Fit With RAPID Roadmapping Results

RAPID has identified several high level knowledge and technology gaps that, if addressed, would significantly advance process intensification and/or modular chemical process processing technologies. Proposals will be scored against their fit within the technical scope defined by these gaps, with projects applying PI and MCPI solutions to address multiple gaps receiving the highest scores.

**Institute Wide Gaps**

- The need for basic “input” data to develop models for PI and MCPI systems and a structure for sharing/accessing such data
- A lack of modeling tools to evaluate and screen potential PI and MCPI applications. Specifically, tools that would allow the screening of new technologies/unit operations (techno-economic evaluations) and evaluate the compatibility with traditional unit operations to allow for the assessment of hybrid process schemes. Beyond tools for process design, models for control and optimization of intensified systems would also be a highly valuable.
- Limited design approaches that balance the benefits from standardization in modular manufacturing with the broad impact of those designs. This gap needs to be addressed by determining what can be standardized and still meet market needs and by focusing on modularization novel process components but also considering modularization of the balance of plant.
- Viable PI and MCPI solutions in water processing – including both aqueous/non-aqueous separations and drying/water removal. Applications range from product recovery and inhibitor removal in biological processing systems to process water purification and management across the chemical and commodity processing space as well as waste water management in unconventional gas production

**Gaps in Chemical and Commodity Processing**

- Novel reaction/separation schemes that are scalable and drive process efficiencies. This includes intensification schemes such as membrane-, electrochemical-, or sorption-enhanced reactors, with applications to processing light paraffins, naphtha streams to increase p-xylene yield, hydrogen production, managing oxygen supply to reactions, etc.
- Non-thermal use of alternative driving forces to activate chemical systems at the appropriate (atomic/molecular) scales.
- Intensification schemes for batch systems. Transferring concepts largely developed for continuous processes to the batch realm could result in increased productivity/lower cost for specialty/fine chemicals.

**Natural Gas Upgrading**
• Highly selective conversion of natural gas, including methane and NGLs, to desired products. This will require fundamental improvements in catalysis, heat and mass transfer and process concepts which could include alternative energy inputs and/or the use of novel reaction systems.

• Energy efficient separations technology to purify the reaction product mix or condition the feed in preparation for conversion. Separations to generate co-reactants for participation in natural gas conversion are also needed, including improved air separation processes to generate oxygen for oxidative conversion of natural gas.

• Process consolidation and modularity to reduce total installed cost by reducing the total number of separate unit operations and by reducing the amount of field fabrication. This gap includes modular solutions addressing the two gaps listed above in this section that would enable upgrading of distributed, unconventional gas resources.

Renewable Bioproducts
• PI technologies for reducing energy demand in primary separation process steps designed to recover organic molecules and biomass components from water.

• PI solutions for dewatering and drying of biomass feedstocks, water removal and drying in pulp & paper process, and drying and removal of low levels of residual water from end products

• Novel chemistries and PI strategies to couple heat transfer and reaction in thermal processing of biomass and/or novel applications of reactive separation technologies in biological conversion technologies such as fermentation.

Modeling and Simulation
• Software tools for integrated reaction and/or separation processes and/or cyclic process such as pressure swing adsorption (PSA) or temperature swing adsorption (TSA). Such tools need to widely accessible and capable of integrating MCPI solutions with existing unit operations.

• Modeling approaches coupled with data generation and/or analysis to generate databases of physical parameters enabling design with mass separating agents

• Tools for the assessment of safety, sustainability, control in PI and MCPI applications. These tools would include dynamic evaluations for cyclic processes and would also address unique issues of uncertainty and reduced control variable options that are present in PI and MCPI applications.

Intensified Process fundamentals
• Scale out methodologies and models to predict performance of alternative energy input approaches for reactions and mixing and decide the suitable scale for modular manufacturing. This would include approaches to deal with scaling for systems with limited penetration depth (e.g. microwaves or ultrasonic mixing)

• Approaches that address key issues with around the lack of data on fluxes, adsorption, and catalyst kinetics for a wide class of materials, limiting the ability to apply novel materials as adsorbents,
membranes, and catalysts. This will include approaches for scale up of novel materials and defect free membranes.

- Modeling capabilities to screen concepts and configurations of all types and predict optimal structures.

**Modular Manufacturing**

- Intensified components that drive down the cost of module pre-assembly, transportation and installation while driving significant energy savings within chemical processes. This could include designs that reduce module manufacturing costs, designs of intensified components to leverage lower-cost manufacturing technologies, and/or modeling tools that drive down the costs of module and component manufacturing and improve reliability of new intensified components.

- Design approaches that limit the amount of non-recurring engineering — during systems integration and installation — needed to support customized modules. This could include work to identify standard module types and sizes for classes of problems that enable economies of mass production and/or designs module that would allow for incremental capacity additions to existing processes.

- Module design and manufacturing approaches to enable economically viable distributed chemical processing applications. These approaches will provide new paths to capital cost reduction and innovative techniques for maintenance and remote access and monitoring.