MODULAR MANUFACTURING WORKSHOP

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Arlington, VA

Co-Organizers:
Dion Vlachos, *University of Delaware*
Marianthi Ierapetritou, *Rutgers University*
Paul Dauenhauer, *University of Minnesota*
Adam Hock, *Illinois Institute of Technology*

U.S. DEPARTMENT OF ENERGY

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Executive Summary

The modular manufacturing workshop (MMW) took place on January 17 & 18, 2017 at the Holiday Inn in Arlington at Ballston in Virginia. The objective of the workshop was to identify the current state of research, the challenges, and the opportunities in modular manufacturing and develop a roadmap that could be used for future fundamental research and eventually enable modular manufacturing with multiple economic, societal, environmental, and workforce development benefits. Key areas that were covered included separations, catalysis, reactors, systems engineering, and cross cutting topics such as modeling, materials, and education, along with important applications that modular manufacturing could have an impact on. The workshop was attended by over 100 people (106 people registered).

The development of modular manufacturing can have a major impact on the US economy, creation of jobs, and sustainability. Untapped resources, such as the shale gas in North Dakota, and lignocellulosic biomass in Midwest, can be converted into valuable chemicals and fuels, while reducing or eliminating CO_2 emissions. Modularization can enable water treatment and purification from nitrates and other organics in the ecosystem. Similarly, it can produce fertilizers on demand in each farm, saving tremendous amounts of energy and reducing CO_2 emissions while using renewable electricity from wind and solar farms. Modular devices enable standardization, fast deployment and assembly, and reuse in various locations for several applications. Their production can stimulate distributed advanced manufacturing and de-risk the billion dollar investments that prevent large companies from investing into manufacturing, limiting further economic growth. Distributed and modular manufacturing in turn necessitate development of software, sensors, and advanced materials for remote operation.

Realizing modular chemical manufacturing requires the development of integrated, multifunctional devices (e.g., reactive distillation, reactive extraction, reactive adsorption, membrane reactor, autothermal reactor), spatial and temporal process intensification strategies, integration of alternative energy forms based on renewable electricity, such as microwaves, plasmas, and electrolysis, into distributed chemical manufacturing, and finally integration of catalysts with reactors and other unit operations (e.g., separations, heat exchangers) into optimal systems.

This report describes the key findings from the workshop. The list of participants along with the agenda of the meeting are appended. A combined PDF of the slides of invited speakers is appended.

Brief Background on Modular Manufacturing

Over the past several years, chemical industry has resorted on best practices to reduce energy utilization, cut down on emissions, reduce cost, and increase overall efficiency and performance. One of the most successful approaches to achieve this has been based on process intensification (PI). Chemical industry has achieved this by, among others, better process and heat integration. As a result of PI, the chemical process industry (CPI) has experienced important economic, productivity, and environmental benefits.

The first pillar of PI entails the integration of multiple functions in a single multifunctional device (Figure 1). Examples include the integration of reactions and separations, reactions and heat exchange, and reaction and mixing. The reactive distillation to produce methyl tetra butyl ether (MTBE) was one of the earlier demonstrations of PI, demonstrated by Eastman Chemicals. A second pillar of PI entails the spatial domain (Figure 1) where structures are purposely arranged in space to increase performance. Well-ordered packings in adsorption and chromatographic columns, fixed bed reactors and reactive distillation units and spatial coupling of exothermic and endothermic reactions in microreactors are examples of spatial structure.

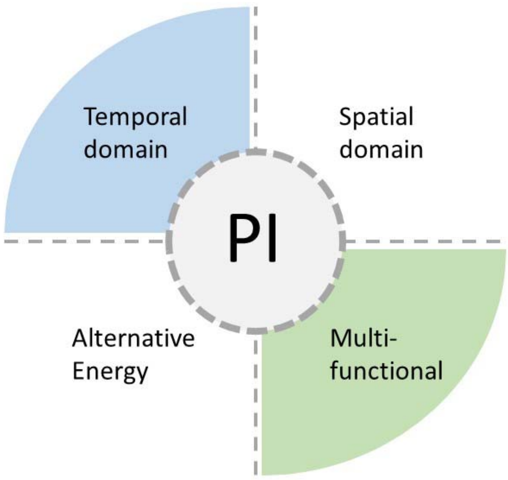

Figure 1. Schematic of pillars of process intensification (PI).

The third pillar entails the temporal domain where periodic operation is employed to enhance performance. The reverse flow operation for combustion of dilute, volatile organic compounds, which conventionally cannot be burned in a self-sustainable manner due to their low calorific value, is one of the earlier adapters of this concept. Temporal operation has also been demonstrated in the laboratory scale for chemical processing, such as methane partial oxidation and methane reforming technologies for remote and onboard production of hydrogen for fuel cells. By trapping the heat in the solid structure, one can improve energy efficiency and increase temperature, leading to self-sustained operation or improved selectivity. The fourth pillar of PI entails the use of alternative energy forms rather than the conventional use of steam and radiation from flames in furnaces for high temperature processes. Examples of this pillar include the use of fields (e.g., microwaves, plasma, ultrasound) and electricity.

While the pillars of PI are by now well established, widespread use of modern PI methodologies has been rather limited. Retrofitting of existing chemical plants and construction of new ones comes at a **high risk** that is often in the billions of dollars. This risk compounded with the high volatility of oil prices can render the operation of new chemical plants uneconomical. As a result, construction of chemical manufacturing facilities in the US has been rather slow. The recent revolution of hydraulic fracking to produce cheap gas and energy has been a game changer but low oil prices have stalled substantial industrial growth. Yet, the abundance of shale oil and gas in the US provides unique opportunities for new manufacturing as the price of oil rebounds.

The traditional cost reduction paradigm of chemical process industry has relied on economy of scales. The so called 2/3 power law, reminiscent of the surface area to volume ratio, implicates that as chemical plants grow bigger (scale up), the cost is being reduced following a 2/3 power low (Figure 2).

In simple terms, large plants exhibit better efficiencies and lower cost due to more efficient process integration. As a result, the past few decades have been demarcated by a clear trend of building chemical plants of an ever increasing capacity.

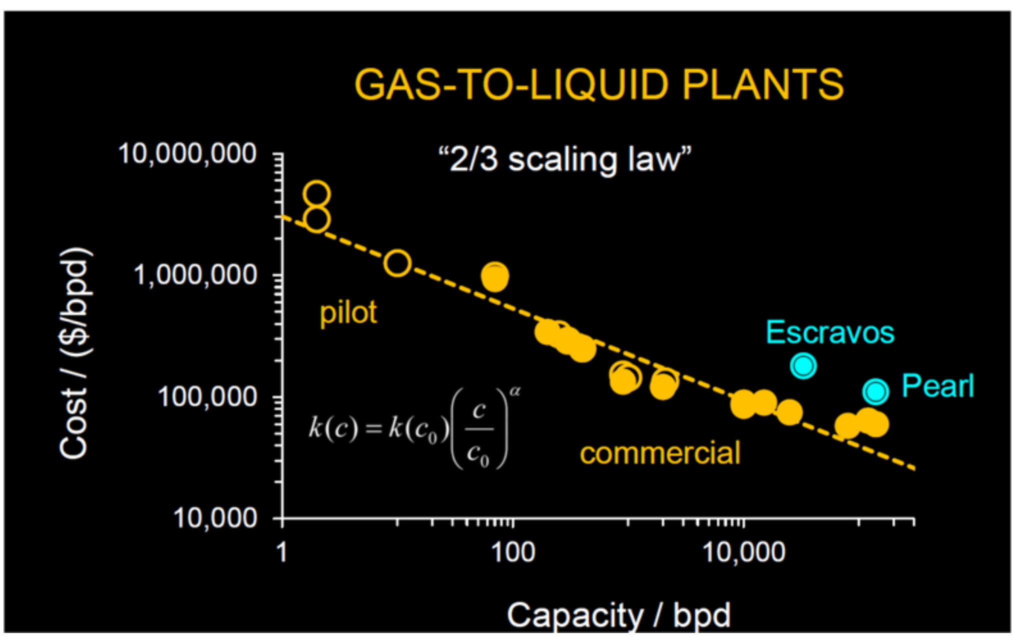

Figure 2. Scaling of cost for gas-to-liquids plants. Courtesy of Dr. Boysen.

A manifestation of this paradigm includes shutting down older and smaller scale refineries in the Delaware/Pennsylvania area and building large ones in the state Texas. Recent examples from construction of some of the biggest chemical plants reveals the potential breakdown of the 2/3 power law. Methods to reduce the cost of future chemical manufacturing are highly desirable. A challenge in scale up of chemical processes is that dominant phenomena from the laboratory to demonstration and pilot scales to actual commercial scale change. While we have become better at coping with this challenge of scale up, the time it takes to commercialize a new discovery remains a decade or longer and risk still stands.

An alternative to constructing large chemical plants entails the manufacturing of small devices and the assembly of numerous identical such devices into modules to achieve a certain throughput. The concept is called **scale out or numbering up**. Small scale devices, often termed microchemical devices, offer enhanced transport rates and as such, a major advantage over their large scale counterparts. In addition, scaling out *lowers the risk of failure for new manufacturing,* provides potentially a *faster path to commercialization* – since phenomena do not change as the number of modules increases – and can be adapted for multiple processes. Small scales offer *inherent safety* and can be used for *on demand and on site production of toxic chemicals* to avoid production and shipping of large volumes. Despite these advantages, microchemical devices have not seen widespread use due to lack of infrastructure, large manufacturing cost, and lack of design principles for such systems.

Over the past three decades, the portable electronics industry has lived its own revolution. Small scale, portable electronic devices (e.g., smart phones, music media, storage media) are part of daily life. Pioneered by techniques developed in the area of microelectronics (e.g., lithography) the production cost is being continuously reduced. Similarly, the automotive industry, including cars, car engines, etc. is another example where **massive manufacturing has led to profound cost reduction**. These examples provide support for reduced cost and improved performance by manufacturing in large numbers. **3D printing** could enable modern PI technologies to be integrated into modules and deployed in remote, offshore, and centralized facilities.

Summary of Workshop Findings

1. Potential Future Applications of Modular Manufacturing

At the workshop, there was general consensus that identification of key applications is essential to enable diffusion of modular manufacturing into emergent markets and create success stories. Potential, key applications include:

Gas Conversion

The revolution of abundant and cheap shale gas provides a technological and economic advantage to the U.S. Manufacturing plants producing on demand propylene from propane have already been commercialized. Yet, utilization of stranded gas in remote locations (e.g., North Dakota) and offshore locations and biogas remains a challenge due to lack of pipelines and chemical infrastructure and high compression costs for transportation. This grand challenge is due in part to the difficulty of activating alkanes and in particular methane and in part to the lack of modular manufacturing for deployment in remote locations in a distributed fashion. As a result, gas is often flared contributing to CO_2 emissions. Solving this problem requires development of low temperature methane activation to syngas and its subsequent conversion to hydrogen and gas-to-liquid technologies, building further on the success of Velocys. Due to high energy and capital intensity of the steam reformer, direct conversion of methane to liquids, e.g., benzene, can be superior to the reforming process. In addition, on demand processing C2-C4 hydrocarbons to olefins and various other chemicals (e.g., butadiene) provides a need and an opportunity for modular manufacturing driven by the low cost of shale gas and the reduced volume of naphtha cracking that used to be the primary source for these chemicals. Production of 'pipeline' acceptable shale gas requires development of modular, energy efficient separation systems. Development of combined carbon capture with conversion of natural gas, biogas, and landfill gas as well as alkene/alkane separation are important topics.

Solids Conversion: Biomass, Waste, and Coal

Solids are abundant. These include lignocellulosic biomass, coal, and waste (food, agricultural, plastics, etc.). Solids handling is often empirical and breaking them down to their constituents is energy intensive. Techniques such as pyrolysis are energy demanding and unselective, producing a large slate of molecules whose use requires challenging separations. Development of methods to effectively handle and deconstruct solids can enable use of diverse feedstocks with significant ecological and societal impact. The low energy density in some feedstocks (e.g., due to high water content in biomass) and short life time (in the case of food waste) require distributed, modular manufacturing at or close to the production site.

Distributed Ammonia Synthesis

Ammonia is the number one chemical in volume produced. Ammonia synthesis requires high temperatures and pressures, and the production of hydrogen from methane steam reforming is extremely energy intensive and inefficient. About 2% of all CO_2 emissions are attributed to the ammonia plants. In addition, over fertilizing the soil and runoff results in more than 50% of the fertilizer finding its way into the water ecosystem, with a tremendous environmental impact. The projected increasing world population will need increased food production that will in turn require more fertilizers. It is thus expected that ammonia production will increase. The significant reduction in electricity cost from solar and wind provide an opportunity for electrified, modular production of ammonia in remote locations and on demand, i.e., at the farm and better fertilizing strategies. There are already reports that in certain windy parts of the world, production of ammonia from wind-farms-electricity is economical. Developing suitable chemical manufacturing technologies and the associated science are needed.

CO_2 Concentration and Conversion

CO_2 is produced over a multitude of scales, ranging from large, concentrated sources (power plants) to small, diluted streams (transportation sources). Given that the carbon is fully oxidized, conversion of CO_2 to chemicals and fuels is thermodynamically uphill and requires energy. The long term solution will require abundant renewable energy to split CO_2 to CO, e.g., via plasma or electrocatalysis, or the conversion ideally directly of CO_2 or from CO to fuels and chemicals. This will require production of renewable electricity at much lower cost, development of catalysts for the selective conversion of CO_2 to fuels and chemicals, and development of integrated modular systems, including intensified reactors, separations, and heat and mass transfer elements, that tap into renewable energy to carry out these transformations at various scales. In transportation sector, CO2 is produced in extremely distributed manner. Capturing CO_2 at sufficiently high Concentration for subsequent conversion requires novel schemes, including reactive capture.

Purification and Recovery of Organics from Water

Many biological processes involve large amounts of water and concentrating valuable organics is extremely energy intensive and inefficient. Fermentation of biomass for the production of glucose is one such example. Development of alterative techniques can significantly impact the economics, and enable the penetration of emerging technologies and utilization of alternative and renewable feedstocks. Water is essential to humans and is one of the top societal challenges. While water is abundant in oceans, its desalination is very energy intensive. The excessive industrialization and use of fertilizers that are washed off create a tremendous ecological problem whose solution requires among other things distributed chemical processing and separation, advanced materials, and integration of renewable energy forms that can operate autonomously and sustainably over long times.

Renewable Hydrogen

Water splitting for H_2 production using renewable energy in electrocatalytic or photoelectrocatalytic systems is essential for many transformations, such as distributed ammonia synthesis and CO_2 utilization and upgrade of fuels and chemicals. Key enablers are similar to those for CO_2 conversion.

Chemical Process Industry (CPI)

Modular manufacturing in established CPI can reduce energy demand, increase productivity, and reduce cost of several energy intensive, low yield processes. Examples include hydrogenation reactions in the liquid phase, autothermal reforming at small scales, propane conversion to propylene via dehydrogenation, ammonia synthesis, etc.

Power Generation and Storage in Chemicals

Due to intermittent nature of renewable energy, energy storage is essential as renewables penetrate more into the market. Due to several challenges associated with batteries including their low energy density, storing renewable energy into chemicals, whose energy density can be as high as 100 times higher than that of conventional Li-based batteries, is an appealing scenario. These chemicals can be used whenever needed or can produce electricity in fuel cells. Development of improved batteries, membranes for fuel cells and flow batteries, and superior catalysts for electrocatalytic transformation is essential to realize this opportunity. At the systems level, fundamental studies are essential to integrate power generation, storage, and smart grids, especially microgrids. Improved batteries and harnessing electric power via catalysis are directions that should be explored.

Biotech

Continuous processes for the production of pharmaceuticals can enable reduced cost, increased reproducibility and product quality. Over the past several years, there has been increasing emphasis on continuous manufacturing, modularization, and process intensification. Personalized medicine and health are expected to increase the need for further developments in this direction.

2. Overarching Goals for Modular Chemical Processing and Manufacturing

The overarching goals, as found in the workshop, are (the order is random):

1. Reduce cost of massive produce for modular manufacturing.

2. Provide technically and commercially, viable de-risked solutions.

3. Create long-lived, robust to impurities, active, and selective catalysts; eliminate or reduce catalyst deactivation; reduce or eliminate membrane fouling; and create easy to regenerate strategies.

4. Develop upstream separations for PI and modular manufacturing.

5. Extend lifetime of entire system and reduce CAPEX.

6. Develop physics-based models across scales.

7. Reduce or eliminate noble metals. Reduce manufacturing cost of high performance materials.

8. Advance process safety, software, and mitigation strategies (tools, standards, regulations) for modular manufacturing.

9. Allow for flexibility in operation to accommodate varying feedstocks and intermittent use of renewable energy and handle transients (start-ups and shut-downs).

10. Improve energy efficiency and use, reduce CO_2 production, and reduce OPEX.

11. Create plug and play modularly designed, assembled, operated and controlled systems.

3. Potential Future Technologies

1. Hybrids of reactors and separations.

2. Electrified chemical production using microwaves, plasma, ultrasound, electrolysis, etc.

3. Smart, active, and effective separation technologies. Reversible reactive sorbents; microwave transparent membranes.

4. Sensors for *in situ* and remote measurements.

5. Frameworks to integrate various types of data to enable discovery, materials discovery and process design.

6. Tools predict long term stability and performance of materials, including catalysts, adsorbents, membranes, etc.

7. Multifunctional materials for separations and reactions.

8. Manufacture of defect-free, large surface area membranes.

4. Challenges and Opportunities for Process Systems Engineering (PSE)

Summary

Process systems engineering (PSE) has been viewed as an enabling technology that can play a critical role in modular manufacturing providing the tools and approaches for design, control and optimization of modular systems. As such, there were discussions in all breakout sessions of the workshop regarding the state of the art of PSE and the challenges in supporting modular systems. These are summarized below.

State of the Art

As discussed during the workshop, there are numerous *computational approaches* that can be used to design and optimize conventional process operations. More specifically Prof. Grossmann emphasized the development of efficient optimization algorithms for the solution of Mixed Integer Linear and Nonlinear problems that are appropriate of the solution of distributed modular systems where the locations of plants are problem variables. In order to address realistic size problems and account for the inherent uncertainty (due to external and internal problem variability), there is a need for more effective decomposition-based approaches to handle the high dimensionality of the problem.

Multiscale modeling has been central in all workshop discussions as a means of enabling the design of innovative processes while accounting for process performance. Although, there is a lot of progress in the literature connecting length and time scales, there are still no available approaches and software that can connect molecular to process levels in order to explore "out-of-the-box" solutions, let alone to incorporate plant level information and account for enterprise-wide connectivity and complexities.

The last important issue that was discussed is the problem of *data acquisition at different levels of process and product development*. How those data can efficiently be integrated and transformed to valuable information and how can be incorporated as part of a software architecture that can seamlessly combine model development with data acquisition. Although there are a lot of recent ideas at the intersection of computer science and engineering, there are a lot of gaps in this area identified during the workshop.

Challenges and Opportunities

The specific challenges and opportunities identified are:

1. Multiscale modeling tools to synthetize, consider, evaluate and design unique and novel intensified and dynamic reactive systems. These tools should connect multiscale models with traditional PSE.
2. Data fusion into models and data mining for robust and real-time optimization, design and control of modules and of entire modular systems. New model libraries for modular and process intensified systems.

3. Information overload; data integrity/standard methods; lack of communication between fields.
4. Operating under fluctuating feedstock conditions as an example of uncertainty considerations in decision making. Development of flexible systems to handle variability and uncertainty.
5. Design and control of integrated systems (e.g., reaction and separation). Development of suitable tools. High level of integration reduces the degrees of freedom.
6. Reliability and controllability of modular reactors, including safety.
7. Lack of systematic design methods for many unit operations.
8. Competing and beating economies of scale; lowering capital and operating expenditures; justifying retrofits to existing assets vs. new installations. Explore the benefits of additive manufacturing. Expansion of the supply chain to significantly cut cost of modules.

Roadmap Action Plan

The topics that have been identified as priority focus areas and suggestions for moving forward are as follows:

1. Multi-scale Modeling Framework for Modular, Intensified Systems. A generalized multi-scale modeling framework is currently lacking to support the design, optimization, control of novel, intensified systems, devices, and discovery of materials for separations and catalysis. This roadmap strategy will develop open-source modeling frameworks, model hierarchies and data structures that can be applied to catalysis and separations. The approach is to define and implement a software architecture with capabilities of mechanistic reaction models, detailed system geometry, and functionality of dynamic optimization, and controller synthesis. The objective is to create software tools/methods that will enable design of modular and intensified chemical processes.

2. Process Control, Systems Analysis and Automation for Modular Plants. Operation in remote and offshore locations and very integrated systems require high fidelity models and control, optimization, and automation of high dimensional systems.

3. Widely Distributed Process Systems with the Necessary Resilience, Safety, and Operability are lacking to fully utilize "stranded" resources. Process design modeling, which addresses reliability, controllability, and safety, does not yet exist to support design of distributed process systems.

4. Rapid Design Process Systems Engineering Tools for Plug-and-Play Integration of Experiments with Computations. Given the uncertainty of models, integration of experiments and computations is essential. This integration should ideally be in real time and enable parameter estimation of models and model-based design of experiments.

5. Business Case and Techno-Economics for PI and Modular Systems. Applying a disciplined approach to develop a state-of-the-art vision and roadmap for a certain application is challenging. This activity will focus on demonstrating economic viability of intensified and

modular processes. The approach will be to work with stakeholders to develop, maintain, and utilize risk analysis, techno-economic analysis, and business case toolsets.

6. Data-Driven Decision Making for Modular Systems. Different platforms currently exist for data collection and storage that make analysis and decision making difficult. Other challenges include current limits of software communication for data analysis; data quality (noise, errors, etc.); capabilities for information extraction; and the temporal and spatial variability of data. This activity will focus on integrated computing architecture and algorithms for data mining and utilization for decision-making. Another element will be the development of approaches for risk mitigation/management.

5. Challenges and Opportunities for Chemical Reactors

Summary

Reactor engineering provides optimal technology facilitating the implementation of process chemistry for modular manufacturing and new approaches for converting feedstocks to products. Due to the importance of novel design in modular and intensified reactors, there were discussions in all breakout sessions identifying the state of the art in reactor design and the challenges related to better and more integrated reactor configurations. These are summarized in the following sections.

State of the Art

Advanced approaches to intensifying chemical reactors for improved throughput, chemical performance, and economic productivity utilize detailed modeling and integration of multiple functions within the same unit operation. Intensity of chemical productivity is achieved through improved reaction rate, selectivity, and controlled reactant addition and/or product removal. The ability to describe and ultimately control reacting flows at the molecular scale occurs through detailed reactor design; optimization of reactors achieves the greatest extent of reaction per unit volume. Additionally, as depicted in

, experimental characterization of reacting flows allows for detailed understanding of the relationship between reactor design and productivity. One approach toward reactor intensification entails *multiscale modeling* combined with *advanced experimental characterization*.

A second approach to reactor intensification *combines chemical reaction with separation* in a single unit. Strategies for separating reacting flows include integration of reaction with a membrane, a sorbent bed or a co-flowing separate phase (liquid or solid). As shown in Figure 2, Professor L.S. Fan demonstrated a multifunctional reactor to separate carbon dioxide using chemical looping. The prospect of using chemical reactions to overcome separations or materials undergoing redox or other catalytic cycles remains relatively untapped.

Another approach to process intensification includes *selective heating and energy integration*, such as the use of microwaves within flow reactors. Selective heating or integrated heating have the potential to improve overall conversion, reduce energy use, and reduce overall capital expenditure. Coupling of energy exchange with reaction, as for example happens in periodic flow reversal, spatially segregated microreactors, or short contact time partial oxidation reactors are such examples. Although there exist numerous potential methods for implementing multiple functions within a single reactor system, a generalized methodology to achieve optimal integration within reactors remains to be developed.

For modular applications, *data collection*, *processing, and feedback within control strategies* remain a key challenge, where applications can include reactors with extreme thermal and/or concentration gradients. Additionally, emerging applications in shale gas, biomass, and carbon dioxide target small-scale systems with *rapid transients* associated with startup, shutdown, and natural variation from the environment (e.g., feed disruption) that require new approaches to *monitoring and control*. Seamless implementation of novel, highly productive reactors requires a new approach to design and control for these applications.

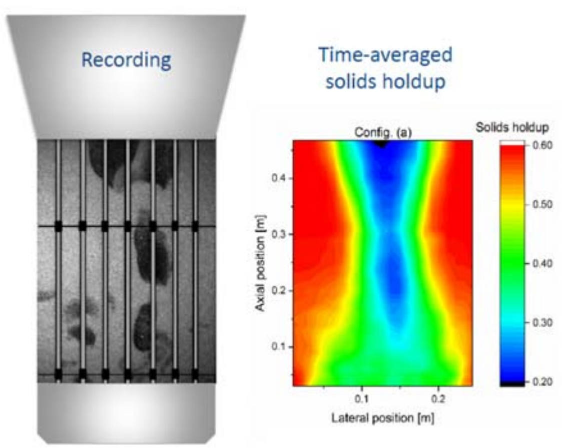

Figure 3. Reactor Fluid Phase Characterization for Intensification. Courtesy of Prof. Martin van Sint Annaland.

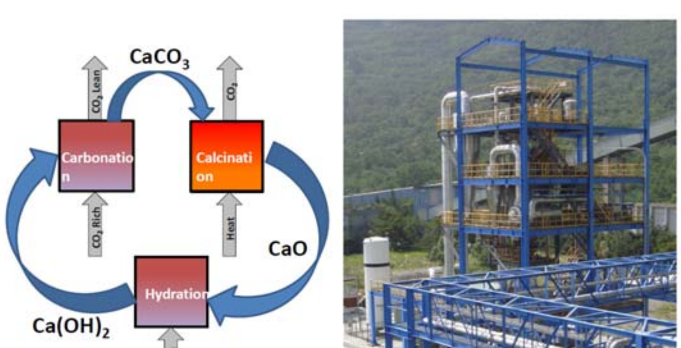

Figure 4. Multi-Functional Reactor – Chemical Looping for Carbon Dioxide Separation. Courtesy of Prof. L. S. Fan.

Challenges and Opportunities

The key challenges and opportunities identified are summarized as follows (in random order):

1. Control of reactor dynamics and stability in small-scale and distributed reactors. Small systems exhibit fast response and rapid change in operating conditions. Additionally, small-scale distributed reactors require independent operation without continuous oversight.

2. Management of solids (i.e., biomass or waste materials, such as food waste, plastics, etc.) or deposits in small-scale reactors – lack of designs for intensified reactors with solid feedstocks. Solids are generally difficult to handle.

3. Heat management in intensified reactors; integrated reaction and temperature control with spatial resolution.

4. Stable materials for systems with rapid thermal cycling or large thermal gradients, such as in chemical looping.

5. Standardized tests for new catalyst evaluation.

6. Lack of fundamental parameters (e.g., reaction kinetic constants, transport properties) for advanced reactor design. These become even more crucial when reaction happens in complex media, such as solvents (biomass processing) and electrolytes.

7. Lowering reactor manufacturing cost through additive manufacturing and/or structured catalysts and reactors.

8. Characterizing reactor performance at interfaces in the presence of strong fields and/or gradients, e.g., electromagnetic fields, temperature and concentration gradients.

9. Development of reaction models including reaction network analysis, reaction network generation, and model validation for steady state and dynamic operation.

10. Reactor design cost optimization of reactors with various methods of heat integration.

11. Identify 'best use' cases for modular reactor technology that provide unique impact for application.

Roadmap Action Map

Priority focus areas and suggestions for moving forward are as follows:

1. Data Fundamentals for Modular and Intensified Reactor Design. Design of intensified chemical reactors with high activity per unit volume and/or integrated separation relies on fundamental parameters related to reaction and separation. For target applications of modular and intensified reactors, kinetic and thermodynamic parameters are needed for reactor design inclusive of multiple reaction and transport phenomena. This roadmap will identify the key fundamental needs for development of advanced intensified reactors and a platform for facilitating and broadly sharing data, models, and parameters. Physics-informed machine learning should be explored as a means of describing and collapsing data into low dimensional, useful tools.

2. Microkinetic Models for Evaluating Complex Reactions. Control of complex reacting flows and surface reactions requires detailed understanding of multi-step chemistry dependent on reactor conditions at steady state and transient conditions. Design of advanced intensified reactors with the potential for rapid transients with varied-scale applications relies on the ability to model complex transient reaction behavior, which is captured by microkinetic models. The predictive ability of microkinetic models should be assessed and improved for reliable model-based design and control. Fusion of data into microkinetic models is another research priority. Use of microkinetic models to predict multifunctional catalysts is another priority. Extension of microkinetic models to account for the complex environment in which the chemistry happens, such as solvent and electrolyte effects, confinement effects in micro and mesoporous materials is crucial.

3. Multiscale Modeling Framework for Design, Optimization, and Control of Modular, Intensified Systems. A generalized multiscale modeling framework is currently lacking to support novel, intensified systems, devices, and materials for separations and catalysis occurring at the atomic scale, particle scale, and reactor scale. Intensified systems with extreme concentration and/or temperature gradients have the potential for rapid transient behavior in varied-scale applications such that robust design and control relies on the ability to define reaction-transport behavior at all scales. This roadmap strategy will develop open-source modeling frameworks, model hierarchies and data structures that can be applied to catalysis, mixing, heat transfer, and separations. Multiscale modeling of electrified systems (electrolyzers, fuel cells, microwaves, plasmas) needs also to be developed. Sustainable modular software, which integrates tools and models across scales, will be essential. Control and optimization modules should be an integral part of this software.

4. Intensification Platforms and Novel Materials for Modular Manufacturing. Implementation of modular systems requires new design strategies for combining reaction, separation, mixing, and heat transfer. Broad application of modularization requires a generalized design platform; examples include reactors with membranes or reactors with chemical sorbents. Modularization and process intensification will further improve with the development of unique materials for integration, such as membranes, sorbents, heat transfer surfaces/fins, or co-flow separate phase reactants (as in chemical looping). Design of smart, robust, self-healing materials as catalysts and adsorbents or membranes is a key priority to enable remote operation for long periods of time and resistance to impurities, varying feedstocks, transient operation, fouling, and corrosion. Additive manufacturing that enables easy incorporation and regeneration/replacement of solid materials into mesoscopic and macroscopic structures is essential. Economic, scalable manufacturing of novel, multifunctional, atomically-controlled catalysts, currently made at bench scale, is a crucial research priority.

5. Techno-economics for Modular Systems. Decisions related to design of intensified reactors can be generalized across numerous applications by developing a disciplined approach to reactor design with economic feedback. The methodology aims to conduct techno-economic analysis of reactor design while identifying and reducing risk of design. Optimization of reactor economic value and minimization of design and implementation risk will be accelerated by establishing standardized methods of design of intensified reactors within a larger system; general design criteria towards this objective need to be developed.

6. Challenges and Opportunities for Separations

Summary

Separations are an enabling technology in modular manufacturing for purifying streams prior to chemical reaction or separating products from reactants. There are also crucial in numerous other applications, including water purification, CO_2 capture, and H_2 storage. As such, there were discussions in all breakout sessions of the workshop regarding the state of the art and the challenges in supporting modular systems. These are summarized below.

State of the Art

Separations are an integral part of chemical and fuel processing. They account for the majority of energy use in a chemical plant, and thus, the development of more energy efficient separations and separations for emerging applications was discussed extensively. Robert J. Giraud of Chemours discussed ongoing efforts to coordinate efforts among various stakeholders for mass separating agents and development of an associated research roadmap. Prof. Belfort of RPI discussed the impact of replacing distillation with low energy separations including synthetic membranes, adsorption, solvent extraction and crystallization and presented an example of reverse osmosis for desalination of water that is practiced in several parts of the world. Opportunities for modularization for pre- and post-treatment of water and integration with renewable (solar, wind) energy were also proposed. He also discussed replacing batch with continuous processing for recovery of biological molecules in biotech and pharmaceutical industry. Prof. Koros of Georgia Tech discussed the challenges associated with small molecular separation, the potential of carbon based materials, and the need for collaboration between multiple domains, as shown in Figure 3. Prof. Tsapatsis of the Univ. of Minnesota discussed highly selective zeolite membranes, recent advances to nanometer scale thick membranes, polymer composite membranes for improved manufacturability and high selectivity, and strategies of healing defects (Figure 4).

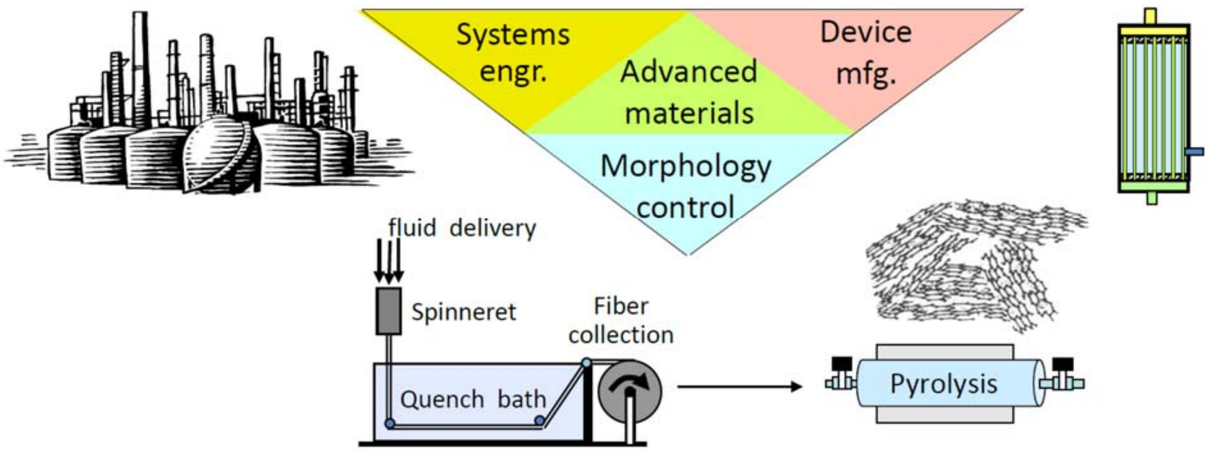

Figure 3. Schematic of integration of multiple domains to enable fabrication of membranes. Courtesy of Prof. Koros of Georgia Tech.

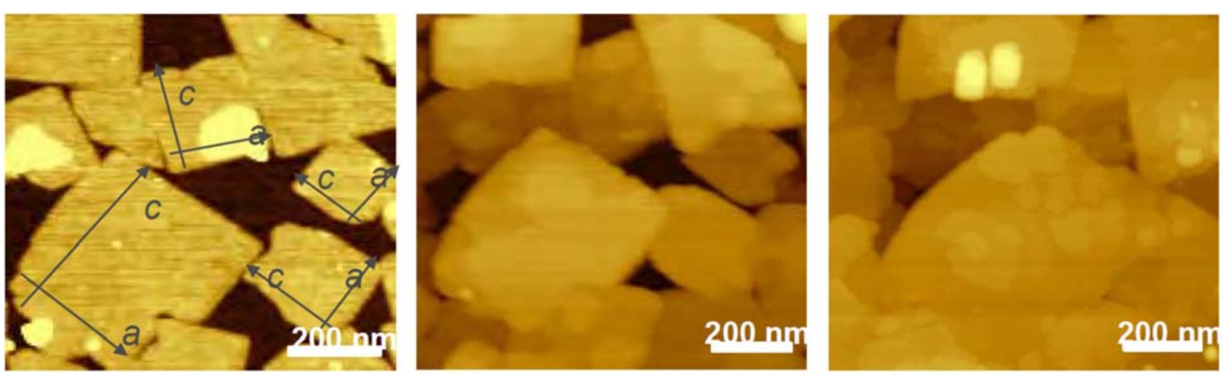

Figure 4. Epitaxial solution-based growth conditions enable filling pinholes and tailoring 2D zeolite thin films at scale approaching single-unit-cell dimensions. Courtesy of prof. Tsapatsis of the Univ. of Minnesota.

Challenges and Opportunities

1. New or improved separations are needed for existing and emerging applications for modular manufacturing. Separations include H_2S management at plants and natural gas wells, separation of CO in steel industry and power plants, H_2 purification downstream of

reformers, air separation, and biologically-based separations, such as water/ethanol separation from fermentation. It is often the case that these streams are very dilute and purification is inefficient and needs significant amounts of energy. The low cost of electricity may provide novel electrochemical separation schemes for example of organics for water purification, electrochemical pumping, and efficient membranes for fuel cells. Separations for biorefineries will be an important research direction and involve low temperature, thermally sensitive substrates; extraction, adsorption, membranes, and chromatography will be more common than distillation.

2. Novel materials for more energy efficient, cost-effective separations, including electrochemical ones.

3. Reduce cost of modules over that of large scale systems. Low cost fabrication methods of high performance materials.

4. Characterization of materials structure including defects, disorder, and other defects across scales.

5. Long lasting materials as adsorbents and membranes. Potential for self-healing.

6. Membrane selectivity and fouling while allowing for high flux.

7. Defect free synthesis and robustness of large membranes.

8. Lack of sufficient data to predict performance, especially with complex, multicomponent feedstocks.

Roadmap Action Map

1. Data Fundamentals and Libraries of Data and Models for Modular and Intensified Separation Design. Fundamental molecular properties obtained from molecular simulation and experiments, a library of models for separation using various materials and for modules are clearly needed.

2. Novel Materials and Manufacturing for Modular Processing. The development of novel materials with multiple functionalities that are resilient to high temperatures and impurities and that possess high flux and selectivity is essential. It is also critically important to rapidly screen and characterize these materials and membranes and find ways to detect and self-heal defects during operation and to manufacture materials and membranes at low cost and at scale suitable for modules.

3. Standardized Testbeds for Assessing Materials and Reproducible Data. There is a need to systematically evaluate adsorbents and membranes for various separations to enable comparison and allow for reproducible data.

4. Multiscale Models. Models that integrate molecular scale to device scale and with an entire flowsheet optimization are needed. This in turn requires a library of models for multicomponent systems, accounting for the composition and microstructure of composite membranes, the effect of materials processing on microstructure, and defects. Models should be assessed against well controlled experiments.

5. Techno-economics for Modular Systems. Accurate, high fidelity, materials-gnostic and computationally efficient models that can be integrated into optimization or control codes and flowsheets are needed to predict best materials, optimal operating conditions, cost and assess the scale at which modularization outperforms economy of scales. Model reduction is an essential research direction to enable systems tasks.

7. Educational Challenges and Opportunities

1. Workforce Development. Lack of books, test cases, and knowledge by professors on process intensification and modular manufacturing is a roadblock. Creating curriculum for various audiences, including technicians, K-12, undergraduate, graduate and postdoctoral fellows is essential.

2. Stakeholders and New Education Paradigm. It is important to bring industry together with academia for the development of curriculum and training of students. Integration of R&D with societal changes and real world application is necessary. Explore practical courses, hands-on and virtual learning, as well as co-teaching with mechanical and electrical engineers on new topics such 3D printing, sensors, etc.

3. Software Tools. There is a need for new tools to support education on PI and modular manufacturing along with the creation of repositories of modular and PI models. Support for open-source software, e.g., OpenFoam, for PI and modular processes.

8. Advanced Materials Challenges and Opportunities

1. Materials durability, selectivity, and efficiency. These are common traits for catalysts, adsorbents, chromatographic separation solids, membranes, etc. Fouling and deactivation are very common. Understanding the failure of materials and methods to remedy them are essential, especially for distributed manufacturing where remote operation may be a necessity.

2. Cost-effective, scalable manufacturing of advanced materials for modular devices. While several techniques have been developed for tailor-made synthesis of multifunctional nanomaterials, e.g., solvothermal methods, atomic layer deposition, development of economically viable and scalable processes are generally lacking. Similarly, while high flux and high selectivity membranes are often demonstrated in the laboratory, the fabrication of module size, defect-free membranes and self-healing techniques remains a challenge.

3. Integration of materials and regeneration in small scale devices. Modular systems that can be used for multiple purposes necessitate the need to easily replace and regenerate materials, such as membranes, adsorbents, and catalysts. Developing novel designs for modules is an important research direction.

Table 2-1. Separations/Systems for PI and Modularization (Blue Group): Future Applications

Gas Separations

- CO_2 from combustion gases (small scale)
- Air separation
- Gas to liquids
- Distributed/stranded natural gas (NG) processing: pre-purification, water removal, acid removal
- H_2 syngas purification downstream of reforming
- Separation of CO from O_2 downstream of a plasma reactor or integrated with plasma reactors
- Separation of CO in steel industry/ power plants
- Small particles from gases/air (continuous)
- O_2/N_2 separation
- H_2S management at plants and natural gas wells (pollution prevention)

Liquid Separations

- Tri-chlorsilane/silane production (reactive separation)
- Water/ethanol (renewables)
- Chemical distillation; azeotrope separation to replace pressure swing absorption
- Replacement or reduction of cryogenic separation (e.g., Alkene/alkane)

Reactive Separations

- Aromatization reaction plus separation
- Reactive separations for improving yield of aromatics (xylenes, …), diesel, gasoline
- Directional solidification: photovoltaics, rectifiers (gallium oxide displaces Al_2O_3)

Electrochemical Separations

- Electrochemistry field-based separation
- Ions from/to water or organic liquids
- Field-based plus absorption step/electrostatics – small particle separations
- Electro-catalytic CO_2 reduction to organics
- Membranes for flow batteries

Water and Wastewater Separations

- Desalination (membranes)
- Remediation: reduction of pumping and treating; in-situ separations and/or treatment
- Local waterway filtration for third world
- Wastewater treatment: reduction of biosolids from biological treatment
- Separation of ammonia and phosphorous fertilizers and byproducts from wastewater for reuse

Biological Separations

- Biomass to chemicals (biorefinery)
- Biorefineries (pyrolysis sugars): extraction, membranes, adsorbents
- Cleaning/upgrading of biogas from organic waste

- Biorenewables: phenolics, furanics, and upstream feedstocks
- Selective molecular separations from liquid in biological processing

Table 2-2. Separations/Systems for PI and Modularization (Blue Group): Goals
• Focus on water and food to start desalination (some way to focus) • Achieve (X) percent reduction of life cycle cost compared to conventional approaches • Be capable of testing small quantities under actual conditions • Enable dynamic, stochastic, economic, and change analysis for modular/PI systems • Achieve better economics: cost reductions, cheaper materials, to drive business case (from university to scale

Table 2-3. Separations/Systems for PI and Modularization (Blue Group): Future Technologies (● = one vote)
Materials for Separations
• Multifunctional materials ●●●●●●●● • Reversible reactive sorbent architecture ●●● • Microwave (MW) transparent membrane for MW-assisted multiphase reactors ●●● • Fouling resistant membranes ● • Corrosion-resistant materials • Low-cost biogas cleaning membranes • Electrochemical membranes that are stable, high flux under both reduction and oxidizing conditions. • Membranes (high-temperature such as H_2 separation; O_2 separation) and sealing • Metal organic-framework based systems applications
Innovative Technologies
• Manufacture of defect free/large area membranes (new fabrication techniques) ●●● • Affordable, flexible manufacturing (additive manufacturing) ●● • Application of high-G field (electrification) to separations (spinning reactor) ●● • Flexible units for dynamic operations/separation (modeling and manufacturing) ● • Advanced manufacturing of complex materials and devices (integrated) ● • Canister based capture systems (like catalytic converters) • Electrification (microwaves vs. fuels) • Ultra-selective removal and low energy recovery from dilute streams: CO_2, H_2S, alcohols, diols, etc. • Pumping/compression without totaling machines • Hierarchical catalytic membranes coupling reactions/transport (cascade) • Chemical looping (or oxygen uncoupling) • Tools to support/enable innovation of PI/Modular (beyond new materials or modular)
Controls/Infrastructure

Table 2-3. Separations/Systems for PI and Modularization (Blue Group): Future Technologies (● = one vote)
• Tools/technology to optimize and control integrated (separation) processes ●●● • Low cost wireless sensors and controls (leads to intelligent modeling) ● • Standardized interconnects and communication ● • Secure wireless ● • Separation agents' properties targets set from system analysis and models • Plug and play, robust and adoptive controls; improved controls • Flexible units for dynamic configurations

Table 2-4. Separations/Systems for PI and Modularization (Blue Group): Challenges and Barriers (● = one vote)	
Modeling and Simulation	
High Priority	• Multi-scale modeling and simulation tools capable of readily handling PI/modular and novel systems, devices, and materials ●●●●●●●
Medium Priority	• Data sharing and validity of data paradigms (literature, operations, better machines, etc.) ●●●
Low Priority	• Lack of data, models integration to speed up materials discovery and increase model predictability ●● • Multiscale modeling – lack of a platform for process design and materials prediction ●● • Open-source modeling frameworks ● • Modeling of multi-scale and multi-temporal processes ● • Lack of accurate data to drive models ●
Controls/Infrastructure	
High Priority	• Systems analysis to identify the relevant bottlenecks (i.e. focus on biggest problems) ●●●●●●
Medium Priority	• Adaptive process control systems (optimization of connected systems) ●●● • Wireless signal and process flow for modular systems (module separation) ●●●
Low Priority	• Standards for sensors, controls, and models (integration of information technology and physical systems) ● • Lack of tools/technology to adapt/learn system dynamics in real time • Lack of systems tools to understand: resources, technology, social interactions and interdependencies for modular and intensified systems • Mismatch of operating windows between reactions and separation systems; unknown optimal conditions
Materials	
High Priority	• Characterization of materials structure (order, disorder, detects, and beyond crystal structure); properties (selectivity, stability) relations from experiment/models ●●●●●●
Medium Priority	• Membrane/material robustness ●●●●
Low Priority	• Improving corrosion control to reduce fouling/chemical purification (reduction of corrosion metal) ●● • Membranes with longer lifetimes than catalysts ●
Other	

Table 2-4. Separations/Systems for PI and Modularization (Blue Group): Challenges and Barriers

(● = one vote)

Low Priority	• New safety paradigms that industry will confidently accept ●● • Multidisciplinary framework to support dialogue and collaboration (vocabulary and touch points) ● • Understanding cost vs. scale ● • Lack of cross-functional development (too many specialized technologies) • Current reward system and non-disclosure (solving the wrong problems) • Conversion of methane to aromatics • Value chain assessment for switching costs (incumbency)

Top Roadmap Priorities

- Materials/membrane/structure/robustness (order/disorder defects, properties, etc.) ●●●●●●●●●●
- Multi-functional materials; corrosion resistant; fouling resistant ●●●●●●●●●●
- Multi-scale modeling/multi-temporal modeling to readily handle PI/modular systems ●●●●●●●●●●
- Systems analysis tools for interconnected PI/Modular systems, resources, data ●●●●●●●●●
- Process controls, sensors, and networks that are adaptive and dynamic for optimization, in real time; sensors that are low cost, standardized, support better corrosion control ●●●●●●●●●●
- Data/data sharing paradigms (drive models, speed up discovery, improve operations) ●●●●●●

Table 2-1. Catalysis and Reactors (Blue Group): Future Applications
Biological Catalysis • Biologics-measurement/test; better analysis and liquid chromatography • Anaerobic digestion (catalyst-modular) • Nutrient recovery from organic waste • Bio oil hydrogenation (stabilizing conditions) • Reactive extraction of bio-processes • Food waste conversion to fuels/chemicals **Gas Conversion** • Stranded gas to liquids (i.e. offshore, remote locations without gas infrastructure) • Conversion of shale gas to locally marketable commodities (BTEX, monomers, etc.) • Low-temperature methane activation (catalyst and reactor concepts) • Syngas production and conversion **Chemical Process Catalysis** • Hydrogenation, liquid phase • Autothermal reforming at small scales • Propane to propylene via catalytic propane dehydrogenation (PDH) • Coal to gas or liquids especially at remote locations or source • Safe organic oxidations with O_2 • Reactors and catalyst for ammonia production (i.e. N_2 activation catalysis) • Non-equilibrium limited reactions: exploit micro-regions for non-steady applications • Water purification and contamination removal • Modularized process plant (“plant-on-demand”) **Energy/Electrochemical and Storage** • Battery, electric storage; distributed and grid integration; stationary modules • Harnessing electrical power (wind) via catalysts • Chemical storage (store energy as chemicals); reversible chemical storage

Table 2-2. Catalysis and Reactors (Blue Group): Goals
• Contaminant-resistant catalysts • Self-repairing, self-sensing, and self-healing catalysts • Reusable, hot, swappable, catalyst tubes/microchannels • Smaller, more manageable, outsource technology for chemicals (components market) • Artificial intelligence-driven reactor (for pharma) that optimizes itself • Exploitation of new shorter, reaction pathways via modularity (entirely new types of chemistry, new products, etc.) • Standardized modular technology – repetitive modules, lower cost

Table 2-3. Catalysis and Reactors (Blue Group): Future Technologies
Advanced Catalysts
• Improved selectivity at reduced temperature • Air and sulfur tolerant non-noble catalysts • Low cost, robust water splitting catalysts • Non-metal catalysts • Plug and play catalyst cartridge-micro-channels (immediate turn-on) • Catalyst switching (e.g., from acid to heterogeneous) • Heterogeneous catalysts for biocatalyst or enzymatic catalyst • Hierarchical catalytic materials for optimal coupling of reaction and transport • Catalytic “guard beds” for impurity management • Low temperature catalysts for renewable feedstocks that are highly distributed (biomass; CO_2; waste (e.g. plastic)) • Far more robust catalysts to reduce need for start-up/shut-down • Technology to deposit catalytic films
Innovative Reactors
• Plasma reactors • Microwave reactors • Single integrated reaction/separation units • Separative catalytic membrane reactors (high temperature and pressure) • Multi-functional reactors • Catalytic reactors for “on-demand” chemicals production via changing operating conditions (pulsed energy input, contact time, etc.); example is CH_4 to C_2 – C_6 products • Methane/biomass/feedstock flexible modular systems (catalysts and reactor concepts) • Reactors and catalysts that can be integrated with adsorbents and membranes • Standardized platform for modular utilities; regeneration reactors (standardized ‘plumbing’) • Lower cost fluid bed technologies – improved models for scale-up to lower risk • Floating modular unit reactors that are non-reactive to gravity (non-fixed gravity; orientation) • Reuse of waste via modular systems
Operations

Table 2-3. Catalysis and Reactors (Blue Group): Future Technologies
• 3-D printing of everything in the plant • Non-stationary (steady-state) operation of catalytic systems (regeneration, periodic operation); switched systems • Modular chemical analysis for field use – standardized and user-friendly

Table 2-4. Catalysis and Reactors (Blue Group): (Challenges and Barriers) (● = one vote)	
Modeling and Simulation	
High Priority	• Multi-scale modeling tools to help synthetize, consider, evaluate and design unique/novel intensified and dynamic reactive systems ●●●●●●● • Reliable models for optimization control and scale up ●●●●●●
Medium Priority	• Lack of knowledge of actual compositions, process conditions and economics (data inputs) ●●●
Low Priority	• None
Catalyst Properties/Materials	
High Priority	• Lack of standardized tests for new catalyst evaluation ●●●●●●
Medium Priority	• Controlling catalyst structure (function) ●●●●●
Low Priority	• Catalyst sensitivity (impurities, thermal deactivation, etc.) ●● • Metal sintering and control and understanding ●● • Lack of validated catalytic property databases and catalyst depositories ● • Lack of design principles for multifunctional materials • Materials scale up • Achieving selective C-X functionalization (X=H,O,S) • Heterogeneous catalyst manufacturing technologies for more process control but cost effective • Material property management; CTE for coating • Defining catalysis – and how to optimize reactivity
Controls/Operations	
High Priority	• Limited sensors and data fusion/mining for robust/real-time optimization and control ●●●●●●●
Medium Priority	• Operating under highly fluctuating feedstock conditions ●●●●● • Heat and water management ●●●
Low Priority	• IP (freedom to operate) ● • Addressing balance of plant issues ● • Tradeoff between volume (flexible system) and efficiency (optimized/specialized limits)
Other	
High Priority	• Defining “killer” applications for modular reactors (integrated IT, analytics, or process) ●●●●●●
Medium Priority	• Cost (“ideal” system will be unaffordable) ●●●●● • Proper definition of techno-economic metrics (resilience, sustainable, flexibility, risk) • Change/risk management (i.e., going to modular systems) ●●● • Sustainability (most flexible systems might not be very sustainable, aka “catalyst cartridge”) ●●● • Industry acceptance: must be simpler and safer to operate than current technology ●●●
Low Priority	• Multiple interpretations and goals of what modular/PI mean; more descriptive terminology ●● • Understanding/awareness of advantage to modularization in the chemical industry (standardizing manufacturing production; socioeconomic; knowing when to integrate ●● • Tensions between exiting technology and infrastructure vs. new modular systems
Top Priorities	
• Multi-scale modeling/models for optimization ●●●●●●●●●●●● • Sensors and data fusion ●●●●●●●● • Defining “best, killer” applications for modular PI ●●●●●● • Controlling catalyst function ●●●●● • Operating under fluctuating feedstock conditions ●●●●●	

Table 2-5. Roadmap Topics (Blue Group)	
High Priority Challenge/Barrier	**Priority Roadmap Topic**
There is a lack of generalized multi-scale modeling framework to support novel, intensified systems, devices, materials.	Multi-scale modeling framework
A challenge is the design new smart, robust materials capable of operating in corrosive environments that a resistant to common destructive perturbations such as fouling and corrosion. Another major challenge is to enhance existing materials in use through the design of modules/construction of systems for a particular material.	Materials for modular manufacturing applications
There is a need for distributed modules that are autonomous with robust "zero" maintenance.	Process control, systems analysis and automation

Table 2-1. Cross-Cutting Topics (Blue Group): Future Technologies
Deployment
• System operations conditions for "proof of value" adoption ●●●● • Better articulation/selling the vision for modular/PI systems ●●●● • Clear documented success stories ● • Societal acceptance of changes (e.g., loss of jobs, etc.) ● • Balance of plant equipment (collaborations with mechanical engineers)
Education
• Industry consortium for education/training ●●●●●● • Bring industry into teaching ●●● • Revised classes to fit in modular manufacturing (MM), not necessarily more classes ● • Ready modules to drop into current curricula ● • Teaching beyond "CHE as usual" (beyond unit ops to techno-economic analysis, supply chain management, entrepreneurship) ● • Incentives for teaching traditional plus new • Bring modern topics into curricula (e.g., micro-channels) • Virtual dynamic books, e-books (develop via grants) • More teaching of entrepreneurship/stimulation • Workforce development (certifications, training, curricula, etc.) • Incentivize entrepreneurship for chemical/mechanical engineers (e.g., school competitions) • Next generation workforce education: skill sets for advanced/innovative materials and manufacturing • More teaching of real-time optimization and control
Technology/Infrastructure
• Research into fluid motion, low maintenance, pumps ●●● • Wireless controls and monitoring • Modular unit operations and auxiliary units (standardized, interchangeable) • New "inks" for flexible 3D printing
Life Cycle
• Life cycle economic case studies with details ● • Flow sheeting integrated with TEE and LCA
Manufacturing/Operations
• Manufacturing at small scale for PI (e.g., micro pumps, turbines and compressors) ●● • Highly optimized operation sensors/adaptive
Safety
• Hazard assessment (lower volume, temperature, pressure, etc.; less skilled operators)

Table 2-2. Cross-Cutting Topics (Blue Group): Goals
• Reduced risk for industry to invest (multiples) • New education paradigm/societal changes to mesh R&D with real world applications • Sufficient programs to create workforce to design, build, install, and operate MM • Vertical integration

Table 2-3. Cross-Cutting Topics (Blue Group): Challenges and Barriers (● = one vote)	
Education	
High Priority	• None
Medium Priority	• Disconnect between R&D and applications/industry ●●●●● • Lack of engineers prepared for traditional fields (pumps, etc.) ●●●● • Placing more value on R&D dollars than teaching ●●●
Low Priority	• Adding credits/workload to graduate curricula • Lack of staff to get funds/do this kind of teaching for MM • Time/cost to develop new curricula (teaching modules) • "Old curricula" that keeps getting revamped/propagated
Deployment	
High Priority	• None
Medium Priority	• Lack of moon-landing target to work toward common goal ●●●
Low Priority	• None

Table 2-1. Separations/Systems for PI and Modularization (Green Group): Future Applications
Gas Separations • Shale gas with "pipeline acceptable" products • Shale gas upgrading • Ammonia synthesis • Multifunctional, modular processes for NG purification • Combined carbon capture and conversion with natural gas, biogas, landfill gas to produce syngas **Liquid Separations** • Non cryo-olefins – paraffin separations • Energy efficient drying processes of chemicals, food, agriculture, forest products. • Distributed products: e.g. fuels, chemicals, plastics • Separation of NGLs in shale gas operations which are highly distributed • Small molecule separation currently performed via distillation **Biological Separations** • Alternate separations for biotech processes • Agricultural (farm waste) biological variability • Separation of low concentration, easily degradable products for biologics application **Electrochemical/Other** • Separation at near ambient conditions; potential to couple with electrochemical processes (distributed) **Water and Wastewater Separations** • Comprehensive modular water treatment in fracking operations to avoid water disposal. • Need separations that can handle heterogeneous distributed waste streams (heterogeneous with regards to composition, seasonal variability)

Table 2-2. Separations/Systems for PI and Modularization (Green Group): Goals
• More cycles for Pressure Swing Absorption (PSA) • Reduce energy consumption by 10%+ in drying/heating processes • Reduce energy use by 50% • Improve separations via modularity and PI – cheaper, better, faster (> 20% energy savings, CO_2 emission reduction, CAPEX savings; cut commercialization time in half) • Safety in design and operation • CAPEX-competitive • Minimal operator needs and maintenance • Achieve modular design in distillation columns • "Plug-and-play" modular controlled systems • Standards that work • Understanding degradation and maintenance costs (health monitoring) • Performance metric: CO_2 • "Good enough" for gathering pipelines to large centralized gas plants

Table 2-3. Separations/Systems for PI and Modularization (Green Group): Future Technologies
Hybrid/Integrated Systems
• Combined separations and catalysis • Integration of reactor with membrane: e.g. C2ODH/ C_2/C_2 = separation • Design of hybrid separation systems • Membrane reactor/sorbent temperature swing/PSA • Integration of design, capacity planning, and location selection approaches (with ability to solve resulting problems) • Tuning syngas composition or ratio through integrated separation and storage • Integrated membranes plus sorbent modular units
Innovative Technologies
• CO_2 concentration (low cost) → from 400 up to 1000+ ppm. For advanced and urban agriculture • Heat integration for SMRs/Heat = Chemistry • Can be conventional but amenable for robust design, operability, and cost. • Wastewater, flue gas treatment • Separation module for electrified chemical production. • Technologies for smart, active, effective separation processes: Electro hydrodynamic (EHD) technology and PCM technologies • Low energy intensive (low water, energy, pressure and temperature) • High temperature natural gas cleanup • Minimum contaminants for pipeline corrosion/aging
Models/Data

Table 2-3. Separations/Systems for PI and Modularization (Green Group): Future Technologies
• Sensors for in-situ measurement • Frameworks for integration of different types of data (material, process, …) to go from discovery to process design • Tools to predict long-term membrane performance (fouling, aging)

Reference: AltSep roadmap (http://altsep.org)

Table 2-4. Separations/Systems for PI and Modularization (Green Group): Challenges and Barriers (● = one vote)	
Processing/Equipment	
High Priority	• Safety of modular equipment to avoid emissions and explosions ●●●●●●●●● • Understanding how additive manufacturing can be used for PI ●●●●●●●●●
Medium Priority	• Varying nature of feedstocks; small compressors, heat exchangers ●●●●● • Design of integrated systems (reaction and separation) ●●● • Smart processes that are needed for separation processes ●●●
Low Priority	• Incumbent technology infrastructure (education through operation) optimized for distillation ●● • Units that can operate with limited on-site personnel (to help with cost challenge) ●● • Mixture complexity – challenging to design alternative separation technologies for biotech (e.g. crystallization, precipitation)
Materials	
High Priority	• Economically process-able high performance materials ●●●●●●●
Medium Priority	• Membrane selectivity and synthetic strategies; collaboration across expertise from academic to commercial processes ●●●● • Long-life stability catalyst/sorbent/membrane materials; insufficient fundamental understanding of what leads to membrane fouling and how to overcome ●●●●
Low Priority	• Robust, selective, cheap materials
Data/Fundamental Science	
High Priority	• Support for systems such as manufacturing test beds for processing of high performance materials; sponsorship for fundamental research needed to advance widespread MSA use. ●●●●●●●
Medium Priority	• How to use existing fundamental understanding/process models and new data to develop new "model libraries" (i.e. ASPEN models) ●●●●● • Using a systems approach for demonstrated operability and cost advantage ●●●●● • How to efficiently integrate molecular simulation with process optimization (multi-scale) ●●●
Low Priority	• Better (more reliable) algorithms for solving optimization problems relevant to PI and modularization ●● • Lack of integration of experimental and computational studies to enable efficient and effective rapid discovery ● • Lack of fundamental understanding of interphase phenomena, mass transfer (diffusion/sorption), and hydrodynamic modeling • Empirical basic data facilities • Process development units and piloting (impurities, run length)
Manufacturability	
High Priority	• None
Medium Priority	• Loss of scale; CAPEX/OPEX trade-off in distributed/standardized systems ●●●
Low Priority	• Conservative industry sectors; capital intensive industry; insufficient funding in the past; lack of cross-disciplining efforts; traditional thinking by process industry ● • Producing modular equipment that is cost competitive • Workforce training for automated modular systems

Table 2-4. Separations/Systems for PI and Modularization (Green Group): Challenges and Barriers (● = one vote)	
Other	
High Priority	• Long cycle times that increase cost; higher costs limit investment in new technology; reduced cycle time with accessible high performance computing ●●●●●●●
Medium Priority	• None
Low Priority	• Risk and risk mitigation for early adopters ● • Support to industrial partners to gain buy in, support, and leadership; collaborations with multiple partners to commercial; IP ownership ● • Disconnect between lab and industry (total cost and scale up)

Table 2-1. Catalysis and Reactors (Green Group):

Future Applications

Gas Conversion

- CO_2 conversion to fuels/chemicals at low cost
- CH_4 conversion to higher carbon molecules with traveling "modular" processes
- Gas-to-liquids for stranded gas (natural gas)
- Modular reactors for C_1, C_2 chemistries linked to shale gas operations
- Alkane conversion at remote sites, low temperature catalysis
- Modular and cost effective biogas to power (distributed solution to distributed problem)

Other

- Load-level solar: produce chemicals, such as NH_3 synthesis during day; convert back to energy at night; at lower cost than batteries
- Convert agricultural byproducts, food waste to biogas
- Low-cost, selective, and robust multi-applications

Table 2-2. Catalysis and Reactors (Green Group): Goals
• Reactor design integrated with separation design • High selectivity, high productivity • Search reaction networks for potential matching of endothermic and exothermic chemistries • Economic/energy efficiency improvement of 75%. • Systematic ways to incorporate PI strategies (e.g. microwave, ultrasound, specialized micromixers) into unit modules and conceptual plant design. • Effective catalysis via earth abundant metals (instead of rare earth elements) • High capital productivity • Low energy intensity • Enable fast time to market • Scale-down of reactors

Table 2-3. Catalysis and Reactors (Green Group): Future Technologies
Advanced Catalysts
• Solid-solid catalysts (i.e. solid catalysts for conversion of municipal solid waste) • Novel catalysts for methane activation and ammonia synthesis • Robust catalysts designed to handle variability in feedstocks • Any catalytic process; Catalyst preparation; catalyst integration with new reactor. • Virtual reality tools to visualize layout of modular plants • More catalysts that can handle wet feedstocks • Catalysts that operate at reduced temperature and pressure to reduce energy cost and improve safety • CO_2 activation catalysts • NH_3 synthesis catalyst for lower pressures and temperatures • Catalyst manufacturing of new materials
Reactor Technologies / Tools
• Dynamic analysis of reactor absorber systems incorporating advances or design in nanotechnology to enhance catalyst selectivity • Gas-to-liquids conversion: high throughput at relatively low volumes • Rational reactor selection guided by fundamentals/scale up • Reactor designs that take advantage of additive manufacturing advances. • Reactors for high exothermic reactions • Lower energy demand reaction systems • Smart/active devices/systems not designed under one specific operation condition (flexible) • Process Systems Engineer (PSE) tools for simulation and optimization of modular reactors
Hybrid/Integrated Systems

- Incorporation of membranes with catalysts
- Close coupling of heat/separation with reactors
- Systematic methods to optimally integrate reactions and separations
- Systematic design methods for combined reaction and separation that are “intense” (including gas-liquid-solid, liquid-liquid-solid, etc.)

Table 2-4. Catalysis and Reactors (Green Group): Challenges and Barriers

(● = one vote)

Processing/Equipment	
High Priority	• Reliability and controllability of modular reactors, including safety ●●●●●●●●●
Medium Priority	• Heat management, removal (exothermic reaction systems), and integration in smaller modular systems. ●●●● • Effective ways to quickly replace catalyst in modular reactor involving catalyst deactivation ●●●● • Reactor design that considers the entire conversion process to better enable modular systems and integrate chemistry, chemical engineering, and mechanical engineering ●●●
Low Priority	• Robust reactors (low maintenance) ●● • Limited availability of cheap, reliable spectroscopic sensors for reactors under extreme conditions (e.g. very high temperature, highly corrosive) ● • Solids handling in reaction environments ● • Integrated sensing • Cheaper analysis equipment
Materials	
High Priority	• Catalysts and catalytic systems with high efficiency at low temperature and pressure; processes with low energy demand suitable for distributed chemical plants at medium/small scales ●●●●●●●
Medium Priority	• None
Low Priority	• Long-term performance data on new technologies ●● • New reactor construction methods and materials • High cost of metals typically needed for many reactions
Data/Fundamentals	
High Priority	• Integration of various forms of data with models for optimization and reactor design ●●●●●●●●●●●●●● • Lack of systematic design methods for many unit operations that combine reaction and separation ●●●●●●
Medium Priority	• Ties between simulation and experiment ●●● • Lack of PSE tools for handling some PI approaches (e.g. ultrasound, microwave, multiphase turbulence in microscale reactors) ●●● • Lack of readily usable methods for multi-scale modeling from Quantum mechanics through reactor simulation and design ●●●
Low Priority	• Prediction of yields in modular reactors with uncertain equilibrium, kinetic, and transport parameters (i.e., from simulation models) ●● • Scale up/scale down rules of new reactors ●● • Open source catalyst/reactor design/analysis tools and university training programs in open source design tools to increase use and accessibility for all ● • Atomically well controlled/understanding of active structure; surface activation kinetics of inert molecules under designed temperature and pressure ● • Reliance on breaking molecular structure and building new structure rather than capitalizing on structures found in nature • Lack of molecular property-based formalism to confidently simulate multicomponent, non-ideal diffusion • Inadequate fundamental knowledge about catalytic mechanisms of catalysts made from earth abundant materials
Manufacturability	
High Priority	• None
Medium Priority	• Additive manufacturing with known design rules and limitation by type of 3D manufacturing; material properties and fatigue properties of 3D printed parts ●●●
Low Priority	• Catalyst manufacturing for new materials ●

Table 2-4. Catalysis and Reactors (Green Group): Challenges and Barriers (● = one vote)	
	• Relatively high capital cost

Table 2-5. Roadmap Topics (Green Group)	
High Priority Challenge/Barrier	**Priority Roadmap Topic**
Process systems that can be widely distributed with needed resilience, safety, and operability are needed to fully utilize "stranded" resources. Process design modeling to address reliability, controllability, and safety do not yet exist to support design of distributed process systems.	Reliable, controllable, and safe distributed modular process systems
Manufacturing currently relies on extremes of temperature and/or pressure to effect transformations to make products.	Catalysts and catalytic systems for low temperature and pressure operations
Current process systems engineering (PSE) tools and simulators are not interoperable (no plug and play capability). There is a lack of accessible models and tools for high-level and detailed analysis. Lack of adequate approaches for feedback loops between experimental and computational studies for validated model development rapidly.	Process systems engineering tools for plug-and-play integration of experiments and computations for validated models

Table 2-1. Cross-Cutting Topics (Green Group): Future Technologies
Education/Training
• Shift in Chemical Engineering (ChE) curriculum to include or introduce more phenomena-based components • ChEs that are creative and effective in designing PI processes • Retraining for chemical plant operators who may be displaced by modular (distributed) process implementation • Include technician/trader in design process • Short courses or online resources for workforce retaining on modular manufacturing and production/PI
Design and Tools
• Conceptual design of intensified processes • Integrated teams of mechanical engineers, chemists, and chemical engineers to "begin with the end in mind" • Design case studies on modular designs • Demonstrated success stories with concrete industrial examples (e.g. www.pinetwork.org) • PSE tool/model repositories • Integrated multiscale process modeling, from molecular to computational fluid dynamics (CFD) to mass and energy balances • Open-source CFD software for "intensified" processes. • Standards for linking "lego blocks" of modular systems • Sensors

Table 2-2. Cross-Cutting Topics (Green Group): Goals
• Less down-time • Continuous high throughput • High purity product • Understanding what economic drivers would push towards modular solution • Integration of feed forward controls with conversion processes for handling variable feedstock composition

Table 2-7. Cross-Cutting Topics (Green Group): Challenges and Barriers (● = one vote)	
Modeling	
High Priority	• Interoperability access scale issues (time, length); techno-economic analysis (learning-by-doing-searching) ●●●●●●● • Limited open-source software for intensified processes ●●●●●●
Medium Priority	• None
Low Priority	• Non-existent comprehensive conceptual design framework for intensified processes ●● • Lack of open-source software for multiscale simulation ● • Most powerful PSE tools are not open source and not "democratic" ● • Algorithms/methods to solve resulting multi-scale models ● • Adequate generality in modeling standards ● • Current design methodologies that cannot be readily applied to modular designs • Ability to work with Aspen to help company understand modularity • Systematic reliable model refinement approaches • Vendor adoption of standards
Education	
High Priority	• None
Medium Priority	• Lack of knowledge by professors; lack of coverage in textbooks or educational material (for PI and modularization) ●●●●●
Low Priority	• Improved K-12 science education to improve science literacy of decision makers ●● • Silos that exist in university education between departments and also with trade schools. ● • Current curricula do not include intensified processes and are constrained in space ● • Modular separation process (e.g. membrane) modules to be routine in junior or senior ChE lab
Economics/Cost	
High Priority	• None
Medium Priority	• Cost estimation of modular designs (vs. conventional cost estimation process units) ●●●●
Low Priority	• Incorporate sustainability analysis into new techno-economic modeling tools ●● • Economically competitive PI designs
Deployment	
High Priority	• None
Medium Priority	• None

Table 2-7. Cross-Cutting Topics (Green Group): Challenges and Barriers (● = one vote)	
Low Priority	• Push back from "drop in", "bolt on" culture. ● • Stakeholder (e.g. public) acceptance of distributed chemical manufacturing • Near term demonstration to assure new modular PI technology is ready to replace existing chemical industry infrastructure as it reaches end of life • Reinstitute the U.S. investment tax credit

Table 2-1. Separations/Systems for PI and Modularization (Red Group): Future Applications
• Distributed processing of wasted carbon into liquid fuel • Low energy mixing • High temperature gas separation in power generation systems/ reactive separation • Olefin production from natural gas; separations is key to product economics • Replacement of energy intensive distillation • Continuous process biotech

Table 2-2. Separations/Systems for PI and Modularization (Red Group): Goals
• Include focus on upstream processing for modular/PI • Economic benefit needs to be exceeding 30% for new technology to take off • Future technical goals: must provide both technical and commercial de-risk • Shift reaction equilibrium with separations (reaction, e-chemical, etc.); rationale is lower temperature for equilibrium limited reactions, higher concentration per pass, also cheaper materials • Lifetime as long as rest of plant, and CAPEX as low as possible • High flow, high separation, low cost vs life, no maintenance, and compact systems • Delta Y = yield ~ 10%, while maintaining purity • Physics-based modeling of transport at nano and meso scales

Table 2-3. Separations/Systems for PI and Modularization (Red Group): Future Technologies
Processing Equipment
• Modular separation processes for small-volume precursors for thin film electronics, PV, energy applications • Separation system consistent with upstream process conditions (avoid intermediate processing); requires studies on temperature, pressure and composition • Non-thermal separations that match or integrate with reactor throughput (~1 mol/m3/s) • Separation pretreatment of spinning membranes; fouling materials prior to membranes with centrifugal filters • Cleaning tail gas with low heat recovery for heat pump utilization • Novel solvent systems and mixing equipment; solvent-free processing • Elimination of separations (minimized) via composite/hybrid catalysts or intermediate treatment streams • Intensified reaction/separation: high temperature membranes with good mechanical/thermal properties, long service life
Materials
• Improved separations via poison-tolerant membranes, sorbents and catalysts • Low energy and high throughput control of pore size for gas separations • Heat absorbing and rejecting materials (metal hybrids) • Robust sorbents with long-term stability (1000s of cycles) • Solvent-stable highly selective membrane separators • Metal Oxide Reaction – engineering for breakthroughs in separation (e.g., cost-effective chemical looping and ionic transport membranes) • High throughput screening of materials • Self-healing materials for remote operations
Data/Fundamental Science
• Scale up or down under model error and uncertainty, with economics • Methods of measuring diffusion (broadly accepted) • Thermodynamics and transport constitutive relations for complex mixtures • Prediction tools for estimating separation expectations; structure – function – process relations at molecular level, connected to economics
Manufacturability
• Easy integration with downstream process • Standard module design for light gas separation (C2/C2 = C1/C2); customize materials in standard hardware to drive adoption, reduce cost and materials design • Manufacturability – scale of separations (ceramics, materials production) consistent with upstream process; Defects in materials during scale-up (or operations) may reduce efficacy or increase costs • Printable sieve membranes
Models
• Techno-economic model to determine which processes can be (1) modular and (2) intensified • Tools for direct intensified process; process synthesis interaction leading to intensification • Models at multi scale all the way to cost/economics
Other
• Online analytics for both desired and undesired components (but at line and not offline) • Real time imaging of molecular separation processes (labs and seals) • Systems that do not need separations X~100% for direct use products

Table 2-4. Separations/Systems for PI and Modularization (Red Group): Challenges and Barriers

(● = one vote)

Economics	
High Priority	• Competing and beating economies of scale; lowering capital and operating expenditures; justifying retrofits to existing assets vs. new installations ●●●●●●●●●●●●
Thinking	
High Priority	• Heat and mass transport currently not advantaged at smaller scales (need new methods); changing entrenched thinking to design technologies that scale-down well ●●●●●●●●●
Standards	
High Priority	• Expansion of the supply chain to significantly cut cost of module; roadmap like semiconductors to guide R&D ●●●●●●●●●
Risk (Return on Investment)	
High Priority	• Lack of current market; need first adopter investment or displacement opportunity; sufficient performance benefit to offset technical risk; cost return on new facilities with unproven design ●●●●●●
Model ●●● (Medium Priority)	
High Priority	• Understanding membrane fouling and aging; equipment degradation ●●●●●●●●
Manufacture	
High Priority	• General equipment industry for module scale systems with high reliability testing not yet developed ●●●●●●●
Data/Fundamentals	
High Priority	• Modeling, analysis, and design tools for PI ●●●●●●●●●
Medium Priority	• Fundamental parameters and separation information on real systems (with composition, poisons, etc.) not available for detailed design (e.g. kinetics) ●●●
Materials	
Medium Priority	• Understanding more on the materials at the molecular level under reactive and non-reactive conditions ●●●● • Chemistry-specific constraints: reaction/separation conditions that do not greatly limit the reaction or the separation. This is very reaction specific. ●●●
Process/Equipment	
High Priority	• Modular + PI equals fewer degrees of freedom for control; new ways to control Intensified and Modular processes are needed (process controls and tools to enable PI) ●●●●●●●●●
Medium Priority	• Complexity: maintenance; controls; product quality; ability to adapt to variability of feedstocks ●●●●
Low Priority	• High energy use in distillations; replace with dividing wall columns (DWC) but control of DWC is difficult; requires better understanding of DWC dynamics

Table 2-1. Catalysis and Reactors (Red Group): Future Applications
• Low temperature (alkane) methane activation to syngas, hydrogen production • Small-scale modular GTL reactor technologies • Small-scale reactors that process solid feedstocks (coal/biomass/waste) • Milder operating conditions (lower T&P) • Distributed systems: water purification; natural gas upgrading • Combined rDNA technology with bioreactor design (cells, enzymes • Photo electrochemical reactors for solar water splitting (artificial leaf)

Table 2-2. Catalysis and Reactors (Red Group): Goals
• Eliminate or reduce catalyst activation/regeneration • Robust, tunable, sustainable, selective, long-lived catalysts • Reactor performance goals: o Inside Wall HTC >= 2000 o Low pressure drop o Catalyst efficiency factor >= 0.90 o Volume loading 0-60% • Metrics: o (reaction rate) / (volume reaction) = (mol) / (m3 – hr) o Conversion efficiency: (reactant emissions rate) / (Feed rate) = pph / pph

Table 2-3. Catalysis and Reactors (Red Group): Future Technologies
Reactor/Reactions and Processes
• Non-thermal activation of reactions (photo, electro) • Low-cost sensors for increasing performance (e.g., sensor for car catalytic converter) • Modular tunable catalytic/heat removal systems for exothermic, equilibrium-limited processes (e.g., clean tail gas, clean up sulfuric acid technology) • Small reactors that can tolerate extreme temperature gradients • Process intensification for biomass reactors: hollow fibers, membranes, CSTR • Reactor versatility, with operating parameter changes to optimize performance • Intensification of batch processes • Working in concentrated solutions/high concentrations to minimize separations systems load • Processes and catalysts that can tolerate intermittent operation (deployed)
Catalysts/Materials
• Hybrid and composite catalysts • Catalyst immobilization in low cost and manufacture form; high heat and mass transfer • Atomically precise catalyst manufacturing processes • Incorporating advances or design in nanotechnology to enhance catalyst selectivity • Capability to cope with variability of feeds/impurities • Improved catalyst activation/regeneration and longevity • Improved anti-fouling technologies • PI for enhancement of reactor performance for the production of 2D and other low dimensional materials (e.g. graphene) • Catalyst versatility to handle feed changes and complexity
Data/Fundamental Science
• Testing/analysis/models to generate data to benchmark new technology vs. old (e.g., performance of high temperature, high flux plasma pyrolysis vs alternatives) • Reactions in and adsorption from liquid phase, especially electrolytic phases (rates, transport, thermodynamics) • Physics-informed machine learning for Ch. Group Applications: adaptive reactors with self-awareness • Flow chemistry
Manufacturability
• Additive manufacturing at scale (size and throughput) for reactor manufacturing for catalyst material classes
Modeling/Design Tools
• From first-principles to requirements models: automate model/theory abstraction • Atomic scale modeling of catalyst; determine optimal catalyst properties (from supports to active sites, etc.) • Modeling of non-traditional reactor geometries (CFD); optimize geometry for specific reaction pathway and catalyst • Design tools for modular technologies that account for total system designs: off sites, piping, turnkeys, etc.

Table 2-4. Catalysis and Reactors (Red Group): Challenges and Barriers (● = one vote)	
Process/Equipment	
Medium Priority	• Heat and mass transfer activity and selectivity maintenance; thermally integrated reactors with spatial temperature control ●●●● • Micro reactors and how to manage solids, deposits, etc. ●●●
Low Priority	• Process dynamics, control, stability, catalyst costs, life cycle volume, and reactivity (too low or too high) ●● • Alternative strategy to adapt high pressure reactors for small scale processes ●● • Built-in balance of plant; integrate circuit (limit values, piping, etc.) ● • Changes induced by modularity scale to reduce unintended chemistry consequences • High efficiency, cost-effective contacting devices that shrink equipment (without downside of delta pressure, etc.); mesoscale best practice
Materials	
High Priority	• Very high temperature materials for redox reaction for integration with thermal cycles ●●●●●●●●●
Low Priority	• Transport limitations, non-fouling materials in bioreactors ●●
Data/Fundamentals	
High Priority	• Characterizing the interface at a solid/liquid boundary especially in the presence of strong fields and other gradients ●●●●●●●●
Medium Priority	• Lack of fundamental parameters (e.g. kinetics) for advanced reactor design/model ●●●●●
Low Priority	• Poor understanding of catalyst deactivation ● • Process chemistries that do not require high pressure ●
Modeling	
High Priority	• Lack of reactor controls to deal with feed changes (lack of an operator) or longevity; modeling reaction dynamics, reaction network analysis, model reduction and validation, and nucleation kinetics ●●●●●●● • Lack of a system level model that optimizes heat integration vs. cost and minimizes balance of plant and footprint; could be used for smart controls ●●●●●●●
Manufacturability	
High Priority	• Lowering reactor system manufacturing cost through additive manufacturing and/or structured catalysts/reactors ●●●●●●
Deployment	
High Priority	• Finding "best" use cases for modular technology; what can modular technology do that is unique; requires a focused application ●●●●●●●●●●
Low Priority	• First adopters: Gas to liquids (GTL), stranded resources, negative value resources ● • Current level of technology maturation and scale-up for ultra-modular processes

Table 2-5. Roadmap Topics (Red Group)	
High Priority Challenge/Barrier	**Priority Roadmap Topic**
Delivering high reactivity reagents at right place and right time to attain the desired selectivity is a major challenge.	Materials to enable chemical looping
There is currently a lack of robust microkinetic models for complex transient reacting systems which prohibits intensified reactor design.	Data and fundamentals in catalysis and reactor in PI
There are no current software tools or packages capable of modeling and analysis of modular and intensified chemical process systems over the relevant space and time scales.	Modeling and control of PI and modular systems
A disciplined approach is needed to develop a roadmap covering the state of the art to final vision for a focused application of modular and intensified systems. Business models showing the value proposition of modularity and benefits of smaller scale are lacking.	Economics

Table 2-1. Cross-Cutting Topics (Red Group): Future Technologies
Technologies
• Design for cartridge replacement of catalysts/sorbents/membranes • Advanced interrogation technologies for in-situ examination • Sensors and analytics development • Pollutants considered • Low cost distributed analytical evaluation of chemical streams
Education
• Software tools to support teaching PI in senior process design • Education not just for students • Workforce development in PI area: operators; analysts; etc.
Manufacturability
• Improved understanding of manufacturability of modular technology
Modeling/Design
• Virtual testbeds approach: data collection; analysis; simulation; design • Identification of specific reactor/system designs that work particularly well for PI • Techno-economic analysis tool for early stage technology (not based on excel) • Technical risk analysis framework for PI • Life cycle analysis, model-base systems engineering, decommissioning costs of intensified processes • Multi-scale/multi-physics models to access PI benefits for given chemistry and configuration
Infrastructure
• Research and development coordination, data sharing, and model sharing • Balance of plant, flow control, compression, and mixing • Maintenance paradigms
Measurement
• Measurement techniques (e.g. solid circulation rate, phase holdup)

Table 2-2. Cross-Cutting Topics (Red Group): Challenges and Barriers
(● = one vote)

Technology	
High Priority	• Analytical equipment that is bulky and expensive for distributed applications ●●●●●●●
Low Priority	• Ease in retrofit or replacement and cost effectiveness ●●
Education	
Medium Priority	• Corporate buy-in to curriculum edits (practical courses, hands-on learning, and virtual learning) ●●●●● • Good textbook with documented good examples (beyond unit operations design) ●●●●
Economics	
High Priority	• Lack of techno-economic analysis tools for novel early stage technology ●●●●●●
Low Priority	• Chicken/Egg economics, which gets resolved only with either regulation, funding or subsidy • Clear applications and first adopters for new technology
Standards	
High Priority	• Common vessel types and connection "seams" to integrate technology (e.g. reaction and absorption) ●●●●●●●●●
Medium Priority	• Standards for simulations and data, open source software ●●●●●
Low Priority	• Lack of modular supply chain which impacts standardization and deployment
Infrastructure	
High Priority	• Investment in data exchange/storage ●●●●●●
Other	
High Priority	• Cross-disciplinary research, communication and engagement ●●●●●●
Low Priority	• Generating management commitment to modular/PI

Table 2-1. Separations/Systems for PI and Modularization (Yellow Group): Future Applications
Gas Separations • NG/shale gas to chemicals via distributed modular processing (separate/package distribute; separation/reaction then distribution) • Flare/flue gas separation (membranes, sorbents, eliminate NO_x, SO_x, HCs) • Methane to ethylene, propylene, and butylene • Utilization of currently uneconomical resources **Liquid Separations** • High energy use or low efficiency or high chemical hazard chemical separations • Processes with large product demand variability to enable large "turn down" (e.g., distillation only has 2:1 turn down) • Small scale NH_3 synthesis for distributed applications • Chemicals production from C_1-C_3 feedstocks • Water resources **Biological/Pharma** • Sustainable energy utilization form renewable resources • Pharmaceutical/biotechnology separations • Food processing **Energy** • Renewable energy integration • Energy production • Green cheap electricity in redesign of exiting separation processes • Utilization of "stranded" resources (water, fuel)

Table 2-2. Separations/Systems for PI and Modularization (Yellow Group): Goals
• Boiling point separation; molecular size/shape; chemical class • Molecular recognition/design of MSA • Energy and "waste" reduction • Membrane selectivity and robustness • Ability to switch on/off modules to change production rates relatively quickly • Unattended operation (1 week monitoring) • Design for heat and mass integration (e.g. use of low grade waste heat)

- Lower pressure and temperature
- Standardization; massive production; low pressure with no minimum recycle
- Make currently uneconomical opportunities viable, not necessarily better than large scale
- Water footprint overall efficiency
- Scale up of alternative separation systems to defined commercial scale (i.e., crude 10 kBPSD, 20kBPSD, etc.)
- Definition of PI
- Real-time optimization and control algorithms (robust, fault tolerant)
- Energy recuperation to minimize irreversibility for chemical/energy conversions
- Safety for remote operation

Table 2-3. Separations/Systems for PI and Modularization (Yellow Group): Future Technologies
Novel Separation Technologies
• European model – reduce size by moving from batch to continuous • Electrochemical pumping separations of organic acids, electrocatalyst/membrane systems • New separation media with targeted performance • High temperature water/hydrocarbon separation (T>500°C) • Enhanced recovery separations: break emulsions; recycle surfactants; heavy oil extraction enabler • Separation of fuel/ feed: ranges of hydrocarbons from crude without traditional distillation column • Hydrocarbon reverse osmosis • Application of additive manufacturing • Renewable feedstocks (comparable cost, performance)
Hybrid/Integrated Systems
• Switchable, adaptive separation and reaction media/processes • Combining reactions with separations (example: chemical looping ODH) • Separation from reactor for energy savings (e.g., membrane reactor) • Heat and mass integration transfer • Novel reactors as efficient separation and heat/mass transport efficiency • Reactive separations; hybrid processes; alternative driving forces
Other
• Process modeling software for PSA • Supply chain optimization: membranes, screening tools/process selection • Conceptual modular design framework for separations • Advanced simulation tools/multiscale models

Table 2-4. Separations/Systems for PI and Modularization (Yellow Group): Challenges and Barriers (● = one vote)	
Processing/Equipment	
High Priority	• Alternative energy systems needed to power equipment (integrated); solar, battery, etc., fit-for purpose ●●●●●●●●●
Medium Priority	• Standardization vs. flexibility vs. optimization; requires input from business and operations ●●●●● • Handling one-way separations (like adsorption) in continuous process (like SA or moving-bed adsorption) ●●●●
Low Priority	• Systems approval lacking for integration • Efficiency constraints of bulk heating of fluids • Lack of standardization to lower manufacturing costs
Materials	
High Priority	• Active/selective catalyst materials for shale gas conversion; low temperature/pressure highly conductive/separative membranes ●●●●●●● • Material robustness for reactors, catalysts, membranes, etc. ●●●●●●
Medium Priority	• Lighter/stronger materials for reaction/separation housing (i.e., vessels) ●●●●● • High temperature materials catalysis (sintering) ●●●
Low Priority	• Catalyst deactivation: temperature, pressure limitations on materials ● • Controlling morphology of materials ● • Separation media: uncertainty about what should be made, rather than what can be made ●
Data/Fundamental Science	
High Priority	• Data mining and fusion of process data with model predictions for real-time operation ●●●●●●●●●
Medium Priority	• Information overload; data integrity/standard methods; lack of communication between fields ●●●
Low Priority	• Understanding aging-degradation as a molecular dynamic process ● • Addressing hazardous research needs and facilities ● • Noisy/sparse/uncertain data sets ● • Lack of fundamental understanding of materials/catalyst ● • Small single PI projects that don't address multiple aspects– lack synergy, potential siloed efforts ● • Fluids/solids under radiation, extreme environments ● • Using existing processing equipment and materials in new areas/uses via cross fertilization
Manufacturability	
Medium Priority	• Consideration of dynamics, control, startup/shutdown at design phase ●●● • Consideration of safety, sustainability, and environmental effects ●●●
Low Priority	• Manufacturing limitations which drive cost up; potential for 3D printing ● • Lack of "creative" process synthesis technique (more related to "systems" – combined reactions/separations in single unit operation) ● • Constrained footprint in unconventional gas or oil location; environmental/physical space ●
Modeling	
High Priority	• Disconnect in multi-scale modeling ●●●●●●●●
Medium Priority	• Design fundamentals: limited/lack of good descriptor models for designs and handling nonlinearities/interactions ●●●●●
Low Priority	• Separation media design: extracting new knowledge from multiple data, including molecular structure-chemistry and reactivity; first principle models; multi-model characteristics; in operando dynamics ●● • Process simulation tools for modular processing and manufacturing; Open source and commercial tools (PSA, membrane, supply chain) ● • Models predict separation media that is not synthesizable with existing techniques • Economic models to set specific targets

Table 2-1. Catalysis and Reactors (Yellow Group): Future Applications
• Catalytic membrane reactors, for example, for equilibrium limited reactions (e.g., to remove product continuously) • Catalytic separative membrane reactors for C_1 (light) upgrading and biomass feedstock valorization • Low temperature nitrogen activation catalysts • Renewable energy systems • Combination of several reactions in one unit operation (reactors) • Combining bio and fossil feedstocks for syngas production • Modular systems for in-field GTL for C_1 to C_4 hydrocarbons at shale locations • Supports to restructure metal migration and stability • Modular waste minimization/treatment

Table 2-2. Catalysis and Reactors (Yellow Group): Goals
• Robust catalyst lifetime, selectivity, yield, recyclability • Decreased use of transition/noble metals • Sufficient level of flexibility to allow operational control for highly intensified process steps • Targeted selective catalysts that put contaminated water or gas streams within specifications in field • Use of exothermic heat release (in catalytic cracking units, for example) • New class of catalytic activity/action and integration providing intensification/yields above the norm (historical: Pt to Pt-RE bio-metallic supported) • Mapping of meta stable carbon thermodynamics • Flexibility for variable feedstocks • Reactive process safety analysis and mitigation solutions (tools, standards, and regulations) • Heat-mass transfer analysis in integrated multi-functional reactors • High fidelity evaluation models for various catalysts and reactor configurations • Alternative catalyst supports to reduce hazards • Minimized inventory of materials (especially hazardous)

Table 2-3. Catalysis and Reactors (Yellow Group): Future Technologies
Innovative Reactors/Catalysts
• Millisecond reactors (at pressure) • Plasma (cold): decouple activation steps from reaction e.g. CH_4 activation • Recycling used chemicals to minimize waste (refining sulfuric acid rather than going through SO_2 or using fresh sulfur) • Horizontal reactor (or distillation) systems – centrifugal • Photo/solar catalysts to possibly shift HC product selectivity in refining "polishing stage" • Modular catalysts for in-situ oil upgrading to a synthetic crude • Heavy HCBN conversion without fluid catalytic cracking reactors or on 2 pressure vessels • Microwave technology "heating where is needed" for catalytic reactors • Water and thermally stable acid catalyst for reaction-based separation • Metal additive manufacturing for materials/catalysts
Hybrid/Integrated Reactor Systems
Hybrid/Integrated Reactor Systems • Integrated reactivity (e.g., TVA auto thermal reactor; reactive distillation column) • Hybrid reactors combining more than one technology (e.g. use of microwaves and zeolites to activate/convert methane) • Integration of catalysts and reactor design (multi-scale modeling) • Combining catalysis with other unit operations (e.g. separation, heat integration, etc.) • Integrated reaction and separation development (e.g. reactive distillation); improved fundamental design methods • Process control for integrated reactors/separators

Table 2-4. Catalysis and Reactors (Yellow Group): Challenges and Barriers
(● = one vote)

Processing/Equipment	
Medium Priority	• Scale up challenges in reactor designs which minimize feed/catalysis interaction/residence time ●●●● • Better metallurgy for refining sour, low pH crudes; material robustness under more demanding environments ●●●●
Low Priority	• Limits of catalytic-membrane reactors
Materials	
High Priority	• None
Medium Priority	• Collaboration/common language between experimentalist and theorists ●●● • Lack of smart catalysts that can perform multiple reactions depending on stimuli/substrate materials ●●●
Low Priority	• Synthesized (non-natural) enzymes and organisms for synthesizing "biological" and commodity and specialty chemicals ●● • Developing new shapes/forms of materials for improved conversions/separations • Limited supply of rare earth elements
Data/Fundamental Science	
High Priority	• Low temperature, low pressure, solution phase catalysts (enzymes, homogeneous catalysts, other biocatalysts) that are more amenable to reactor membrane hybrids ●●●●●●
Medium Priority	• Collecting better health safety, and environment safety data on catalyst toxicity; fast quench to stop runway reactions; transportation friendly ●●●●● • Lack of a unified database for experimental data (for example, comparison of catalyst materials in chemical reactions) ●●●●● • Catalyst design and fabrication tools lacking for PI ●●● • Deducing poisoning/deactivation mechanisms in addition to reaction mechanisms ●●●
Low Priority	• New analytical techniques that help improve understanding of processes ●● • Chemical basis of hydrogen dissociation in oxide and sulfide catalysts • Understanding of microwave-hetero solids interaction and quantitation • Valuing the conversion of low energy materials (e.g., CO_2 to higher value products)
Manufacturability	
Medium Priority	• Startup of heat-integrated catalytic reactors, e.g., moving "hot spots" (a process control consideration) ●●●●●
Low Priority	• Incorporating human factors design ●● • Integration of smart grid with electric power infusion reactors (microwave, etc.) ●● • Loading/unloading catalysts in remote (inhospitable) regions ● • Scale-up of membrane reactors for industry practices ● • Equipment manufacturing capabilities
Modeling	
High Priority	• Inadequate resolution of catalyst, stability, activity, and selectivity in aqueous systems in models ●●●●●●●
Medium Priority	• Integration of material science and reactor design in models ●●● • Standardizing inputs/outputs for modeling the same interface ●●●
Low Priority	• Truly predictive modeling strategies ●● • Forced concentration: temperature cycling, control strategy ●

Table 2-5. Roadmap Topics (Yellow Group)	
High Priority Challenge/Barrier	**Priority Roadmap Topic**
Currently, there is a lack of renewable systems readily available for distributed energy resources that could be applied to modular or intensified processes.	Alternative energy systems
Chemical upgrading of stranded gas is currently difficult and/or not cost-effective.	Chemical upgrading of stranded gas
Modular process safety requires greater focus due to the increased number of facilities and their interconnections.	Process safety
Different platforms exist for data collection and storage; software communication for data analysis; information extraction; and data quality (noise, errors, etc.). Temporal and spatial variability of data also poses a challenge.	Decision making using data
Catalyst/reactor technologies that could aid integration of reaction and separations are currently lacking and require development.	Integration of reactions and separations

Table 2-1. Cross-Cutting Topics (Yellow Group): Future Technologies

Education/Training

- Educate the educators: classics on separations/reactions vs. transformative alternatives
- Communication of separation challenges to materials and reactor/reactions engineering community
- Teaching innovation principles
- Program for exchange of scientists between industry and academics
- Modular design construction course work for engineering students
- Development of a challenge problem with current complexity (modular vs large scale problem) for education/training
- Tap European experience: micro-devices; mirco-channel reactors; connection; wealth of experience
- Inclusion of PI concepts in unit operations training and SR design
- Education on concepts rather than units
- Separations education that covers practical operations (e.g., poor coverage of real-time, non-steady state distillation)
- Determine what should be added or championed in ABET to drive correct focus
- Dedicated sessions in AIChE to cover modular/PI

Infrastructure

- Wireless sensors and actuators and standardized cloud sharing IT software and hardware
- Development of transportation infrastructure for shipping modular systems
- Fast prototyping capabilities
- Cloud data security for plant data
- Government regulations: minimum emission; charges/forced fines/ incentives

Table 2-2. Cross-Cutting Topics (Yellow Group): Goals

Economic Goals

- Economics of number [of units] greater than economies of scale (e.g., beating economics of scale with modularization/PI)
- Definition of “value” of modular/PI
- Funding mechanisms (promotion of private investment)
- Joint industry partnerships (JIP) on the modularization topic
- Suitable or niche technologies that may be economically more amenable/ready/advantageous for modular PI
- Measurements to decide when to go modular; could be based on economics
- Evaluation of economics with industrial partners at each stage (TRL) of development
- Baseline commercial performance (Marshall Swift equivalent)

Performance Goals

- Environmental impact that may be different
- Life cycle analysis to enable comparison to state-of-art
- Self-sustainable, economic, environmentally friendly modular process/system for chemical/fuel production
- Understanding of unintended consequences such as: security, environmental, public safety, total cost of ownership
- U.S. chemical engineering focuses on products (material, biotech) vs process (rebalance of education)
- Integration of different business units
- Ability to make two products in a modularization process to leverage value chain
- Overcoming of chemist/molecular biologist prejudice toward batch reactors
- Chemical engineers (ChEs) work more with social scientists and industrial engineers (not just MEs, EEs, technicians)

Table 2-3. Cross-Cutting Topics (Yellow Group): Challenges and Barriers

(● = one vote)

Collaboration/Development/Deployment	
High Priority	• Intellectual property (IP) “finding common ground”; sharing of IP; ability to publish; commitment/complexity of IP ●●●●●●●● • Difficulty creating diverse teams-social science, etc. with engineers (multidisciplinary solutions) ●●●●●
Medium Priority	• Lack of communication between different communities ●●●●
Low Priority	• Risk aversion of industry adopters/developers ● • Difficulty estimating (quantity) “modular impact” (economic, environment, etc.) ● • Anti-collaboration pressure (NIH) ● • Tendency to focus on small problems and hope the sum of the parts is greater than the whole • Peer review silos • Changing political environment • Maturity level of modular technologies for many applications • Joint venture “buy-in” for trailing a new technology • Cross cutting areas means different incentives

Table 2-3. Cross-Cutting Topics (Yellow Group): Challenges and Barriers (● = one vote)	
	• Environmental metrics differ by media and government policy • Routine/standard vs. state-of-the-art differs by field
Education and Training Challenges	
Medium Priority	• Education covering concepts rather than units ●●●●● • Reduced number of process-oriented ChE faculty means new ideas are harder to incorporate; ChE academic research involvement in products helps co-development of processes ●●● • Lack of facilities for hands on training at right (pilot/demo) scale ●●● • Communication of separation challenges to materials and reactor/reactor engineering community; educating the educators: classics of separation/reaction energy plus transformative alternatives ●●●
Low Priority	• Lack of knowledge or education or appreciation for modular/PI ● • Curricula is already extensive/full
Economic Challenges	
High Priority	• More NSF/DOE initiatives aimed at joint academic/industry collaboration ●●●●●●
Medium Priority	• Concepts of economy of scale skepticism from industry (perspective that modular is expensive) ●●●●●
Low Priority	• Inadequate support for research/education in this field ●● • Changes in business climate/market challenges ● • Lack of corporate incentives for innovation • Limited operation data to provide OPEX (operating expenditures) for techno economic models • Short-term return requirements by businesses inhibiting innovation • Downward funding pressure in academia, government, and industry (process engineering not a focus)

Modular Manufacturing Workshop Participant List

Last name	First name	Affiliation
Adams	Thad	Savannah River National Laboratory
Adomaitis	Ray	University of Maryland
Aurand	Emily	National Science Foundation
Balan	Prakash	National Science Foundation
Baldea	Michael	The University of Texas at Austin
Belfort	Georges	Rensselaer Polytechnic Institute
Bequette	B. Wayne	Rensselaer Polytechnic Institute
Bielenberg	James	ExxonMobil
Bollas	George	University of Connecticut
Boysen	Dane	Cyclotron Road
Bridge	Nicholas	Honeywell UOP
Bruce	Tatarchuk	Auburn University
Calloway	Thomas	Savannah River National Laboratory
Carole	Read	National Science Foundation
Castaldi	Marco	City College of New York, CUNY
Chadwell	Brad	Energetics Incorporated
Chang	Qing	Stony Brook University
Cremaschi	Selen	Auburn University
Dauenhauer	Paul	University of Minnesota
Davis	Jim	University of California, Los Angeles
Dindi	Hasan	DuPont
Eichner	Melissa	Energetics Incorporated
Epling	William	University of Virginia
Fan	L.S.	Ohio State University
Fisher	James	Department of Energy/NETL
Fletcher	Karen	RAPID
Fulay	Pradeep	West Virginia University
Gaffney	Anne	Idaho National Laboratory
Gatzke	Edward	University of South Carolina
Georgakis	Christos	Tufts University
Giles	Lauren	Energetics Incorporated
Giraud	Robert	The Chemours Company
Goyal	Amit	Southern Research
Grassi	Vince	Lehigh University
Grossmann	Ignacio	Carnegie Mellon University
Gupta	Raghubir	RTI International
Hanjing	Tian	West Virginia University

Hasan	Faruque	Texas A&M University
Herzfeld	Jennyfer	Energetics Incorporated
Hock	Adam	Illinois Institute of Technology
Hu	John	West Virginia University
Ierapetritou	Marianthi	Rutgers University
Jenks	Cynthia	Ames Laboratory
Jiao	Feng	University of Delaware
Jones	Andrew	Activated Research Company
King	Cindy	University of Delaware
Koros	William	Georgia Institute of Technology
Kokkinos	Angelos	Department of Energy
Kovvali	Anjaneya	ExxonMobil
Krause	Theodore	Argonne National Laboratory
Kusiak	Andrew	The University of Iowa
Lage	Jose	Southern Methodist University
Lee	Jennifer	Royal Society of Chemistry
Lerou	Jan	Jan Lerou Consulting, LLC
Li	Fanxing	North Carolina State University
Lighty	JoAnn	National Science Foundation
Lima	Fernando	West Virginia University
Lin	Hongfei	Washington State University
Liu	Dongxia	University of Maryland
Lobo	Raul	University of Delaware
Lueking	Angela	National Science Foundation
Makila	Tommi	Energetics Incorporated
Marler	David	ExxonMobil Research & Engineering
Marton	Andras	Analysis, Inc.
McCabe	Robert	National Science Foundation
Mehta	Rajesh	National Science Foundation
Miller	David	U.S. Dept. of Energy, National Energy Technology Laboratory
Moloy	Kenneth	National Science Foundation
Mountziaris	T.J.	National Science Foundation
Ohadi	Michael	University of Maryland
Patience	Gregory	Polytechnique Montreal
Peden	Chuck	Department of Energy
Pellegrino	Joan	Energetics Incorporated
Pereira	Carmo	DuPont
Pfromm	Peter	Kansas State University
Read	Carole	National Science Foundation
Reynolds	Michael	Shell Exploration and Production
Rezaei	Fateme	Missouri University
Ribeiro	Fabio	Purdue University

Rimer	Jeffrey	University of Houston
Rownaghi	Ali	Missouri University
Sastri	Bhima	Department of Energy
Schottel	Brandi	National Science Foundation
Schwartz	Viviane	Department of Energy/BES
Schwartz	Harrison	Energetics Inc.
Scott	Susannah	UC Santa Barbara
Shiflett	Mark	University of Kansas
Stefanidis	Georgios	University of Leuven
Thompson	Levi	University of Michigan
Tonkovich	Anna Lee	Tonkomo
Tsapatsis	Michael	University of Minnesota
Tway	Cathy	The Dow Chemical Company
van Sint Annaland	Martin	Eindhoven University of Technology
Veser	Goetz	University of Pittsburgh
Vlachos	Dion	University of Delaware
Weber	Robert	PNNL
Westmoreland	Phillip	North Carolina State Univ / CESMII
Wilhite	Benjamin	Texas A&M University
Wong	Hsi-Wu	University of Massachusetts Lowell
Xu	Bingjun	University of Delaware
Yagoobi	Jamal	Worcester Polytechnic Institute
Ydstie	Erik	Carnegie Mellon University
Yoon	Seongkyu	University of Massachusetts
Zavala	Victor	University of Wisconsin-Madison

Workshop Agenda

Tuesday, January 17, 2017

7:00 am Registration

8:00 am Opening Session

- Welcome and Workshop Objectives – Lakis Mountziaris, NSF
- Energy and Modular PI – Angelos Kokkinos, DOE

8:20 am TOPICAL PLENARY: Separations/Systems for PI and Modularization

- Robert Giraud, The Chemours Company – Sustainable Separations for Modular Chemical Manufacturing
- Georges Belfort, Rensselaer Polytechnic Institute – Challenges and Research Needs for Modular Design of Synthetic Membrane Separations with Liquids
- Michael Tsapatsis, University of Minnesota – Porous Materials for Adsorption and Membrane-based Separations and for Reaction-Separation Processes
- William Koros, Georgia Institute of Technology – Gas Separation Systems: Modular Tools for Process Intensification
- Ignacio Grossmann, Carnegie Mellon University – Centralized versus Distributed Manufacturing: A Continuous Location-Allocation Problem
- Erik Ydstie, Carnegie Mellon University – Vistas for Process Operation and Control: Integrating Physics, Computation and Communication Networks

10:00 am Break

10:15 am BREAKOUT SESSION: Separations/Systems for PI and Modularization

- Future Applications, Technologies, Performance, and Goals
- Challenges and Barriers / Priorities

11:50 am Lunch: Dane Boysen, Cyclotron Road, Lawrence Berkeley National Laboratory – Democratizing Energy Technology

1:10 pm TOPICAL PLENARY: Catalysis and Reactors

- Cathy Tway, Dow Chemical Company – Catalysis and Reaction Engineering as Critical Components to Modularity and Process Intensification
- Mike Reynolds, Shell Oil Company – Upstream Opportunities in Modular Molecular Manufacturing
- Martin van Sint Annaland, Technische Universiteit Eindhoven – Challenges in Designing Fluidized Bed Membrane Modules
- Liang-Shih Fan, Ohio State University – Chemical Looping Gasification and Reforming: Modularization Strategy for Syngas Generation with CO2 as Feedstock
- Georgios Stefanidis, University of Leuven – Electrification of Chemical Reactors for Process Intensification: Power-to-Chemicals using Plasma and Microwaves
- Nicholas Bridge, UOP LLC – Honeywell – Modular Fuels Processing: Serving the Demands of the Future

2:30 pm Break

2:45 pm BREAKOUT SESSION: Catalysis and Reactors

- Future Applications, Technologies, Performance, and Goals
- Challenges and Barriers / Priorities

4:20 pm Report Outs

5:00 pm Adjourn Day 1

Wednesday, January 18, 2017

7:00 am Arrive and Network

8:00 am Welcome

- Opening Remarks from Organizing Committee

8:15 am Keynote

- Smart Manufacturing and Modular Systems – Jim Davis, UCLA – Vice Provost, Information Technology and Chief Academic Technology Officer – Smart Manufacturing and Modularization

8:45 am BREAKOUT SESSION: R&D Roadmap

- Separations/Systems for PI and Modularization and Catalysis/Reactions – Participants break into interactive groups within breakouts to develop R&D roadmap and pathways

10:15 am Break

10:30 am PANEL SESSION: Cross-Cutting (Modeling, Education, and Economics)

- Anna Lee Tonkovich, Tonkomo LLC – Accelerating Development of Modular Process Intensification Technology
- Susannah L. Scott, University of California, Santa Barbara – Designing Resilient Catalysts
- Levi Thompson, University of Michigan – Using Cascade Concepts to Design More Energy and Atom Efficient Heterogeneous Catalysts
- Phillip Westmoreland, North Carolina State University – Developing an Intellectual and Educational Framework for Modular Process Intensification
- Michael Baldea, University of Texas, Austin – Modular Chemical Production Systems: Economics, Design and Operations

12:00 pm Lunch: Raghubir Gupta, RTI International – A Case Study in Technological and Business Challenges of a Modular Process Technology

1:20 pm BREAKOUT SESSION: Cross-Cutting Topics

- Desired Future Applications, Technologies, Performance, and Goals
- Challenges and Barriers / Priorities

2:45 pm Open Forum and Wrap-Up

3:15 pm Adjourn