

Breakout Session 1: Chemical Reactions and Reactors

Technology Needs, Barriers, & Challenges

- Catalysts
- Thermal integration:
 - Control of heat in reactions
 - Rapid efficient heating (thermal transfer) methods
- Scale-up: reactor designs
- Simulation and modeling
- Process control, sensors and automation
- Scale-down:
 - Design of small scale systems
 - Define which applications can be addressed
- Separations and selectivity
- Business case/economics
- Environmental/sustainability

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R&D Needs

- Catalysts:
 - Engineered and optimized for microreactors, methane conversion catalysts, hydrothermally stable materials, non-precious metal catalysts
- Reactions/Reactors
 - Compact heat exchanger reactors, reactive separations, minimizing fouling for microreactors
- New processes
 - Process development to reduce process steps, solutions for utilizing flared gas, CO₂ to make products (e.g., alcohols)
- Modeling and design
 - Mixing and dispersion modeling, better kinetic modeling, cloud-based simulations, design for manufacturability, integrated design
- Sensors and control
 - New integrated sensor control technology, smarter sensors
- Other
 - Demonstration platform/facility, cost modeling, supply chain assessment

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Metrics and Impacts

- Energy efficiency (20-50% energy reduction for commodity chemicals and 50+% reduction for specialty chemicals)
- Eliminate gas flaring (100% utilization)
- Industry defined goals for specific materials (e.g., cost or BTU per lb; productivity improvements, operating/capital costs)
 - Metrics may vary by sector/output
- Catalysts: reduce activation energy by some percent of free energy of reaction
- Capitalize on underutilized waste streams
- Zero effluent manufacturing
- Technology adoption metrics
- Based on on-stream time and particular feedstock

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Other Considerations

- What will it take for industry to collaborate on these issues?
- Effort needs to make money for industrial involvement
- How to handle IP (first mover advantage?)
- Industry will collaborate on process safety
- Clearinghouse for technology pathways: what would be the best structure?
- Test bed for modular production
- Need to de-risk the technology
- Look at prior consortium models for lessons learned
- Needs to address crosscutting challenges (less on application specific challenges)
- Update objectives occasionally
- Needs a well-defined focus regardless of modality
- Chemical industry slow to change
- Is PI too close to company competitive advantages?