparent to millimeter-wave electromagnetic energy) should be explored.

Efficient Thermal Conversion: Methods and technologies are needed to lower heating system costs, including efficient heat transfer systems; optimized oxygen/fuel ratios; heat flux, microwave, radio-frequency, ultraviolet, plasma, and infrared technologies; induction resistance heaters; graphite electrodes; and convection plus convection-coefficient fluid-flow devices (e.g., fans, agitators, baffles, impingement heating).

Investment Justification and Value Proposition: Thermal intensification processes should address energy productivity and not just energy efficiency. Energy productivity needs to be coupled with a payback period and the ROI. Technology development and economic analysis are needed to explain the cost-benefit of new PI methods.

METRICS FOR THERMAL INTENSIFICATION

Suggested Targets

- Thermal intensification processes with 50% less footprint and 50% to 100% more capacity.
- Reduction in waste heat of 50% and redirection for other use with 75% efficiency.
- Thermal conversion/efficiency:
  - Watt per square inch increase by 25%
  - Conduction/convection coefficient increase by 25%
  - Turndown equal to 100% within maximum/minimum endpoints
  - Heating rate equal to or greater than 25% of the current baseline for heating systems
- Reduction in energy operating cost baseline by 25% (baseline equivalent to capital per unit output).
- Reduction in energy use, material and capital costs, and manufacturing time by 50%.

INSTITUTE CONSIDERATIONS

An institute could provide access for small and medium manufacturers to R&D capabilities and resources, and could assist smaller companies to drive innovation and allow for maturing of technologies. It could assist in the creation of user test beds where academia, laboratories, and industry can work and validate new materials/processes and aid in transitioning technology to market.

Mixing and Mass Transfer

> ***Framing Statement****: Mixing and mass transfer are key to manufacturing operations. Improvements in mixing and mass transfer could achieve significant reductions for processing time and improve efficiencies. In some applications, time requirements for specific processing operations could be reduced by more than 50%.*

Two basic processes used in a majority of chemical and industrial applications are mixing of various components and mass transfer between two or more components resulting in a final product. Both mixing and mass transfer can be accomplished using either dynamic rotating equipment or static in-line mixers. Although these technologies have been used for centuries, more efficient, cost-effective, and energy-saving methods may be achieved for mixing and mass transfer through PI if investments are made in appropriate areas. This can take the form of applying minimum energy to a medium in order to decrease reaction time, size, and cost while simultaneously increasing quality and yield. Improper mixing can result in excessive agitation, cavitation, or an inconsistent blend of materials with poor quality of the final product. Improper mass transfer can reduce the rate of a chemical reaction which in turn could be limited by mixing. Both can expend more energy than would be required with a more effective process. Highlights of discussions are outlined below; the full results of discussions are provided in Appendix B.

CHALLENGES/BARRIERS FOR MIXING AND MASS TRANSFER

Modular Systems: Challenges to replacing current in-plant processes with new modular systems include reducing the risks and costs associated with downsizing manufacturing processes where adoptability is key. Modular versus economies of scale capital planning is a major barrier to implementing modular technologies.

Heat Transfer: A key challenge is addressing energy losses in large-scale mass transfer devices where heat transfer results in dispersion, complicating effective energy management. Energy losses can also be significant in mixing applications on a scale of tons per day due to friction.

Modeling and Simulation: Use of simulation-based design and scale-up is currently limited. More investments are needed to enable product design especially for organic and inorganic interactions on micron-submicron scales. Specific R&D needs include validated first principle models and advanced measurements for multi-phase mixing, including phase distributions, and techniques for modeling and measuring particle packing, (including tomography as well as multi-physics models that are adaptable to large-scale systems. A self-sustaining computational tool for use in mixing and mass transfer applications would benefit many industries. Easy access by private and public users to high-performance computing resources at a federal facility would encourage technology maturation.

R&D NEEDS FOR MIXING AND MASS TRANSFER

Membranes: One key R&D need is new membrane technologies that use composite materials and nanomaterials that resist extreme environments, enhance mass transfer, improve the efficiency of gas separation and reduce costs in mixing and mass transfer processes. Performance targets should include the cost of membranes and the reduction of fouling and scaling.

Equipment and Process Effectiveness: Move efficient and cost effective combinations of mixing and mass transfer equipment are needed. Advanced, materials-driven mass transfer devices that are robust relative to conventional systems could improve the cost-effectiveness of many manufacturing processes. For example, bringing nanocomposites into industrial use requires better mass transfer processes in order to convince manufacturers to make a cost investment for early stage development. Downsizing manufacturing processes to modular systems to replace current in-plant processes requires an assessment of both risks and costs.

METRICS FOR MIXING AND MASS TRANSFER

Suggested Targets

- Material utilization and cost benefits.
- Degree of homogeneity per unit of energy used relative to the end product cost.
- Quantification of time and cost of energy used as inputs into the total product manufacturing cost.
- Cost of membranes and materials and the reduction of fouling and scaling for longer membrane lifetimes.
- Energy used to mix and transfer, including reduction in cooling.

INSTITUTE CONSIDERATIONS

Pilot-scale and Demonstration Facilities: Flexible, instrumented, and staffed demonstration facilities (or user facilities) and more pilot-scale testing facilities may be a good modalities to advance new mixing and mass transfer technologies.

Technology Transfer: A method for identifying, evaluating, prioritizing and moving the most promising technologies from lab-scale to pilot-scale is required for effective technology transfer. This method would include partners, expertise, and funding. A better process is needed for transitioning breakthrough technologies to industry through an institute, center of excellence, or shared demonstration facilities.

Chemical Separation and Crosscutting Technologies

> ***Framing Statement:*** *Separation technologies are estimated to consume 22% of in-plant energy in the U.S. manufacturing sector, with particularly high usage in the chemical industry. Membranes and other advanced separation processes could reduce the amount of energy required for chemical separations by 20-45% for specific high volume chemicals.*

Separations processes, including but not limited to distillation, filtration, and adsorption, are integral elements of most if not all chemical manufacturing operations. The ability to isolate or purify a process stream is critical in ensuring the integrity of the final product. A single process may undergo multiple separations. Separations are also critical to treating waste streams and meeting environmental regulations, but they consume a significant fraction of process energy. R&D on new technologies for PI research could reduce the energy and costs associated with existing process technologies. Chemical separations may also have analogues in other sectors, i.e., advances in chemical separations could impact water treatment and oil and gas extraction. Highlights of discussions are outlined below; the full results of discussions are provided in Appendix B.

CHALLENGES/BARRIERS IN CHEMICAL SEPARATION AND CROSS-CUTTING TECHNOLOGIES

High Cost of Separations: Separations processes typically have high operating costs. Absorbent-based separations, or those utilizing thermal separation processes, have high operating costs. Strong drivers exist in industry for lower cost systems that do not compromise on performance. Lower cost separations technologies could dramatically impact the ability to conduct separations on smaller scales.

Fouling: Membranes must be cleaned or replaced often to retain performance. Fouling is especially challenging in in high-concentration applications (15-30% input stream).

Membrane Characteristics: Membrane lifetime, efficiency, and durability are all barriers to the greater use of membranes. Achieving sufficient stability of the membrane and seals over long periods of operation can be a challenge, depending on the industrial operating environment.

Operating Requirements: Separations in chemical manufacturing often require quite specific operating conditions, or are sensitive to environmental conditions (e.g., acidity, concentration). Widening the operating conditions under which the separation processes is a challenge but would better enable greater integration of separations.

R&D NEEDS FOR CHEMICAL SEPARATION AND CROSS-CUTTING TECHNOLOGIES

Water Treatment: Water treatment, with regards to both desalination and wastewater, were identified as target focus areas for separations research. Aqueous processes are quite common in chemical manufacturing, food manufacturing, and the forest products industry.

Gas Separations: Gas separations, particularly CO_2 capture, is of interest because CO_2 is a major by-product of industrial operations and power generation as well as a significant contributor to global warming. However, streams of the gas are generally quite dilute. The ability to better separate CO_2 from its component streams would enable further processing and improve the economics surrounding its storage or utilization. Knowledge learned from CO_2 research could likely also be applied to hydrogen, nitrogen, and oxygen.

Continuous Processing: Many chemical reactions in industrial processes are reversible and often exist in equilibrium. The ability to remove the desired product from an active reaction vessel while leaving the reactants would drive reactions further towards completion. It would also help avoid undesirable side reactions and enable continuous process operations. Combinations of reaction and separation operations are key consideration in such large-volume processes as ammonia and alkane dehydrogenation.

Advanced Materials and Processes: Innovative materials and processing techniques have the ability to enable PI. These materials could lead to increased performance and/or decreased costs. For example, 3-D printing, low-cost sorbents, and metal organic frameworks provide potential opportunities for advancement. The availability of a pilot facility to test and validate these innovations would accelerate their adoption by industry.

METRICS FOR CHEMICAL SEPARATION AND CROSSCUTTING TECHNOLOGIES

Suggested Targets

- Minimum of 20% reduction in volume and 20% reduction in energy.
- Increase of process energy efficiency by 20% in 2 years and greater than 50% in 5 years.
- A 50% water efficiency improvement over best available technology measured in dollars, yield, or conversion.
- New separation technology with at least 10% lower capital and operating costs than existing technology (especially distillation), with a goal of 50% lower costs.
- At least 20% improved economics (without carbon tax considerations) as a result of improved process performance (based on thousands of hours of demonstration).
- A 20% reduction over state-of-the-art in CO_2-equivalent mass (emissions).

INSTITUTE CONSIDERATIONS

Membranes research via an institute model could contribute significantly to advances in this area by providing support for scale-up and supply chain for advanced materials; and a testing facility would independently verify materials for separation at relevant conditions. It would also encourage partnerships between engineering contractors, allow for demonstration of economically viable modular technologies (reducing risk), and provide an accessible venue for modeling and simulation and model validation.

Other Process Intensification Applications-Water, Food, Energy

PI technology improvements are usually discussed within the context of a specific part of a production process during the manufacture of chemicals, metals, plastics, cement, glass, and ceramics. However, other manufacturing processes and application areas can also take advantage of PI. Examples include food processing, water treatment, and energy transformation.

> ***Framing Statement:** Many manufacturing processes are not designed with full consideration of the life-cycle aspects of energy, materials, and water consumption. Process intensification approaches can be undertaken in areas such as food processing, water treatment, and energy transformation to significantly reduce operating costs. For example, industrial water treatment energy requirements could be reduced by more than 50%.*

A key objective was consensus on energy efficiency as a key productivity metric and identification of advances that could have significant benefits to the manufacturing sector. Highlights of discussions are outlined below; the full results of discussions are provided in Appendix B.

CHALLENGES/BARRIERS FOR OTHER PI APPLICATIONS

Resource and Energy Efficiency: Requirements for transporting water in food/agriculture, electricity production, and industrial applications are challenging to meet. Large plants are already relatively energy and water efficient, which makes further improvements more difficult. In addition, current manufacturing business models do not always account for the resources, value, and other aspects of efficiency. Many plant operators are also reluctant to 'own' life-cycle issues that go beyond plant boundaries.

Large Scale vs. Modular: Robust technical and economic analyses are lacking to help decision-makers understand how manufacturing processes are costed and to determine feasibility at different size scales. Scaled-down, cost effective approaches are lacking for waste treatment and recovery of materials and energy to support greater resource efficiency.

R&D NEEDS FOR OTHER PI APPLICATIONS

Processing Flexibility: Manufacturing processes should be designed to achieve production flexibility across a range of utilization capacities without sacrificing energy efficiency. Flexibility in raw material and products should be considered in process design (i.e., use of the same production line for multiple products). Transient distributed processes that utilize renewable energy or feedstocks are needed to make use of intermittent renewable resources for grid leveling.

Modeling and Simulation: Multi-scale, multi-physics models that run faster for design iteration (e.g., hours or days) are critical to technological advancement. Better methods need to be developed for process simulation and techno-economic analysis to confirm the cost benefit of new methods/technologies for PI.

Life-Cycle Analysis: Quantitative analysis is needed on the life-cycle of products that contain PI in the processing or PI-processed material. Studies are also needed to determine scaled-down and cost effective approaches for new PI technology.

Materials Substitution and Reuse: Enabling routes for PI are material substitution strategies and materials development using advanced manufacturing processes. Recycle-friendly materials (RFMs) as markers are also needed to aid in standardization efforts for RFMs/products.

Renewable-Based Technologies for PI: New transient distributed processes that utilize renewable energy or feedstocks or that make use of intermittent renewable resources for grid leveling should be explored. Process methodology for integration of concentrated solar thermal and thermochemical energy with industrial processes would help to reduce fossil carbon consumption (e.g., traditional gas/oil). In addition, alternative thermal process research is needed, focusing on wave/material data, measurement technologies, and cross-cutting materials/data measurement issues.

Water Use and Treatment: Improved technologies are needed for water treatment at the industrial scale to enable internal re-use, including determination of critical parameters in various industries, and level of cleaning required. Smaller, modular systems should be developed to enable water treatment and heat integration at industrial or agricultural sites.

METRICS FOR OTHER PI APPLICATIONS

Suggested Targets

- Recovery of previously unrecoverable materials and energy from a given process.
- Cradle to cradle type metric; i.e., material/product degradation/ number of cycles of reuse (yield times fitness).
- Performance metrics for modular technologies for distributed systems that match the cost/unit product of large, centralized processes.
- Metrics for biggest impact versus nearest-term impact and distributed applications versus large, established production facilities.
- Savings for operational capital expenditures (capital investments).
- Net consumption per unit production (e.g., energy, water) that could equate to net savings.
- PI hardware metrics for productivity following Moore’s Law (doubles approximately every two years).

INSTITUTE CONSIDERATIONS

Technology to Market Considerations: Test beds or pilot demonstrations where academics, laboratories, and industry work together and validate new materials/processes would accelerate technology commercialization. An Institute could also assist smaller companies to drive innovation and allow for technologies maturation with reduced risk for introduction into industrial markets.

Process Intensification for Environmental Management

Since the formation of the Environmental Protection Agency in 1970, industrial and manufacturing processes have been required to take the necessary measures to reduce the amount of pollutants to protect the environment. Beyond protecting the environment, conservation of materials and energy used in manufacturing processes can result in cost savings through reducing scrap material and re-using waste energy. R&D of novel technologies that result in a dramatic improvement in manufacturing and processing while substantially decreasing energy consumption or waste production must address the requirement for effective environmental management. Sustainability is considered a key metric. Environmental management considerations go hand-in-hand with PI approaches that decrease equipment footprint relative to production capacity and achieve cheaper, sustainable technologies. Highlights of discussions are outlined below; the full results of discussions are provided in Appendix B.

> ***Framing Statement:*** *Opportunities abound to achieve more sustainable operations and reduce environmental impacts. Greater recovery and recycling of in-plant wastes and increased end-of-life recycling are just two opportunities. Over 200 trillion Btu of energy could be saved by increased utilization of recycled material in five selected industries alone.*

CHALLENGES/BARRIERS TO PI FOR ENVIRONMENTAL MANAGEMENT

Cost: Industry's focus is reducing cost and increasing bottom line profit. Industry is reluctant to take the extra steps for better environmental management without a government or corporate mandate because it reduces available capital for product development or other improvements. Capital investment and stakeholder awareness are both barriers to improving environmental management for a given industry or business.

Education: Even with regulations, people need to be educated on effective environmental management practices. Considerations should include how to implement a cultural shift, such as what was done with automobile seatbelts. There is a need for a greater number of science/technology education programs certified by the Accreditation Boards for Engineering and Technology (ABET) that could impact PI and environmental management.

R&D NEEDS FOR PI FOR ENVIRONMENTAL MANAGEMENT

Separation Technologies and Processes: Low-energy separation technologies and processes are needed for liquid-liquid extraction:

- High-throughput, low-energy filtration including solid/aqueous/organic separation and high-throughput/low-energy separation for water.
- Gas separations (for oxygen, nitrogen, carbon dioxide and volatile organic compounds) on a large scale, or as an add-on.
- Trace metal separations.
- Inorganic, organic and water separation in pulp and paper products.

Water Treatment: Transposable wastewater treatment processes, including generic solutions based on first principles, and enhanced, less energy-intensive water extraction from gas, solid, and liquid effluents, including extraction/separation of very dilute concentrations, are needed. Mitigating the effect of impurities on the performance of separation technologies, such as fouling and degradation, should be considered during development of these wastewater treatment processes.

Modeling and Simulation: Enhanced modeling and simulation of industrial processes (especially lifecycle analysis) and computational simulation and analytics development are needed to understand modeling mechanisms. Companies do not yet have the business case for purchasing the type of high performance computing capabilities needed.

Process Integration and Modularity: New technologies should have the capability to be readily added to existing processes using a plug-and-play approach. Simple add-on approaches for heat recovery to existing equipment need to be investigated. Manufacturers should have flexibility to build a new plant away from existing infrastructure. Process integration for heat and material recycling and recovery should be included early in the technology development stages.

Green Energy and Recycling: Cost-effective technologies that apply green energy for reducing energy use, and green chemistry and recyclability for waste reduction are needed. Two key opportunities are techniques for handling waste on site and reducing process water requirements. Other potential solutions for reducing waste include increasing yield and selectivity, reusing polymers from waste streams, "erasing" the thermal history of waste streams, and co-locating processes to reuse waste heat (i.e., different companies that are co-located could devise a method of mutual waste heat recovery for re-use in each other's processes). Recovery of chemicals and nanoparticles from water at dilute concentrations is also of interest.

Life-cycle Considerations: Initial product design and life-cycle analysis should address long-term environmental management requirements. Secondary source inventories to feed the supply chain should be part of the technology development process. Industry needs a capability to test, identify, and evaluate pollutants or toxics created unknowingly in processing before an environmental violation occurs. Two additional opportunities are subsurface characterization without excavation for contaminants and metrology that enables characterization of environmental issues resulting from legacy waste.

METRICS FOR ENVIRONMENTAL MANAGEMENT

Suggested Targets

- Capital costs reductions of 50%, possibly by using global solutions.
- A 75% reduction in energy per pound for liquid-liquid extraction and 50% reduction in energy per pound for water separations.
- A 50% increase in throughput at the same energy per pound for solid-liquid separations.
- Minimal (<1%) added for product, production time, and maintenance.
- Metric for measuring consumer and industrial awareness of PI for environmental management.

INSTITUTE CONSIDERATIONS

Opportunities exist for an institute to address various industrial needs for environmental management for chemical processes and manufacturing methods. Additional investments in environmental management research are needed to keep up with current research efforts in Europe and China where environmental laws have become more stringent. The commercial sector needs research supported by national laboratories and universities for applications such as biofuels, environmental biological-geological-chemical interactions, transforming metals in an energy-efficient manner, transforming carbon dioxide into useful carbon products, removal of mercury from air emission sources, and investigating emerging pollutants. Industry requires access to small and mobile laboratories, pilot test facilities, and user facilities for broad R&D and testing. An institute could address some environmental management issues across small, medium, and large businesses.

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APPENDIX A: AGENDA

Process Intensification Workshop

Alexandria, VA | September 29-30, 2015

Day 1	
Time	**Activity**
8:00 am	Registration
8:40	Welcoming Remarks; and AMO: Introduction and Interest in Process Intensification by *Mark Johnson, Director, DOE Advanced Manufacturing Office*
9:10	Panel Discussion on Process Intensification (Invited Participants)
10:20	Instructions
10:30	Break
11:10	**Topic Area Sessions**
	● Chemical Reactions and Reactors ● Thermal Intensification – High Temperature Processes ● Mixing and Mass Transfer
12:20 pm	Lunch
1:20	Resume sessions
4:00	Break
4:30	**Comments from Sessions**
4:30	● Chemical Reactions and Reactors
4:45	● Thermal Intensification – High Temperature Processes
5:00	● Mixing and Mass Transfer
5:15	Adjourn

Day 2	
Time	**Activity**
7:45 am	Registration
8:15	Facility Public-Private Partnerships in AMO by *Mark Shuart, DOE Advanced Manufacturing Office*
8:45	Panel Discussion on Process Intensification (Invited Participants)
9:40	Instructions
9:45	Break
10:15	**Topic Area Sessions**
	• Chemical Separations and Crosscutting Technologies • Other Process Intensification Applications – Water, Food, Energy • Environmental Management
12:15 pm	Lunch
1:15	Resume sessions
3:00	Break
3:30	**Comments from Sessions**
3:30	• Chemical Separations and Crosscutting Technologies
3:45	• Other Process Intensification Applications – Water, Food, Energy
4:00	• Environmental Management
4:15	Closing comments
4:30	Adjourn

APPENDIX B. DETAILED BREAKOUT RESULTS

Chemical Reactions and Reactors

FOCUS QUESTION 1: *What are the critical technological challenges/barriers for chemical reactions and reactors?*

Table B-1. Barriers and Challenges for Chemical Reactions and Reactors

Challenges and Barriers
Catalysts
• Dealing with input streams that vary in composition (whether seasonal or source). • Managing micro-channel catalysts (replacement of existing catalysts). • Capturing transient high-efficiency catalyst performance. • Developing robust processes that take into account feedstock change and associated conditions and the catalyst lifetime. • Increasing variety of iron and non-iron substrates and impacts on multi-layer coating stacks.
Separations
• Difficulty performing selective product separation. • Lack of technology to handle unwanted side reactions at industrial scale. • Challenges that arise from integrating processes, combining steps, or requiring fewer reaction steps.
Reactor Design
• Limited reliability of current computational fluid dynamics (CFD) models. • Designing for safety; some reactions operate in unsafe regions or where cogeneration requires use of unsafe chemicals.
Scale Up and Modularity
• Risks associated with scaling up reactions from the bench top. • Lack of knowledge about areas where PI can play a role in overcoming economies of scale. • Integrating all unit operations during scale-up. • Cost and difficulty of transporting large reactors from supplier site to the plant site. • Achievement of nth plant economics.
Thermal Integration
• Lowering reaction temperatures. • Economical utilization of stranded (gas) resources. • Heat control during reactions (e.g., hot spots). • Thermodynamic constraints that limit improvements.
Process Synthesis
• Lack of technology for large volume oxygen capture. • Addressing unique requirements for individual plants based on product slate.

FOCUS QUESTION 2: *What are the critical technology developments that will be required in chemical reactions and reactors?*

Table B-2. R&D Needs for Chemical Reactions and Reactors
Membranes
• Chemically and thermally resistant membranes for separation (that are also fouling resistant). • Easily configurable membrane material systems for targeted separations. • Manufacturing of robust membranes capable of being servicing (e.g., cleaned) by nano- and micro-equipment. • Better understanding of the cost drivers for membranes (e.g., ion-exchange membranes can be expensive for some applications) to drive costs down. • Hydrothermally stable materials for membranes (e.g., for fermentation).
Catalysts
• Engineered and optimized catalysts for specific reactions or reactors, including micro-reactors, methane conversion catalysts with reduced coking (e.g., dry reforming), hydrothermally stable materials (low and high temperature), non-precious metal catalysts, selective alkane activation, and selective oxidation reaction design. • Improved catalysts with characteristics of greater selectivity, easier recoverability, faster reaction, lower cost, and increased durability and impurity tolerance. • More durable nano-structured catalysts. • Homogenous catalyst separation/recovery. • Approaches for catalyst regeneration/replacement in multifunctional reactors. • Molecular-level design of catalysts to improve difficult reactions; along with molecular engineering of catalysts and sorbents. • Catalyst management replacement opportunities. • Highly selective and commercially viable oxygen transport catalysts.
Reactions / Reactors
• Integration of exothermic and endothermic reaction (or separation) processes. • Low-energy drying processes. • Advancements for electrochemical organic reactions (e.g., CO_2 to alcohols). • Advanced state-of-the art flow control within micro-reactors, heat exchange reactors, and separators (active and/or passive). • Improved reactor design tools (manufacturing, kinetics, etc.). • Batch reactor optimization to reduce downtime (requires value stream integration). • Better uniformity of reaction conditions. • Approaches to minimize micro-reactors and micro-channels fouling. • Multi-function reactors via additive manufacturing. • Compact, scalable, and robust separation devices compatible with reaction conditions. • Flexible PI technologies for adaptive processing. • Fluid/moving bed designs for non-classic petrochemical applications. • Approaches for separating and upgrading complex mixtures such as pyrolysis bio-oil or process integration fluids. • Hydrothermal de-polymerization mechanisms for processing biomass feedstock. • Alkane dehydrogenation. • Sequentially scaling up reactor design to reduce risk (e.g., scale up of chemical reactions from bench top). • Modular reactors for highly exothermic reactions. • Modular reactors able to economically convert distributed feedstock.
New Processes
• Advancements for transient reactor design/electrochemical systems (e.g., hydrogen electrolysis). • Process control systems for integrated systems that combine unit operations and steps.

Table B-2. R&D Needs for Chemical Reactions and Reactors

- Approaches for value-added capture of product from purge and waste streams.
- Process approaches using novel directed energy (e.g., vibration, light, and ultrasound).
- Risk mitigation approaches to external fields applied for process enhancement such as electrical fields.
- Reactive separation technologies.
- Non-phase change separation processes.
- Reduction in second law losses in chemical processes (e.g., better thermal integration and reduction of other irreversible processes).
- Rapid and efficient transient heating for endothermic reactors, along with heat utilization in exothermic reactors.

Improved Modeling and Design

- Better mass flow phenomena models, including phase changes.
- Multi-scale optimization methods.
- Integrated design of processing systems (sensors, chemistry, separation reactions, and materials).
- Designs with concurrent simplification and intensification of feed systems, products systems, and separations.
- Rapid kinetics measurements and turbulence in modeling and design.
- Advanced fundamental science of materials behavior coupled to energy.
- Basic science for impurities to model beyond the ideal.
- Designs and models for heat integration and waste heat recovery to reduce energy use.

Sensors and Controls

- Smart sensors for improved PI operations.

FOCUS QUESTION 3: *What are the most appropriate metrics and types of impacts for assessing chemical reactions and reactors?*

Table B-3. Metrics and Impacts for Chemical Reactions and Reactors

Energy

- Extent to which catalysis reduces activation energy.
- Production energy vs. heat of reaction ($/barrel (bbl)) produced.
- Cost of production per reaction or BTU per reaction and savings resulted.
- Decrease in BTU per unit of product.
- Energy used by the PI process relative to the calculated theoretical minimum of the process.
- *Suggested Target:* Energy reduction of at least 20% over the current state of the art.

Material Usage and Waste

- Footprint reduction.
- Progress toward achieve zero-effluent manufacturing.
- Efficiency of raw material usage.
- Percent capture and utilization of flared natural gas (through strategies and technologies that are cost competitive).
- Yield of skid-based platform stranded gas recovery (for gas to liquids production).
- *Suggested Action:* Develop a set of case studies showing minimum 10% cost savings and 20% greenhouse gas emissions reduction.
- *Suggested Target:* CO_2 emissions reduction; for example, CO_2 emissions reduction of at least 15% over the current state of the art.

Table B-3. Metrics and Impacts for Chemical Reactions and Reactors

- *Suggested Target (with particular relevance for ammonia production and bio-oil to products):* Report on ability to decrease cost by 10% and greenhouse gas emissions (unspecified amount).

Economic

- Cost per pound of production.
- Overall life extension of the system.
- *Suggested Targets:*
  - Life-cycle cost analysis indicative of ROI less than 3 years.
  - ROI multiple after 3, 5, and 10 years.
  - Operating and maintenance (O&M) and capital cost better than existing processes by 50% at pre-pilot stage.
  - O&M and capital cost better than existing processes by 20 to 25% at technological readiness level (TRL) 5.
  - Cost reduction (per unit mass of product): e.g., cost reduction of at least 15% over current state-of-the-art.

Other Metrics

- Higher value distributed volatile organic liquid separations.
- *Suggested Actions:*
  - By 2020, develop computational tools that scale from molecules to reactor and validate against real life reactions/reactors.
  - Develop and disseminate industry tools and best practices (both new and retrofit).
  - When developing metrics, set them for a given timeframe at a given scale on real feedstocks (e.g., thousands of hours at pilot scale).

FOCUS QUESTION 4: *How would chemical reactions and reactors best contribute to a public-private partnership institute framework?*

Table B-4. Chemical Reactions and Reactors – Contributions to a Public-Private Partnership

Proposed Institute Structure and Operation

- The public-private partnership must be beneficial, sustainable, and money-making to attract corporate sponsors.
- A partnership should consider energy intensity, catalysis, raw materials, expenses, and recovery-separation.
- The partnership must adequately address the issue of intellectual property.
- An independent third-party statistical analysis could lower the perception of risk.
- The institute would target a particular national need rather than a specific industry and its waste stream.
- PI becomes more sustainable if the waste stream is well understood.
- A flexible test bed and an integrated system would enable a modular test bed system in which pieces of equipment could be swapped in and out.

Performance Guarantees

- Performance guarantees are considered unrealistic; alternative approach is to conduct pilot projects that scale up so that the institute acts as a test bed. The proposed institute would likely have to be process-specific, which may allow the establishment some kind of performance guarantee related to the chosen process.
- Prioritization of projects would be required if the institute was a testing facility for multiple processes.

Partnership/Institute Sustainability

- A sustainable institute would be one in which industry pays a user fee.
- To get industry to pay such user fees requires some commercial applications (e.g., the EPRI consortium's pilot project on combustion technology).

Table B-4. Chemical Reactions and Reactors – Contributions to a Public-Private Partnership
• The Solid State Energy Conversion Alliance (SECA), which had a set of common features such as shared intellectual property but with individual competitive cost-sharing projects, resulted in both vertical teams and a horizontal baseline.
Steering Committee of Proposed Institute
• The institute would need to create a mechanism to scope out viable new ideas and products. • The institute would need to create an external board and a mechanism to sunset nonperforming projects.
Basic Fundamental Research and Application-Specific Reactions
• All companies face common basic R&D problems. • Companies have interest in basic research that is pre-competitive in a way similar to many other consortia. • The institute should include both collaborative work and specific competitive projects, which shares some traits with a CRADA (cooperative research and development agreement, now called Strategic Partnership Projects). • The proposed institute would need to have targeted applications with modularity and down-scaling. • The project-specific RFP strategy has suited industry players since they do not feel they are giving away their competitive advantage to other companies. • Such RFPs still help make process improvements for the industry as a whole. • Ultimately, PI is core to the businesses in the chemical industry, which could make it harder to establish a single institute or consortium.
Modality of Approach versus Focus
• The focus of the current DOE approach is more important than its modality; a good example is the DOE's SunShot program with its goal of $1 per watt of generation. • In the case of PI, one such goal could be ending all flaring of natural gas. • The form of the partnership could be either a DOE initiative or an institute.

Table B-5. Chemical Reactions/Reactors Contributors	
Name	**Organization**
William Ayers	Ayers Group, LLC
Billy Bardin	The Dow Chemical Company
Mary Biddy	National Renewable Energy Laboratory
David Bruce	Clemson University
Maria Burka	National Science Foundation
Louis DiNetta	Compact Membrane Systems, Inc.
David Edwards	Zeton Inc.
Anne Gaffney	Idaho National Laboratory
Daniel Ginosar	Idaho National Laboratory
Diane Graziano	Argonne National Laboratory
Raghubir Gupta	RTI International
Greg Harris	U.S. Army/OSD
Faruque Hasan	Texas A&M University
Jamie Holladay	Pacific Northwest National Laboratory
Cassidy Houchins	Strategic Analysis
Greg Jackson	Colorado School of Mines
Cynthia Jenks	Ames Laboratory, U.S. DOE
Zhijun Jia	CompRex, LLC
Mark Johnson	DOE Advanced Manufacturing Office
Denis King	DJKing & Associates
Gary Luce	Eastman Chemical
Sudip Majumdar	Compact Membrane Systems
Mike McKittrick	DOE Advanced Manufacturing Office
Sankar Nair	Georgia Institute of Technology
Randall Partridge	ExxonMobil Research and Engineering Co.
Veena Rao	University of Maryland
Robert Ritchie	Corning Incorporated
Sharon Robinson	Oak Ridge National Laboratory
Mayur Sathe	LSU Chemical Engineering
Costas Tsouris	Oak Ridge National Laboratory
Mario Urdaneta	Advanced Manufacturing Office
Eric Wachsman	University of Maryland
David Walters	PPG Industries, Inc.
Robert Wegeng	Pacific Northwest National Laboratory
Mark Wright	Iowa State University

Thermal Intensification

FOCUS QUESTION 1: *What are the thermal intensification technical challenges/barriers?*

Table B-6. Barriers and Challenges for Thermal Intensification

Challenges and Barriers
Materials
• Lack of data on changes in mechanical properties (e.g., corrosion, fatigue, and tensile strength), thermal behavior/properties (e.g., range of tolerance of thermal gradient), and conductivity during operation in high-temperature environments. • Lack of specific standards to describe/quantify material characteristics at high temperature. • Availability of materials with unique properties to meet the conditions experienced in extreme environments (e.g. high temperature/extreme thermal gradients) without a loss of material strength or ductility. • Limited availability of corrosion-resistant and high-temperature materials for improving manufacturing processes through thermal intensification. • Lack of methods for manufacturing materials/material interfaces (e.g., refractories) at a smaller scale for applications in harsh conditions.
Process Methods and Technologies
• Lack of a process for efficient rapid heating of molten metal/glass on demand (e.g., intensive rapid heating on demand). • Relatively poor thermal conductivity of the interfaces between heat exchangers and devices. • High thermal/energy intensity of carbon fiber production (80% of the cost of carbon fiber manufacturing is energy) and high associated energy losses. • Inability of thermal intensification alone to always reduce size or time (e.g., diffusion limits, drying, and bubble removal in glassmaking). • Ineffective material utilization (e.g., limited reuse of scrap material) in injection molding processes. • Inconsistent heat distribution and containment within processes and energy leakage throughout the entire process. • High energy requirements for product cooling.
Modeling
• Lack of robust thermal process equipment models. • Difficulty managing high-temperature complex-geometry heat/thermal management systems and technologies. • Limitations of current modeling techniques of high-temperature processes for design coupled with integrated measurements.
Other Thermal-Intensive-Process Enabling Technology
• Lack of accurate knowledge on micro-channel systems, which do not bring about a change in pressure penalty (i.e., scale-up by numbering up does not apply). • Limitations in amount of energy that can be applied in a cost effective manner in large-scale applications of certain electro-technologies such as microwave technologies.

FOCUS QUESTION 2: *What are the critical technological developments that will be required in thermal intensification?*

Table B-7. R&D Needs for Thermal Intensification

Processes

- Cost-effective, durable, variable-frequency microwave technology (allows more uniform heating with less arcing potential, but requires shielding to prevent spurious emissions).
- Rapid heating systems with infinite turndown through minimum-maximum power output.
- Uniform heating using 3-D zone control heating to the pixel level.
- Methods and technologies to lower heating system costs, including efficient heat transfer systems; optimized oxygen/fuel ratios; heat flux, microwave, radio-frequency, ultraviolet, plasma, and infrared technologies; induction resistance heaters; graphite electrodes; convection plus convection-coefficient fluid-flow devices (fans, agitators, baffles, impingement heating), conduction-convection materials; and nano-materials.
- New processes for rapid heating of molten materials.
- Secondary processes that combine new heat recovery methods and that are adaptable to existing furnace/kiln systems.
- Heat recovery methods to extract heat from finished products.
- Highly efficient, concentrated closed-loop heating processes that take advantage of the heat loss as an energy source, maximize efficiency, and reduce cycle time.
- Uniform heating of parts with various geometries and/or section thicknesses.
- Thermoelectric devices and improved thermal-to-electric energy converters as methods for harvesting recovered heat energy.
- Systems with uniform heating that make use of susceptors, chamber/containment design (radiation, convection), energy focusing (laser, microwave), sensors (in situ- high temperature) and tailored material-handling approaches.
- Modified additive manufacturing that does not require prior heat treatment for development of technologies that use multi-materials.
- Systems that demonstrate the ability to drive backend thermal cycles using waste heat recovery, vapor compression, and refrigeration approaches.
- Advanced design and manufacturing tools such as Design for Manufacturing and Assembly to reduce the need for high temperature requirements.
- Application of three-dimensional (3-D) printing for areas where heat recovery and re-use can be achieved during parts and components manufacture.
- Engineered resilient systems that are process gradient tolerant and can automatically re-baseline from process upsets (i.e., self-healing processes and systems).
- Total ecosystem solutions for improvements and utilization of materials injection molding.
- On-site, low-cost concentration/generation of ambient gases (sometimes only need 50% purity oxygen rather than mixing in expensive 99% purity oxygen).
- Reuse/recycling of gases, exit gas scrubbing, local generation, and collection of by-products for re-use in order to lower total cost of value-added gases (e.g., nitrogen, hydrogen).
- Adoption of improvements in the insulating, reflecting, and corrosion resistance of refractory materials.
- Adoption of technologies such as low emissive coatings, nanostructure catalysts, flow bailing films, and two-phase-flow heat exchangers.
- Modular, portable, durable equipment to process/distribute resources (e.g., natural gas) at the source (wellhead).
- Advanced/low-cost heat pumps that can operate in high temperatures and are inherently safe.
- New reactor geometrics to replace current brick-lined reactors.
- Alternative low/no thermal process technologies that use little or no heat to accomplish the job (e.g., ultra-violet curing as a replacement to thermally driven processes).
- Submerged combustion melting (mixing fuels and oxidant with the raw materials and firing fuels directly into and under the surface of the batch material being melted).

Table B-7. R&D Needs for Thermal Intensification
Materials
• Improved methodologies for characterizing material properties at high temperatures (e.g., how do materials behave at high temperatures?). • Standards to describe material characteristics at high temperatures. • Novel materials that improve the heat transfer coefficient in heat exchanger design. • Further investigation of exotic alloys and superalloys to determine if they can replace existing materials. • Fine-grained resolution simulations for material analysis and development. • Understanding and quantification of the theoretical limit for thermal intensification. • New materials with high thermal conductivity. • Affordable technologies to fabricate materials that can survive the harsh environments in many thermal processes. • Improved refractory materials (e.g., high thermal insulation and corrosion resistance) for high- temperature containment applications (e.g. molten glass/metals processing). • Advances in industrially robust energy/heat control containment materials (e.g., thermally insulating materials that are transparent to millimeter-wave electromagnetic energy). • Ceramic matrix composites (to reduce costs) for high temperature applications. • Database of processing requirements of functionally graded materials typically used in manufacturing. • Enhanced conductivity, thermal expansion, and dissimilar-materials joining processes that can be coupled to advanced manufacturing technologies. • Materials with phase-change properties that can be used for waste heat recovery management. • Low-emissivity coatings that can be applied on materials to enable high-temperature containment/insulation, reduced radiation from surfaces, and minimal thermal losses. • New materials for application in high-temperature concentrated solar panels that can operate at extremely high temperatures without degradation and enhance system efficiency. • Advanced bulk materials (e.g., refractories, ceramics, and high-temperature metals) that result in lower cost products and large tonnages production capabilities. • Techniques to tune material thermal properties over wide ranges (variation with part location by a factor of 10). • Advanced alloys for combined/multicomponent application in extreme environments (e.g., oxidation, sulphidation, chlorination). • Determination of fundamental material constants under high-energy radiative processes. • Materials that respond to the energy used for radiative processes (e.g., increasing the heat flux and lowering the radiant cost). • Materials with near zero thermal expansion, high temperature insulation, and low radiation/conduction. • Coating techniques for modifying surfaces.
Analysis and Modeling
• Software models of existing thermal process equipment in order to optimize setup and utilization for load changes and zero down time. • High-temperature models for sensors to monitor the material being processed. • Manufacturing process models for technologies used in complex-geometry heat/thermal-management systems (e.g., hydrogen fuel cell vehicles). • New and advanced computational approaches to aid with lower-cost scale-up and systems integration of high temperature technologies. • Heat recovery and utilization modeling of carbon fiber. • Pressure vessel zero-radius corner modeling and heat exchanger standards for power control monitoring and cooling to minimize thermal energy requirements during manufacture of high-temperature applications pressure vessels. • Advances in the integration of first principle models that can be adjusted with the actual process data to yield real-time process behavior visualization and control product quality prediction.

Table B-7. R&D Needs for Thermal Intensification

- Simulations and other computational analysis tools that enable studies of multi-material phase change materials.
- Thermo-physical and thermodynamic properties database that includes physical and chemical characteristics on glass, ceramics, metals and liquids.
- Characterization of the link between manufacturing process parameters and resulting material properties through simulation of the manufacturing environment with the resulting material.

Process Control

- High-temperature process parameters that enable accurate control and optimization of thermal heating on the material.
- New low-cost, wireless, cyber-secure sensors able to measure multiple parameters, survive harsh environments, and are immune to electromagnetic interference.
- Feedback systems for real-time monitoring of thermally intensive processes.
- Methods for improved gas and temperature control across adjacent spaces to reduce the footprint of furnaces, kilns, and other thermal equipment.
- Robust, cost-effective systems based on real-time, and in-situ, non-contact measurements of process materials properties (e.g., to enable measurement of dielectric properties to infer the state-of-cure of a polymer).
- Sensors that provide an accurate, robust, longer life with 0.01°C resolution and a temperature range of 1,200C to 2,000C which is required for accuracy and process control.

FOCUS QUESTION 3: *What are the most appropriate performance/impact metrics for thermal intensification?*

Table B-8. Metrics and Impacts for Thermal Intensification

Manufacturing Approach/Process Design Metrics

- Distributive, portable, and modular capabilities with smaller footprints, lower transportation costs, use of custom heat exchangers, and lower capital, energy, and maintenance costs.
- Minimization of additional capacity increment addressed by the process.
- *Suggested Targets:*
  - Thermal intensification processes that have 50% less footprint and 50% to 100% more capacity.
  - Processes need to be developed consisting of modular motion and product diversity with capabilities for easily making product changes with at least 50% reduction in product changeover.

Energy Metrics

- Energy productivity (not just energy efficiency), coupled with a payback period.
- Energy density (gravimetric, volumetric, cost, production time), converted into cost.
- Value of gas reclamation/recycle/reuse to reduce energy losses.
- *Suggested Target:* Energy cost reduction by 50% should be the target across the injection molding ecosystem through raw material reduction, resin reuse, reduced injection, molding waste, and reduced energy consumption to grind for reuse, and transportation throughout the process.

Table B-8. Metrics and Impacts for Thermal Intensification

Performance Metrics

- Percent increase in the insulation value for the material used in high-temperature containment applications.
- *Suggested Targets:*
  - Watt per square inch increase by 25%.
  - Conduction/convection coefficient increase by 25%.
  - Turndown equal to 100% within maximum/minimum endpoints.
  - Heating rate equal to or greater than 25% of the current baseline for heating systems.
  - Reduction in waste heat of 50% and redirection for other use with 75% efficiency.

Environmental Impact and Safety Metrics

- Reduction in carbon footprint and greenhouse gas emissions generation.
- *Suggested Targets:* Reduction in utility/water usage by 50-100%, and by-products and waste by 50-70%.

Economic Metrics

- Life expectancy of assets that could be doubled while achieving a positive ROI.
- Ratio of scale/absolute cost (i.e., minimum economic production per minimum profitable capital expenditures).
- Labor costs, process time, and energy consumption in terms of capital expenditures/unit output, labor dollars/unit output, process time/ unit output, and energy/unit output.
- Reduction in capital expenditure/operational expenditures while producing the same product.
- *Suggested Targets:*
  - Reduction in energy operating cost baseline by 25% when the baseline is equivalent to the capital per unit output.
  - Reduction in energy use, material and capital costs, and manufacturing time by 50%.
  - A 50% reduction in the percentage of high temperature processes eliminated by introduction of other materials and processes.

FOCUS QUESTION 4: *How would thermal intensification technologies best benefit from a public-private partnership institute framework?*

Table B-9. Thermal Intensification – Contributions to a Public-Private Partnership

Cross-Cutting

- Uniqueness of some pilot and demonstration projects.
- Means for combining resources for transport technologies (such as micro-channels) and improved kinetics through use of nanostructured films and catalysts.
- Enhancements to existing processes.
- One-stop shop for a depository of information (e.g., databases for material properties), highlighting what information is available and what is not available.
- An understanding of industry needs early in the development cycle and access to customers and suppliers to share both new products and problems.

Operational Approach and Exploring New Markets

- Encouragement of industry participation and leadership, enabling field-of-use care in intellectual property or recommend cross-industry teaming in projects for Funding Opportunity Announcements (FOAs).
- Self-sustainability.
- Opportunities for new and/or high-value added materials/products where value makes sense.
- Opportunities where PI improves product quality and enables new products.
- Technology advancement outside of a manufacturer's core capabilities.

Table B-9. Thermal Intensification – Contributions to a Public-Private Partnership
Resource Availability, Workforce, and Education
• Access to expertise across full-scale system development. • Path to educate the community on new technologies, manufacturing processes, and factory operations through various educational programs. • Creation of an educated workforce to feed back into technology development, marketing and end user process development. • Encouragement of industry participation through strong education/academic engagement, creating a talent pipeline in advanced technology development. • Exposure of customers and suppliers to new opportunities.

Table B-10. Thermal Intensification Contributors	
Name	**Organization**
Thad Adams	Savannah River National Laboratory
Balu Balachandran	Argonne National Laboratory
Rolf Butters	U.S. Department of Energy
John Carpenter	RTI International
Suzanne Cole	American Chemistry Council
Joe Cresko	DOE Advanced Manufacturing Office
Qi Dang	Iowa State University
Serguei Dessiatoun	University of Maryland
Charles Freeman	Pacific Northwest National Laboratory
Hossein Ghezel-Ayagh	FuelCell Energy, Inc.
Alison Gotkin	UTRC
Tilak Gullinkala	Owens-Illinois
Robert Hyers	Boston Electromet
Jackie Kulfan	PPG Industries, Inc.
Patrick Kwon	Michigan State University
Saniya LeBlanc	George Washington University
Alan Liby	Oak Ridge National Laboratory
Vahid Motevalli	Tennessee Tech (Center for Manufacturing Research)
Michael Ohadi	University of Maryland
Gina Oliver	American Chemistry Council
Michelle Pastel	Corning, Inc.
Brian Paul	Oregon State University
Frank Pfefferkorn	University of Wisconsin-Madison
Bhima Sastri	DOE Office of Fossil Energy
Amir Shooshtari	University of Maryland
Mark Shuart	DOE Advanced Manufacturing Office
Stephen Sikirica	DOE Advanced Manufacturing Office
Ratnesh Tiwari	University of Maryland
Joseph Vehec	U.S. Steel
Conghua Wang	TreadStone Technologies, Inc.
Esther Wilcox	National Renewable Energy Laboratory

Mixing and Mass Transfer

FOCUS QUESTION 1: *What are the technological challenges to implementation and deployment of process mixing and mass transfer for industrial applications?*

Table B-11. Barriers and Challenges for Mixing and Mass Transfer

- Reducing risks and costs for downsizing manufacturing processes to modular systems.
- Managing energy injection and distribution inside equipment, and the impact of fluid mechanics on mixing and mass transfer.
- High cost of nanocomposite technologies.
- Lack of available data for implementing existing technologies into mass transfer applications.
- Prevention of material corrosion and abrasion in mixing applications.
- Energy losses associated with heat/friction in large-scale mixing applications.
- Dispersion caused by heat transfer, which equals attrition (physical versus chemical properties).
- Effective heat (energy) management.
- Modular capital planning versus economies of scale capital planning.
- Determination of a cost-effective endpoint.
- Decision whether or not to retrofit.
- Mixing energy efficiency.
- Low value of clean water technologies.

FOCUS QUESTION 2: *What are the research and development needs for mixing and mass transfer processes and how could an institute address these needs?*

Table B-12. R&D Needs for Mixing and Mass Transfer

Research Needs

- Technology to transfer waste streams back into the process.
- Advanced characterization capability of materials and processes during operations based on a fundamental understanding of complex processes.
- For paper-based products, smaller volume, more rapid-mixing or continuous-mixing paper coating formulations, and improved heat and mass transfer of water in paper drying.
- Method for mixing large-scale powders without separation of feed components.
- Processes for desalination and water production and re-use.
- Processes for preventing fouling and control of scaling on membranes.
- Combinations of mixing and mass transfer equipment that is more efficient and cost effective.
- Method to minimize the differences in gas mixing processes.
- Optimization of liquid/gas mixing contact area.
- Advanced, materials-driven mass transfer devices that are robust relative to conventional systems.
- Consolidated approach for R&D of common mixing and mass transfer processes that have application to various individual industries.
- Identification of commonalities for mixing for various physical states (solid/solid, solid/liquid, liquid/liquid, liquid/gas, and solid/gas mixtures).
- Micro-bubbles, liquid-water, air-liquid-water mixing, and other techniques to address bubble mixing.
- Improved static mixing processes such as electro-hydrodynamic mixing, particularly for microchannel applications.
- Validated first principle models and advanced measurements for multi-phase mixing, including phase distributions.
- Membranes to resist extreme environments and rapid, efficient separations of gases and nitrogen.

Table B-12. R&D Needs for Mixing and Mass Transfer

- Modeling and measuring organic and inorganic interactions on micron-submicron scales.
- Modeling and measuring particle packing, such as high solids loading conditions including tomography.
- Multi-physics models that are adaptable to large-scale systems, especially models that do not need a supercomputer.
- Local application of energy, and modularization and miniaturization of mixing and mass transfer devices, with an emphasis on adoptability.
- Efficient energy recovery, improved stability of materials-enabled mixing and mass transfer devices, and increased contact areas.

Technology Development Needs

- Continuous jet injector technology.
- New processes to de-couple strength and water retention in paper manufacturing processes.
- Membrane-based technology for mass transfer, such as composite materials and nanomaterials.
- Heating without using natural gas or hydrocarbons.
- Predictive temperature/power controls for systems with long time intervals and sensors/measurements.
- Fractal mixers to control macro- and micro-mixing.
- Desalination technologies for U.S. coastal areas that experience annual water shortages.
- Technologies for mass transfer applications where surface morphology and effects on transportation of pastes/solids/high-viscosity liquids is a concern.

FOCUS QUESTION 3: *What metrics should be used and what are the impacts of breakthrough technologies in Mixing?*

Table B-13. Metrics and Impacts for Mixing and Mass Transfer

- Throughput per floor area, such as space area.
- Manufacturing footprint needed for a particular product. .
- Energy used to mix and transfer, including reduction in cooling.
- Waste heat utilization.
- Material utilization and associated cost benefits.
- Cost of membranes and materials and the reduction of fouling and scaling for longer membrane lifetimes.
- Degree of homogeneity per unit use of energy as it relates to the cost of the end product.
- Number of patents on new designs of mixers.
- Time and energy as inputs into the total cost of manufacture.
- ROI for process changes (in existing facilities).
- Amount of water evaporated per square foot of product as part of mass transfer.
- Method to adjust metrics appropriately based on the TRL.

FOCUS QUESTION 4: *How would Mixing and Mass Transfer best contribute to a public-private partnership Institute framework?*

Table B-14. Mixing and Mass Transfer – Contributions to a Public-Private Partnership

Contribution to an Institute Framework

- Flexible, instrumented, staffed demonstration facility (or user facility) for advancing new mixing and mass transfer technologies.
- Self-sustaining computational tool for use in mixing and mass transfer applications.
- Opportunity for study of nature-inspired engineering and architectures such as oxygen transfer from the lungs to the blood.

Contribution to Technology Advancement

- Recycling waste on-site for enhanced efficiency and/or secondary value products (e.g., waste heat used to filter water).
- Ability to use add-on-site capability (e.g., instead of flaring, using separation to funnel methane back to process and carbon dioxide to algae growth).
- Contributions of lower TRL FOAs to transitioning technologies at a TRL 5-8 to a demonstration facility.

Table B-15. Mixing and Mass Transfer Contributors	
Name	**Organization**
Marcy Berding	SRI International
Charles-Francois de Lannoy	PARC
David Hardy	DOE Advanced Manufacturing Office
Michael Heitkamp	Savannah River National Laboratory
Ryan Lively	Georgia Tech
Liyuan Liang	Oak Ridge National Laboratory
Krishnaswamy Nandakumar	Louisiana State University & Agriculture
Ron Schoon	National Renewable Energy Laboratory
Ratnesh Tiwari	University of Maryland
Sarah Topper	PPG Industries, Inc.
David Turpin	Agenda 2020 Technology Alliance
Elizabeth Vileno	Corning Incorporated
Justin Weiss	LNE Group

Chemical Separations and Crosscutting Technologies

FOCUS QUESTION 1: *What are the critical technological challenges and barriers for process separations and their crosscutting technologies?*

Table B-16. Barriers and Challenges for Chemical Separations and Crosscutting Technologies
Membranes
• Fouling in high-concentration applications (15-30% input stream). • Incompatibility of current membrane materials with pH/temperatures of some industrial applications. • Low membrane flux rates at high separation efficiencies. • Limited temperature range for membrane operation for reactions/separations. • Membrane lifetime, efficiency, and durability. • Stability of membrane and seals. • Membrane cleaning. • Trade-off between membrane flux and selectivity. • Separation of azeotropes.
Distillation and Other Separation
• Displacement of distillation as the primary separation method in chemical process industries (existing assets). • Distillation or separation of chemicals with very close boiling points. • Separation selectivity. • Efficiency of removing dilute product from process streams. • Undesirable back mixing of extraction columns.
Cross-Cutting
• Impact of transport and thermodynamic limitations on selectivity and specificity. • Pre-cleanup requirements of some contaminants. • Targeting micro-pollutant or emerging contaminants. • Logistical demands of storing products as multiple components are separated. • Inability to easily "tune" separations alternatives. • Reduction in capital costs as systems are scaled down. • Sunk cost of investment in existing design, equipment, and operations at existing facilities.

FOCUS QUESTION 2: *What are the critical technology developments that will be required for chemical separations and crosscutting technologies?*

Table B-17. R&D Needs for Chemical Separations and Crosscutting Technologies
Membrane Technologies
• Membranes capable of operating at process temperature and pressure conditions. • Straightforward "platform" membrane system for similar separations yet has specialty applications that are typically funded by industry. • Thermally integrated membrane separation and catalytic processes. • Non-noble metal hydrogen-selective membranes to facilitate reactive separations. • Membrane reactors with increased tolerance to impurities. • Acid gas stability of adsorbents and chloride stability for reverse osmosis (RO) membranes. • Gas separation membranes, specifically for CO_2 separation and nitrogen/methane separation.

Table B-17. R&D Needs for Chemical Separations and Crosscutting Technologies

- Membranes with improved selectivity and lifetime for applications including reactors, batteries, platform systems, and water purification.
- Membrane-based solvent recovery.
- Robust (polymer) membranes to meet the temperature needs of membrane reactors; H_2, O_2, CO_2 membranes that can be integrated with dehydrogenation, oxidation, and other catalytic reactions for higher yield and lower cost.
- High-temperature fluorinated membranes (for chemical separation and batteries).
- Membrane reactor and separation hydrogen production from bio-liquid.
- Membrane separation of light olefins and alkanes with similar boiling points.
- Facilitated transport membranes for oxygen-enriched air, nitrogen-enriched air, and CO_2.
- Alternatives for Nafion-based (sulfonated fluoropolymer) electrochemical systems.
- Novel anti-fouling technologies, including nozzles, additives, or self-cleaning processes.
- Non-chemical additive fouling control (i.e., membranes that are biofouling resistant or can prevent scale formation).
- Dual/combined membrane separation and reaction used in contaminant degradation, bio/pharma production, and chemical synthesis.
- Super acid catalyst for catalytic membrane reactor (with broad application).
- Membrane materials that can withstand high temperatures.

Sorbents

- Novel sorbent development for environmental remediation and water clean-up.
- Low-cost sorbents and metal organic frameworks (MOFs) that operate in relevant environments.
- Novel sorbent/process development for critical material extraction.

Distillation Technologies

- Distillation alternatives (e.g., more energy-efficient – with no phase change).
- Combining separation with reaction in order to save energy (e.g., reactive distillation to increase selectivity and product purity).
- Improved distillation column technology (temperature control and mass transport), including drop-in equipment, new packings and controls, and double wall column.
- Compact separation device for catalytic process distillation/absorption.

Other Separation Technologies

- Separations enhanced by external fields (e.g., electric, magnetic, microwave, etc.).
- High impact industrial separations (e.g., C_2 – C_5; olefin – paraffin separation).
- Oxygen/nitrogen separations for air enrichment in fossil plants.
- Ionic liquid separations.
- Magnetic field-assisted separation of oxygen/nitrogen.
- Separation of products from aqueous media at low product concentrations.
- High gravity separations.
- Intensified gas/liquid/solid 3-phase separation for gas/oil production.
- Environmentally friendly extraction of rare earths.
- New technological/device for surface refreshing and internal mixing.
- Ability to do chromatography on a distributed and large-scale.
- Computer-aided design of highly selective ligands for adsorption.
- Condensation and separation of pyrolysis vapors and bio-oil.
- Continuous bio-based process technologies, including continuous reaction with separation (e.g. continuous fermentation).
- Rotating separation devices with improved mechanical performance (reliability).
- Magnetic separation for use of metal organic frameworks (MOFs) and others for low concentration chemical recovery.

Table B-17. R&D Needs for Chemical Separations and Crosscutting Technologies

- Temperature swing adsorption for rapid gas purification.
- Separation technology tunable to variations in process stream inputs (self-adjusting).

Other Technologies and Manufacturing Techniques

- Manufacturing techniques to add specific ligands on various substrates such as polymers and inorganic materials.
- Compact techniques and new structural designs for improved mixing.
- Support structures and architectures on which to conduct the separations (e.g., membranes).
- New manufacturing techniques for new designs (e.g., brazing of membranes).
- Additive manufacturing to make membranes.
- Roll-to-roll technology for membrane production.
- Design and 3-D printing of reaction/separation units/devices, including modular ones.
- Process for CO_2 to dimethyl ether, a diesel substitute, to other products (distributed locations).
- New/improved mining methods that are environmentally benign and produce less waste.
- Technologies for turning stranded natural gas into products at generation site (products by new processes and/or modular facilities).

Modeling, Simulation, and Controls

- New visualization and complex controls development for process control.
- Combination of separation reactor design knowledge with data 3-D visualization to design systems and overcome technical challenges before construction.
- Realistic testing in conjunction with modeling.
- Advanced separation sequencing, modeling control, and integration.
- Fundamental models for reactive separation and control coordinated with testing protocols.
- Combinational chemistry modeling to design membrane materials/compositions.

FOCUS QUESTION 3: *What are the most appropriate metrics and types of impacts for assessing chemical separations and crosscutting technologies?*

Table B-18. Metrics and Impacts for Chemical Separations and Crosscutting Technologies

Energy

- Energy intensity and energy capital intensity.
- Life-cycle assessment metrics such as water usage, greenhouse gas emissions, and fossil energy consumption (e.g., reduce by greater than 30% in 3 years).
- Modular (approach) meets efficiency of existing processes in conversion and energy.
- *Suggested Targets:*
  - In 5 years, development of a case study showing cost and energy savings; minimum of 10% improvement at the nth plant and a life cycle assessment.
  - Minimum 20% reduction in volume; 20% reduction in energy.
  - 30% reduction in energy consumption in 5 years for methane to syngas.
  - Inverse of energy efficiency of process by 20% in 2 years and greater than 50% in 5 years.

Economic

- *Suggested Targets:*
  - 50% water efficiency improvement (twice as effective) over best available technology measured in dollars, yield, or conversion.
  - In 5 years, 1,000 hours of demonstration in a relevant environment and demonstrating cost decrease of 10%.
  - New separation technology must have at least 10% lower capital and operating costs than existing technology (especially distillation), with a goal of 50% lower costs.

Table B-18. Metrics and Impacts for Chemical Separations and Crosscutting Technologies

- Normalized capital at small/modular scale at least two times smaller than full scale.
- At least 20% improved economics (without carbon tax considerations) as a result of improved process performance (based on thousands of hours of demonstration).
- Cost-effective implementation within 10 years.
- Demonstration of robust modular conversion of distributed feedstock at capital expenditures cost of $50,000 per barrel of oil equivalent per day.

Other

- Brine disposal for reverse osmosis.
- Flaring (methane and CO_2 release).
- Leakage at well; number of abandoned wells.
- Computational code that enables membrane design for specific chemical applications (pass/fail evaluation).
- Flux, sensitivity, operating temperature, chemically robust, stable market, cost, manufacturability, and economics of application.
- Waste intensity (kilogram waste/kilogram product).
- *Suggested Targets:*
  - At least three technologies "adopted" by industry by the end of five years.
  - A 20% reduction over state-of-the-art in CO_2-equivalent mass (emissions).
  - At least three modular 3-D printing operations at three different scales in five years.

QUESTION 4: *How would a chemical separations and crosscutting technologies best contribute to a public-private partnership institute framework?*

Table B-19. Chemical Separations and Crosscutting Technologies – Contributions to a Public-Private Partnership

Contribution to Institute Framework

- Technology groupings that allow comparison via modeling and simulation to current state-of-the-art.
- Recognition that adaptive membranes (with wide applicability) are not like current membrane technologies.
- Focus on energy productivity (dollars per unit).
- Support for advanced materials scale-up and supply chain.
- Testing facility to independently verify materials for separation at relevant conditions.
- Methods to engage engineering, procurement, and construction firms.
- Partnerships between engineering contractors (crossing technology silos).
- Demonstration of economically viable modular technologies.
- Modeling and simulation, model validation, and upgrading process modeling to plant model.
- De-risking of separation options for smaller processes (biomass, fuels, chemistry; modular systems).
- Public database for best practices.
- Publicly available analysis tools to support pinch integration analysis.

Contribution to Technology Advancement

Table B-19. Chemical Separations and Crosscutting Technologies – Contributions to a Public-Private Partnership

- Big data modeling and simulation and advanced/dynamic modeling.
- Smaller, more distributed technologies that could address localized needs for separations and extractions.
- Reactive membrane technology and scale up for improved cleanup, and water purification/separation.
- Collaboration on reactive separations such as alkanes dehydrogenation.
- Membranes for shale gas clean-up (could involve gas companies; national laboratories, SBIRs, and universities).
- Carbon capture and utilization by a bio-refinery (power companies, universities, national laboratories, small companies).
- Encouragement of pilot-scale implementation of CO_2 capture at plants (through collaboration with academia and national laboratories).
- Pilot test facility to test/validate separations (including membrane performance).
- Rethinking wastewater as a recoverable, valuable resource instead of a waste.
- Membranes and materials (sorbents and solvents) for scale-up including addressing supply chain issues.
- Distributed waste and biomass to enable distributed supply chains, allowing better use of feedstocks.
- Technology for separations for dilute aqueous streams, broadly applicable to biofuels, forest products, chemical, drinking water, and oil exploration and production industries.
- Demonstration facility for improved distillation (could include adsorption, extraction, etc.).
- Separation and reaction; dry CO_2 reforming; any available CO_2 stream.
- Novel small-scale separations (integrated reaction and separation systems).

Table B-20. Contributors to Chemical Separations and Crosscutting Technologies	
Name	**Organization**
Balu Balachandran	Argonne National Laboratory
Robert Baldwin	National Renewable Energy Laboratory
David Bruce	Clemson University
Billy Bardin	The Dow Chemical Company
Marcy Berding	SRI International
Mary Biddy	National Renewable Energy Laboratory
Maria Burka	National Science Foundation
David Constable	ACS Green Chemistry Institute
Louis DiNetta	Compact Membrane Systems, Inc.
David Edwards	Zeton Inc.
Charles Freeman	Pacific Northwest National Laboratory
Daniel Ginosar	Idaho National Laboratory
Faruque Hasan	Texas A&M University
Jamie Holladay	Pacific Northwest National Laboratory
Cynthia Jenks	Ames Laboratory, U.S. DOE
Zhijun Jia	CompRex, LLC
Patrick Kwon	Michigan State University
Dongxia Liu	University of Maryland
Ryan Lively	Georgia Institute of Technology
Sudip Majumdar	Compact Membrane Systems
Randall Partridge	ExxonMobil Research and Engineering Co.
Robert Ritchie	Corning Incorporated
Sharon Robinson	Oak Ridge National Laboratory
Mark Shuart	DOE Advanced Manufacturing Office
Bhima Sastri	DOE Office of Fossil Energy
Costas Tsouris	Oak Ridge National Laboratory
David Turpin	Agenda 2020 Technology Alliance
Eric Wachsman	University of Maryland

Other Process Intensification Applications

Question 1: *What are the challenges and barriers for other process intensification applications?*

Table B-21. Barriers and Challenges for Other Process Intensification Applications

Material Use and Recovery

- Limitations of current conversation/utilization technologies.
- U.S. supply chain inefficiencies (leading to attractiveness of transfer outside the country).
- Requirements for transporting water in food/agriculture, electricity production, and industrial applications.

Manufacturing Process and Life Cycle

- Limitations of current control systems for operation of process-intensive systems.
- Inability of additive manufacturing to address porosity and surface finish tolerance requirements.
- Residual stresses that occur during manufacture of certain products, which affect surface finish tolerance.
- High energy and water efficiency of large plants, making further improvements more difficult.
- Reluctance on the part of many operators to “own” life cycle issues.

Institutional Factors

- Inability of small and medium-sized companies to effectively manage supply chains because of lack of resources.
- Lack of information/education for staff operating plants, and lack of buy-in for advances.
- Regulatory and process “overkill” efforts (could more energy be lost than created?)
- Current manufacturing business models do not account for resources, value, and safety.
- Shifting government research priorities leading to TRL 2, 3, and 4 technologies losing funding.
- Academic rather than practical nature of many data in the public domain.

QUESTION 2: *What critical technology development will be needed for other process intensification applications?*

Table B-22. R&D Needs for Other Process Intensification

Basic and Applied R&D

- Improved distributed processes for biomass and waste-tolerant materials.
- Integration of diverse technologies that might be mutually beneficial (e.g., algae for biofuel utilizing industrial stock gases and liquid effluents).
- Material substitution strategies and materials development via advanced manufacturing processes.
- Alternative thermal process research such as wave/material data, measurement technologies, and cross-cutting materials/data measurement issues.
- Recycle-friendly materials (RFMs) as markers that could also aid in standardization efforts for RFMs/products.
- New transient distributed processes that utilize renewable energy or feedstocks that make use of intermittent renewable resources for grid leveling.
- Process methodology for integration of concentrated solar thermal and thermochemical energy with industrial processes to reduce fossil carbon consumption (traditional gas/oil).
- Processes and feedstocks that provide alternatives to petroleum for hydrogen, carbon and energy use in manufacturing.

Table B-22. R&D Needs for Other Process Intensification

Hardware

- Low-cost, reliable sensors and actuators for control and monitoring.
- Low-cost manufacturing methods for PI hardware that allow determination of hardware mass production economics to compete with economies of scale.
- Consolidation of operational characteristics of micro-reactors, heat exchangers and separators (e.g., an engineering handbook).
- Technologies for water treatment at an industrial facility scale to enable internal re-use, including determination of critical parameters in various industries, and level of cleaning.
- Smaller, modular systems to enable water treatment and heat integration in industrial sites or agricultural sites.

Demonstrations

- Waste water filtration pilot plants for proof of concept and large scale demonstration of new technologies.
- PI system demonstration for meaningful applications (e.g. producing liquid hydrocarbons from landfill biogas).
- Demonstration process to determine feedstock and catalyst flexibility, catalyst longevity and resistance to poisoning, and reactor design requirements for municipal waste and waste plastic.
- Demonstration of feedstock flexibility and catalyst longevity, improved selectivity and tune-ability of the catalyst to the target product development, and catalyst poison resistance and regeneration.

Material Use and Recovery

- Technologies for maximum conversion/utilization of raw materials regardless of the process without reverting to current technology capabilities.
- Life-cycle consideration of all secondary sources.
- Scaled-down, cost effective approaches for waste treatment and recovery of materials and energy to support distributed modular, continuous-flow manufacturing.
- Materials recovery and reuse for municipal solid wastes and waste plastics, catalytic conversion of wastes to chemical products, and domestic waste recovery (supply chain issue).
- Efficient, smart recycling technology to process localized feedstocks.

Analysis

- Supply chain management across industries and markets and integrated processes and communication methods to determine connectivity (how can PI connect those areas?).
- Models that analyze the impact of using water for manufacturing as opposed to agriculture.
- Fresh view of early-stage technologies that could be moved forward in the development cycle if new metrics are considered.
- Technologies that address R&D needs in different parts of DOE (e.g., an algae roadmap).
- Cost-effective balance of plant evaluations for small-scale applications in order to determine the cost-effectiveness of scale-up from small plant scale to full production levels.

Life Cycle Cost

- Understanding of recovery costs for reuse/recycle of materials to determine if certain items are cost effective.
- Methodology for quantifying the life-cycle of products (particular chemicals) from raw material, production use, and recycling, and a database on life-cycle information (e.g., degradation of material, cost of material, cost of recovery, etc.).
- Life-cycle analyses, guidelines, and standardization, including for water consumption.
- System-level evaluation of the cost change due to technology development, cost on environment and on health, and cost due to process variety.
- Better definition of the role of technology development for end-of-life-cycle requirements for products transitioning to the commercial sector.
- Minimization of material use during production in order to minimize waste produced.

QUESTION 3: *What are the most appropriate performance/impact metrics for other process intensification applications?*

Table B-23. Metrics and Impacts for Other Process Intensification Applications

Performance Improvement

- Ratio of hydrocarbon product per unit to the hydrocarbon feedstock input required.
- Performance metrics for modular technologies for distributed systems that match the cost/unit product of large, centralized processes.
- Business-model-dependent metric such as unit of productivity equal to the dollar value added/unit of interest.
- Metrics for biggest impact versus nearest-term impact and distributed applications versus large, established production facilities.
- Savings for operational capital expenditures (capital investments).
- Net energy and water consumption per unit production that could equate to net savings.
- Product intensification hardware metrics following Moore's Law in equivalency (doubles approximately every two years) as it pertains to productivity.
- Evaluation metric of dollars of investment per unit of production of shale gas (value should go down if proper PI is applied); shale gas will drive new investment over the next 10 years.

Resource Recovery and Savings

- Use of previously unutilized gas streams that can be applied to other waste streams to drive them closer to zero (e.g., plastics in the waste stream, zero gas flare, recycle by-products).
- Number of products that can be easily communicated and sold to the public.
- Recovery of previously unrecoverable materials and energy from a given process.
- "Cradle to cradle" type metric; i.e., material/product degradation/ number of reuse cycles (yield times fitness).
- Negative feedstock value to positive value for high margin chemicals using in-situ recycling, and recycling by-products (e.g., benzene-toluene-xylene recovery and recycle).
- Amount of process effluent stream recycled back to reactor during an alkylation process for chemicals such as p-xylene and polyethylene terephthalate plastics.
- Reduction in fossil carbon emissions (i.e., carbon utilization).

Other

- Relationship between size of production system size and distribution scale (if the chemical requires a large system, must the distribution be on a large scale?).
- Expansion of life-cycle analysis beyond energy life-cycle.
- Clear metrics and ranking process to prioritize the most promising early TRL separation technologies for potential relevance to distributed, modular manufacturing.

QUESTION 4: *How would other process intensification applications best contribute to a public-private partnership institute framework?*

Table B-24. Other Process Intensification Applications – Contributions to a Public-Private Partnership

Industry Impact

- Development of new business models.
- Fostering community engagement throughout the chemical process industry.
- Reduction in the "time to commercial application" for various PI systems.
- Support for continued improvement of PI systems.
- Evaluation of carbon footprint effects as a social engineering problem.
- Definition of the importance of PI to industry and determination of players interested in a PI institute.
- Evaluation of process equipment exportation (e.g. in the international shale gas market) to determine the impact to U.S industry.
- Access to cheap feedstock and portable technology for basic chemicals.
- Positive public viewpoint and local support.
- Regional job creation/education.
- Impact of regulations on institute performance (e.g., automotive CAFE standards).
- Research facilities available to allow ready access to micro-components for developers to evaluate cheap hardware, short lead times and other experiments.
- Research facilities for development of design rules and evaluation of material and design choices, functional grading materials, and passage controls.

DOE Role

- Establishment of a defined area of PI to make an impact on technology development and transfer to industry.
- Definition of the areas for investment under PI, how a PI effort will be described and defined to potential investors, and how the list of requirements will be narrowed down for the purposes of an Institute.

Education

- Collaboration with universities.
- Education on PI by providing availability of faculty/industry/classroom; training and curriculum development (industry would provide academic problems).
- PI training to the next generation of process engineers.
  - Requirement for an engineering curriculum that focuses on processes in a modular way.
  - Need for teaching on modularity and de-centralization of processes that are not "business as usual.
- Establishment of scholarship programs for mostly graduate students using a Nation Science Foundation (NSF) I-Corp model.
- Incorporation of graduate students, industrial representatives, and academics into an institute.
- Creation of roles for associate-level degree seekers and community colleges.
- Education on PI applications as part of modular training on aspects of specific technologies – not necessarily degree related or CEUs (continuing education units).

Showcase Activities

- Focus on a new business model for small and medium-sized companies.
- Driving the development of cross-platform modeling tools.
- Dual-focus R&D efforts: small, medium, and large companies.
- Techno-economic analysis (e.g., as a function of yield, customer, or need).
- Showcasing advancements in manufacturing that make an economic impact.
- Demonstration for large-scale production of needed materials using PI approaches.

Table B-24. Other Process Intensification Applications – Contributions to a Public-Private Partnership
Public Impact
• Formation of health/environment/safety alliances to benefit community relations and company relations with unintended effects (e.g. wastewater treatment regulations from the 1970s that have helped clean up rivers). • Positive effects of institute/public alliances on local support that could lead to job creation and community involvement in the industry. • Enhanced national competitiveness.
Partnership Model
• Likelihood of various companies joining a public-private partnership.   ▪ Example: The Advanced Composite Group has 120 companies willing to join because they are trying to make a low cost carbon fiber. Carbon fiber is one of the few advancing technologies over the next 10 years. There could be common goals for carbon fiber technology and PI efforts.

Table B-25. Contributors to Other Process Intensification Applications	
Name	**Organization**
John Carpenter	RTI International
Joe Cresko	DOE Advanced Manufacturing Office
Anne Gaffney	Idaho National Laboratory
Tilak Gullinkala	Owens-Illinois
Gregory Harris	OSD/US Army
Michael Heitkamp	Savannah River National Laboratory
Greg Jackson	Colorado School of Mines
Patrick Kwon	Michigan State University
Alan Liby	Oak Ridge National Laboratory
Gary Luce	Eastman Chemical
Vahid Motevalli	Tennessee Tech (Center for Manufacturing Research)
Krishnaswamy Nandakumar	Louisiana State University & Agriculture
Ron Schoon	National Renewable Energy Laboratory
Robert Wegeng	Pacific Northwest National Laboratory
Justin Weiss	LNE Group

Environmental Management

Focus Question 1: *What are the challenges and barriers regarding Environmental Management for processes used in industrial applications?*

Table B-26. Barriers and Challenges for Environmental Management

Energy and Other Resources

- Energy requirements for current water separation processes.
- Energy needed for waste cleanup (separators are normally energy intensive).
- High process water requirements.

Supply Chain and Infrastructure

- U.S. supply chain inefficiencies (leading to attractiveness of transfer to outside the country).
- Inability of small and medium-sized companies to effectively manage supply chains because of lack of resources.
- Need for transporting waste from manufacturing facilities.
- Co-location of processes to reuse waste heat.
- Academic rather than practical nature of many data in the public domain.

Technical

- Limitations of current conversation/utilization technologies.
- Design of a method or technology for separating a by-product and a waste stream within a single process.
- Reducing waste by increasing yield and selectivity.
- Reusing polymers from waste streams and "erasing" the thermal history of waste streams.
- Technology development needed to drive the process of setting technical requirements for environmental regulations (regulations need to be good stewards, e.g., regulations for lead settling ponds).

Economic

- Limitations of current conversion/utilization technologies.
- Current manufacturing business models do not account for resources, value, and safety.
- Few ROI drivers except for energy reduction, which creates barriers for environmental management.
- Financial barriers (i.e., companies are less likely to invest money if there is no ROI or government/customer mandate).
- Few motivations to put resources towards environmental management other than recognition.

Focus Question 2: *What are the research and development needs that would assist environmental management of industrial processes and how could an institute address those needs?*

Table B-27. Research and Development Needs that would Assist Environmental Management of Industrial Processes

Water

- Recovery of the water from biofuels production, including cleaning water sufficiently for a municipal waste treatment plant.
- Recovery of chemicals and nanoparticles from water at dilute concentrations, with a focus on mitigating impurities using advanced separation technologies.
- Low-energy water separation.
- Faster method of removing pollutants from water other than boiling.

Table B-27. Research and Development Needs that would Assist Environmental Management of Industrial Processes

- Enhanced, less energy-intensive water extraction from gas, solid, and liquid effluents, such as alternative evaporation techniques and trace metal extraction including extraction/separation of very dilute concentrations.
- Models that analyze the impact of using water for manufacturing as opposed to agriculture.
- Transposable PI technologies for wastewater treatment, including generic solutions based on first principles.

Waste Reduction/Reuse

- Access to "mobile" laboratories and pilot plants for quick turnaround, onsite testing and characterization of waste streams and product lines for contaminants such as carbon dioxide.
- Transforming carbon dioxide into useful carbon products.
- Scaled-down, cost effective approaches for waste treatment and recovery of materials and energy to support distributed modular, continuous-flow manufacturing.
- Materials recovery and reuse for municipal solid wastes and waste plastics, catalytic conversion of wastes to chemical products, and domestic waste recovery. This is a supply chain issue.
- Efficient, smart recycling technology to process localized feedstocks.
- Recovery of chemicals and nanoparticles from water at dilute concentrations, with focus on mitigating impurities using advanced separation technologies.
- High-throughput, low-energy filtration, including solid/ aqueous/organic separation and high-throughput/low-energy separation for water in order to reduce pollutant discharge to the environment.
- Subsurface characterization, specifically to examine subsurface characterization without excavation including liquids and contaminants, and metrology that enables characterization of environmental issues resulting from legacy waste.
- Environmental case for burning waste such as wood chips and recycled tires.

Other Technology

- Process for trace metal separation.
- Low energy liquid-liquid (separation) extraction technologies similar to rare earth separation technologies (multi-stage units are available in Europe); multi-stage units in a single device.
- Technologies for inorganic, organic, and water separation in pulp and paper products.
- Energy-efficient metals transformation methods.
- Cheaper methods for separating nitrogen and oxygen.
- "Green" chemistry research to develop a wider choice of green feedstocks.
- Methods to mitigate the effect of impurities on the performance of separation technologies, such as fouling and degradation.

Modeling, Analysis, and Knowledge Base

- Enhanced modeling and simulation of industrial processes, especially life-cycle analysis.
- Energy, resource, value, and safety knowledge for distributed manufacturers.
- Fresh view of early-stage technologies that could be moved forward in the development cycle if new metrics are considered.
- Initial product designs that address long-term environmental management requirements (e.g., nanoparticles found in cosmetics that are now polluting lakes).
- Consideration of capital investment for gas separations (for oxygen, nitrogen, carbon dioxide and volatile organic compounds) on a large scale, or as an add-on, relative to environmental management requirements.
- Assessment of the entire life-cycle of biofuels.
- Understanding of environmental biological-geological-chemical interactions.
- Investigation of emerging pollutants.
- Enhanced modeling and simulation of industrial processes, especially lifecycle analysis.

Other

- Supply chain management across industries and markets and integrated processes and communication methods to determine connectivity (how can PI connect those areas?).

Table B-27. Research and Development Needs that would Assist Environmental Management of Industrial Processes

- Availability of pilot plants and pilot test facilities, including small and mobile test facilities, for testing pre-production materials and processes (e.g., removal of mercury from air emission sources).
- Development of secondary source inventories to feed the supply chain.
- Improvements to the environmental management of manufacturing processes, such as those that are taking place in Europe and even China.

Focus Question 3*: What metrics should be used and what are the impacts of breakthrough technologies that improve environmental management of industrial processes?*

Table B-28. Metrics and Impacts for Environmental Management of Industrial Processes

Metrics

- Time to affect environmental control before waste migrates out of the feed reservation (e.g., groundwater).
- Toxicity of waste per unit products, and life-cycle waste production or reduction (e.g., toxicity of waste/unit products for laundry detergent); life-cycle analysis considers these materials and factors their environmental impact into production decisions.
- Ultimate goal of zero waste in production and in the environment under life-cycle analysis including product packaging; initial goal of zero waste in production, expanding to zero waste throughout the supply chain.
- Ecosystem and human health (processes versus mortality rates and occupational health).
- Percent reduction in materials, water, and energy use achieved by a target year.
- Volume of waste and the cost of disposal.
- Separation efficiency (D:F ratio/stage) (fraction evaporated per stage) for liquid/liquid extraction.
- Flux/area for solid/liquid separation.
- Flux/area/BTU (energy) for water separation.
  Cost savings achieved through green chemistry implementations.
- *Suggested Targets:*
  - 75% reduction in energy per pound for liquid-liquid extraction.
  - 50% reduction in energy per pound for water separations.
  - 50% reduction in capital cost.
  - 50% increase in throughput at the same energy per pound for solid-liquid separations.
  - Minimal (<1%) added for product, production time and maintenance.

Impacts

- Education:
  - Awareness efforts, since small businesses do not understand benefits as well.
  - Metric for measuring consumer and industrial awareness.
  - Cultural shift, such as what occurred with automobile seatbelts.
- Greater number of science/technology education programs certified by Accreditation Board for Engineering and Technology (ABET).
- Bio-diversity and species attrition.
- Encouraging industry to set and meet sustainability goals.
- Development of global solutions to pollution reduction.
- Improvements to environmental management technologies for city versus rural/urban areas (smaller housing and more intense processes closer together could impact the environment).

Focus Question 4: *What are other considerations for technology advancement with contributions to an Institute framework and their impact on environmental management?*

Table B-29. Environmental Management – Contributions to a Public-Private Partnership
Contribution of Environmental Management to Institute Framework
• Addressing environmental management issues from large and small businesses; easier for large industries to utilize internal resources for environmental management. • Industry input to help direct fundamental research to maximize industry impact. • Environmental management as a good platform for PI technology R&D in a non-competitive space. • Environmental management as organic to the structure of a PI institute structure that considers life-cycle processes. • Contribution of technology developed by an institute to small and medium-sized companies' R&D needs. • DOE encouragement to entrepreneurs and small businesses to innovate and be competitive by issuing funding opportunities for environmental management technologies. • Government user facility for industry as part of an industry-government partnership. • Institute as an education center.
Contribution of Environmental Management to Technology Advancement

• Ability to assess environmental management issues from pollutants/toxics created unknowingly in processing, which would help industry test, identify, and evaluate pollutants or toxics before a violation occurs.
• Ability of national laboratories and universities to address fundamental technology advancement for which industry does not have the time or money.
• Confidential industrial partner access to intellectual property (e.g., more assured ownership of intellectual property by stakeholders, and/or greater protections to use developed intellectual property).
• Voluntary programs to highlight achievements, an Environmental Star award similar to ENERGY STAR, which would increase the number of recognition programs for environmental management.
• Better organization/collaboration on environmental management R&D, including demonstration facilities or centers of excellence.
    ▪ The DOE Office of Environmental Management (EM) funds university centers.
    ▪ Of DOE's budget, EM is $6 billion, and $40 million is floating in R&D that goes to three facilities under construction.

Table B-20. Contributors to Environmental Management	
Name	**Organization**
Bond Calloway	Savannah River National Laboratory
Qi Dang	Iowa State University
Diane Graziano	Argonne National Laboratory
David Hardy	DOE Advanced Manufacturing Office
Liyuan Liang	Oak Ridge National Laboratory
Mike McKittrick	DOE Advanced Manufacturing Office
Elizabeth Vileno	Corning Incorporated
Esther Wilcox	National Renewable Energy Laboratory

APPENDIX C. COMPLETE LIST OF WORKSHOP PARTICIPANTS

Name	Organization
Thad Adams	Savannah River National Laboratory
Lakeyshia Alexander	TCG Consulting, Inc.
William Ayers	Ayers Group, LLC
Balu Balachandran	Argonne National Laboratory
Robert Baldwin	National Renewable Energy Laboratory
Billy Bardin	The Dow Chemical Company
Marcy Berding	SRI International
Mary Biddy	National Renewable Energy Laboratory
Richard Bogacz	New West Technologies
Dane Boysen	Gas Technology Institute
Megan Brewster	DOE Advanced Manufacturing Office
Joe Broz	SRI
David Bruce	Clemson University
Maria Burka	National Science Foundation
Rolf Butters	U.S. Department of Energy
Bond Calloway	Savannah River National Laboratory
John Carpenter	RTI International
Charles Chen	Energetics Incorporated
Anne Clawson	Alcoa Inc.
Jonathan Cohen	Agency of Trillions
Suzanne Cole	American Chemistry Council
David Constable	ACS Green Chemistry Institute
Joe Cresko	DOE Advanced Manufacturing Office
Fred Crowson	Energetics Incorporated
Qi Dang	Iowa State University
Charles-Francois de Lannoy	PARC
Serguei Dessiatoun	University of Maryland
Louis DiNetta	Compact Membrane Systems, Inc.
David Edwards	Zeton Inc.
Laura Fabeny	New West Technologies
Aaron Fisher	Energetics Incorporated
Charles Freeman	Pacific Northwest National Laboratory
Anne Gaffney	Idaho National Laboratory
Daniel Ginosar	Idaho National Laboratory
Alison Gotkin	UTRC
Diane Graziano	Argonne National Laboratory
Tilak Gullinkala	Owens-Illinois
Raghubir Gupta	RTI International
David Hardy	DOE Advanced Manufacturing Office
Gregory Harris	OSD/U.S. Army
Faruque Hasan	Texas A&M University
Michael Heitkamp	Savannah River National Laboratory

Name	Organization
Jamie Holladay	Pacific Northwest National Laboratory
Cassidy Houchins	SA, Inc.
John Hryn	Argonne National Laboratory
Robert Hyers	Boston Electromet
Greg Jackson	Colorado School of Mines
Keith Jamison	Energetics Incorporated
Cynthia Jenks	Ames Laboratory, U.S. DOE
Zhijun Jia	CompRex, LLC
Mark Johnson	DOE Advanced Manufacturing Office
Denis King	DJKing & Associates
Jackie Kulfan	PPG Industries, Inc.
Patrick Kwon	Michigan State University
Saniya LeBlanc	George Washington University
Liyuan Liang	Oak Ridge National Laboratory
Alan Liby	Oak Ridge National Laboratory
Ryan Lively	Georgia Institute of Technology
Gary Luce	Eastman Chemical
Sudip Majumdar	Compact Membrane Systems
John Marano	JM Energy Consulting, Inc.
John Marra	U.S. Department of Energy
Mike McKittrick	DOE Advanced Manufacturing Office
Vahid Motevalli	Tennessee Tech (Center for Manufacturing Research)
Sankar Nair	Georgia Institute of Technology
Krishnaswamy Nandakumar	Louisiana State University & Agriculture
Stephen Nunez	DOE Advanced Manufacturing Office
Gina Oliver	American Chemistry Council
Randall Partridge	ExxonMobil Research and Engineering Co.
Michelle Pastel	Corning, Inc.
Brian Paul	Oregon State University
Frank Pfefferkorn	University of Wisconsin-Madison
Amara Projansky	Agency of Trillions
Veena Rao	University of Maryland
Robert Ritchie	Corning Incorporated
Sharon Robinson	Oak Ridge National Laboratory
Bhima Sastri	DOE Office of Fossil Energy
Mayur Sathe	LSU Chemical Engineering
Ron Schoon	National Renewable Energy Laboratory
Diane Schuster	American Institute of Chemical Engineers
Amir Shooshtari	University of Maryland
Mark Shuart	DOE Advanced Manufacturing Office
Stephen Sikirica	DOE Advanced Manufacturing Office
Ratnesh Tiwari	University of Maryland
Richard Todaro	New West Technologies
Sarah Topper	PPG Industries, Inc.
Costas Tsouris	Oak Ridge National Laboratory
David Turpin	Agenda 2020 Technology Alliance
Mario Urdaneta	DOE Advanced Manufacturing Office

Name	Organization
Brian Valentine	DOE Advanced Manufacturing Office
Joseph Vehec	U. S. Steel
Elizabeth Vileno	Corning Incorporated
Eric Wachsman	University of Maryland
David Walters	PPG Industries, Inc.
Conghua Wang	TreadStone Technologies, Inc.
Robert Wegeng	Pacific Northwest National Laboratory
Justin Weiss	LNE Group
Esther Wilcox	National Renewable Energy Laboratory
Mark Wright	Iowa State University
David Zaziski	Siluria Technologies, Inc.

APPENDIX D. PANELIST BIOGRAPHIES

NGO SMEs – Process Intensification Workshop Panel

Dr. John Marra is currently a Senior Technical Advisor with the U.S. Department of Energy – Office of Environmental Management. During his near 30 years as a technologist, he held various technical staff and management positions at the Department of Energy's Savannah River Site, Savannah River National Laboratory. His work focused on management and treatment of high-level radioactive waste, development and application of advanced materials, and advanced chemical process applications. Dr. Marra is a past president of the American Ceramic Society (ACerS). He is an ACerS Fellow and a past chair and past director of the Nuclear & Environmental Technology Division. He holds degrees in Ceramics Science and Engineering and in the Arts, from Alfred University and the Ohio State University.

Dr. Darlene Schuster presently serves as the Director of the Institute for Sustainability, an American Institute of Chemical Engineers (AIChE) Technological Community. Previously she served in the non-profit technology/society sector as the Senior Director of Institute Alliances and Director of Government Relations for AIChE. She has also been a Science Policy Fellow for the American Chemical Society, where she worked to educate congressional staff and Congress on technical policy issues. Previously, Dr. Schuster was the Clare Boothe Luce Chair of Chemical Engineering at Bucknell University, and an Engineer, Senior Engineer, and Research Engineer with Gulf Oil Production Research, which subsequently became Chevron Oil Field Research Company. She holds a bachelor’s degree from West Virginia University, a master’s from the University of Pittsburgh, and Ph.D. from West Virginia—all in Chemical Engineering.

Mr. David Turpin is executive director of the forest products industry’s Agenda 2020 Technology Alliance, an industry-led consortium that promotes development of advanced technologies for the pulp and paper industry. As executive director, he oversees identification of the industry’s technology research priorities and development of strategies to address them, building partnerships and identifying potential funding sources. Prior to joining Agenda 2020 in 2014, he served for more than 25 years with MeadWestvaco and its predecessor Mead Corporation. Most recently, he was Vice President, Innovation Systems, and prior to that served as Vice President, Packaging Materials and Processing. He holds a B.S. degree in Paper Science from North Carolina State University.

Mr. Phil Callihan is currently the Director, Strategic Projects and MIS, National Center for Manufacturing Sciences. Previously, he also held positions as Editor-in- Chief of UMGoBlue.COM, principle contributor of the Bleacher Report, Go2Tape at the University of Michigan and was Publisher & Founder, Go2Tape. He has a B.A. from the University of Michigan and completed executive education programs at the University of Chicago.

Mr. Denis King has over 40 years of domestic and international experience in the energy and electric power industry and has worked in engineering and project management on power plant projects utilizing a variety of technologies. Mr. King has had assignments as Independent Engineer, Owner’s Engineer, and Technical Advisor and has worked on projects for public utilities, private utilities, industrials, and independent power producers. He is a principal in the firm D. J. King and Associates, Inc. He was formerly the Managing Director of Technical Services, K&M Engineering and Consulting, LLC and previously worked for PG&E National Energy Group, KMR Power and Bechtel Power Corp. Mr. King is a Professional Engineer and attended the University of Maryland, the Catholic University of America, Golden Gate University, and Queen Mary - University of London. He has earned undergraduate and graduate degrees in Electrical Engineering, Nuclear Engineering, Business Administration and International Commercial Arbitration.

Dr. Brian Paul has been a faculty member at Oregon State University for about 20 years. He is currently a Professor within the schools Industrial and Manufacturing Engineering and the Co-Director of its Microproducts Breakthrough Institute. There he conducts research on arrayed microfluidics for green nanosynthesis; microreactor-assisted materials processing: precision bonding for microsystem packaging; and packaging of arrayed microfluidic systems for distributed and portable energy, chemical, and biomedical applications, especially via microlamination. His work is committed to developing technologies for sustainable energy, healthy environments, and improved lives. He holds degrees from the Pennsylvania State University (Ph.D.), Arizona State University (M.S.) and Wichita State University (B.S.).

Industry SMEs – Process Intensification Workshop Panel

Dr. William Ayers is the CTO of Ayers Group, LLC, a consulting organization focused on research and investments in alternative energy and chemicals. He is a SME, who has had an extensive career, focused on energy and electrochemical technology with nearly 30 years' experience in developing, patenting, and commercializing new products. His efforts have resulted in a large number of new product concepts based on advances in chemical physics, electron transfer, plasmonics, and radioisotopes. He is the founder and past CEO of Electron Transfer Technologies, which was acquired in 2004 by Air Products and Chemicals Inc. Additionally, he has been the principal Investigator on grants from the Department of Energy, Department of Defense, and the National Science Foundation. He is an inventor with multiple patents, which includes on-site electrocatalytic hydride generators, electrocatalytic materials, photovoltaic hydrogen productions, fuel cells, carbon dioxide to liquid fuels, and Li battery electrode state of charge sensor. He holds degrees from the University of Pennsylvania (Ph.D. Chemical Engineering), Massachusetts Institute of Technology (M.S. Chemical Engineering), and Princeton University (B.S.E. Chemical Engineering)

Mr. Billy Bardin is the Global Operations Technology Director for the Dow Chemical Company. His responsibilities include driving technology and innovation strategy within Manufacturing and Engineering and oversight of all commercial technologies as well as development of technical talent across manufacturing and supporting operations. He began his career in 2000 with Union Carbide/Dow in the Catalyst Skill Center in South Charleston, WV where he led alternative feedstock and catalytic process development programs. Billy holds a B.S. in Chemical Engineering from North Carolina State University, and M.S. and Ph.D. degrees in Chemical Engineering from the University of Virginia. He is a registered Professional Engineer in the state of West Virginia. He is chair of the Industrial Advisory Board for the School of Chemical Engineering at Purdue University, and a member of the advisory board for the Department of Chemical Engineering at the University of Virginia.

Ms. Michelle Pastel currently is the Manager for Measurements, Controls, and Systems Innovation, in Corning's Manufacturing Technology and Engineering Division, Advanced Engineering Directorate Corning Inc. She joined Corning in 1993 as a Systems Engineer. In her current position, she is focused on collaborating with Science & Technology, as well as Corning's businesses, to deliver differentiating technology solutions in the areas of measurements, advanced process control, laser processing, imaging systems, and systems integration technologies for products and processes to enable Corning's research and development programs to innovate new products and manufacturing processes. She earned her B.S. degree in Electrical and Computer Engineering from the University of New Mexico.

Dr. David Constable is the Director of American Chemical Society - Green Chemistry Institute. Previously, he was owner and principal at Sustainability Foresights, LLC, a consulting firm that assisted companies with sustainability, sustainable and green chemistry, energy, environment, health and safety (ESH) programs. Prior to this, Constable was with Lockheed Martin as the Corporate Vice President of Energy, Environment, Safety & Health and the Director of Operational Sustainability in the Corporate ESH Department at GlaxoSmithKline and a Group Leader of the SHEA Analytical Services group at ICI Americas. In his professional roles, he led development of sustainability-based programs, systems, tools and methodologies. David has a Ph.D. in Chemistry from the University of Connecticut and a B.S. in Environmental Sciences, Air and Water Pollution from Slippery Rock University.

Dr. Dane Boysen is the Executive Director, Research Operations for the Gas Technology Institute. Prior to joining the Gas Technology Institute, Dr. Boysen was a program director within the Advanced Research Projects Agency—Energy (ARPA-E), a researcher at the Massachusetts Institute of Technology and was the founder of Superprotonic, Inc., an energy technology company established to market and commercialize an innovative solid acid fuel cell. He possesses degrees in Materials Science and Engineering from the California Institute of Technology (Ph.D.) and the University of Washington (B.S.).

Mr. Gary Luce is the Technology Manager for Corporate Innovation at the Eastman Innovation Center at Eastman Chemical Company. Overall, he has over 35 years' experience in technology, intellectual property management and business growth for Eastman Chemical Company; 18 years at the Longview, TX site and 17 years in Kingsport, TN. During his tenure, he has gained experience in acquisition, divestiture, business growth, technology development and intellectual property management.

APPENDIX E. ACRONYM LIST

3-D	3-dimensional
ABET	Accreditation Boards for Engineering and Technology
AMO	Advanced Manufacturing Office
ASTM	ASTM, formerly referred to as the American Society for Testing and Materials
Bbl	Barrels
Btu	British thermal unit
^{o}C	Celsius (degrees)
CAFE	Corporate Average Fuel Economy
CEU	Continuing education unit
CFD	Computational fluid dynamics
CHX	Custom heat exchanger
CO_2	Carbon dioxide
CRADA	Cooperative Research and Development Agreement
DME	Dimethyl ether
DOD	U.S. Department of Defense
DOE	U.S. Department of Energy
EERE	Office of Energy Efficiency and Renewable Energy
EM	Office of Environmental Management
FOA	Funding Opportunity Announcement
IP	Intellectual property
MBTU	Million British Thermal Unit
MII	Manufacturing Innovation Institute
MOF	Metal organic frameworks
NNMI	National Network for Manufacturing Innovation
NO_x	Nitrogen oxide
NSF	National Science Foundation
O&M	Operating and maintenance
PI	Process intensification
Quad	Quadrillion British thermal units
R&D	research and development
RD&D	research, development and demonstration
RFI	Request for Information
RFM	Recycle-friendly materials
RO	Reverse osmosis
ROI	Return on investment
SBIR	Small Business Innovation Research
SPP	Strategic Partnership Project
TBTU	Trillion British Thermal Units
TRL	Technology readiness level

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