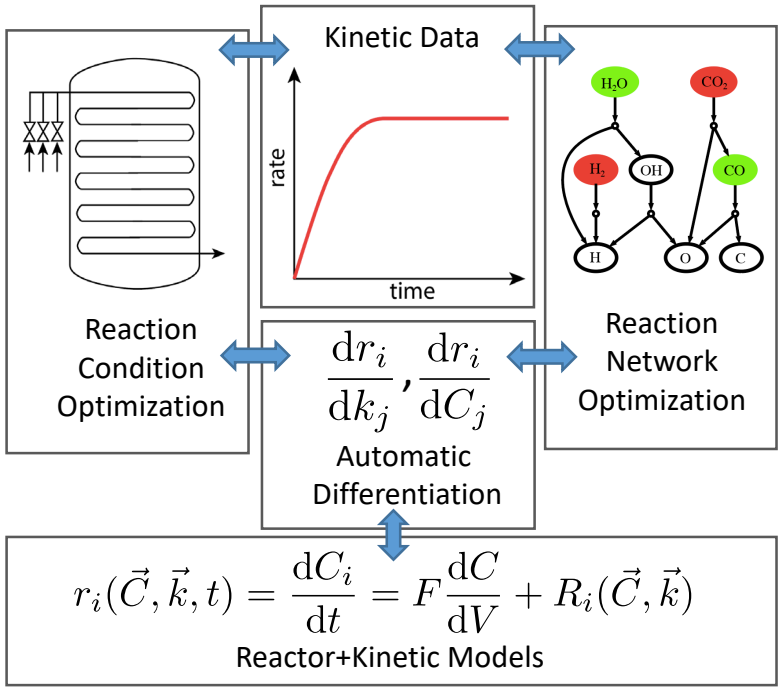
Adaptive Catalyst Testing and Optimization

Andrew J. Medford, School of Chemical & Biomolecular Engineering

Objectives: Integrate micro-kinetic models with transient and steady-state reactor models in computational frameworks that enable automatic differentiation. This will enable efficient model optimization and adaptive experimental design. A quantitative experiment-model feedback loop will provide a route to simultaneously understand the reaction mechanism and optimize the catalyst operating condition.

Concept Illustration:



Technical Approach: The platform will consist of the following components:

- A software tool to automatically generate reaction networks and corresponding kinetic models based on product and reactant specifications.
- A reactor modeling framework capable of handling stiff partial differential equations corresponding to the transient reaction-transport problem. The solver will be capable of automatic differentiation via model adjoints, enabling calculation of derivatives in linear time with accuracy limited by machine precision.
- Hardware-software interface coupling reactor/kinetic modeling software to mass-flow and temperature controllers to automatically adjust reaction composition, flow rate, and temperature.

Impact: The proposed approach will establish a route to accelerate the understanding of a catalytic reaction mechanism and optimization of operating conditions. The integration with reactor models will enable the approach to be directly coupled to reactors that can operate under industrially-relevant conditions with complex supported catalysts. This will accelerate the development and deployment of catalyst materials, and the fundamental information extracted from the micro-kinetic model will provide understanding of the fundamental catalytic mechanism and support the discovery of improved materials.