An open-source framework for the computational analysis and design of autothermal chemical processes

DE – EE0008326
Iowa State University of Science and Technology
June 1st, 2018 – May 31st, 2020

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U.S. DOE Advanced Manufacturing Office Program Review Meeting
Washington, D.C.
June 11th – 12th, 2019

Overview

Project title

An open-source framework for the computational analysis and design of autothermal chemical processes

Project timeline

Project Start Date:	June 1st, 2018
Budget Period End Date:	May 31st, 2019
Project End Date:	May 31st, 2020

Barriers and challenges

- Formulate a chemical kinetic mechanism for biomass autothermal pyrolysis
- Reduce the computational cost to perform scale-up calculations from days to minutes

AMO MYPP Connection

- Advanced sensors, controls, platforms and modeling for manufacturing
- Process intensification
- Process heating

Project budget and costs

Budget	DOE share	Cost share	Total	Cost share %
Overall budget	854,039	214,012	1,068,051	25%
Approved budget (BP-1)	466,268	116,569	582,837	25%
Costs as of 5/31/19	255,986	85,330	341,316	n. a.

Project team and roles

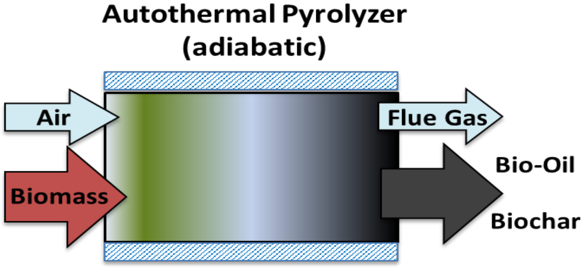
- PI: Alberto Passalacqua (CFD modeling/kinetics)
- Mark Mba-Wright (Reduced-order modeling)
- Robert Brown (Experiments on biomass pyrolysis)
- Shankar Subramaniam (Homogeneous modeling and kinetics)

Project objectives

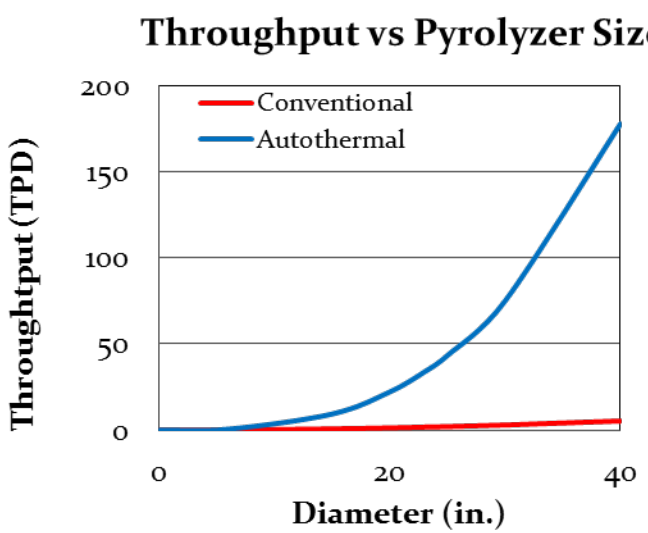
- Scale-up of biomass fast pyrolysis is limited by heat transfer constraints in the pyrolyzers.
- Autothermal biomass fast pyrolysis addresses this limitation by leveraging partial-oxidation reactions of biomass to locally generate heat inside the pyrolyzer.
- **Objective**: develop an experimentally-validated computational tool for autothermal biomass fast pyrolysis to perform design and scale-up of pyrolyzers
  - Difficulty: uncertainty in the kinetics due to partial oxidation processes
- Relevance to AMO:
  - Modeling for manufacturing
  - Process intensification

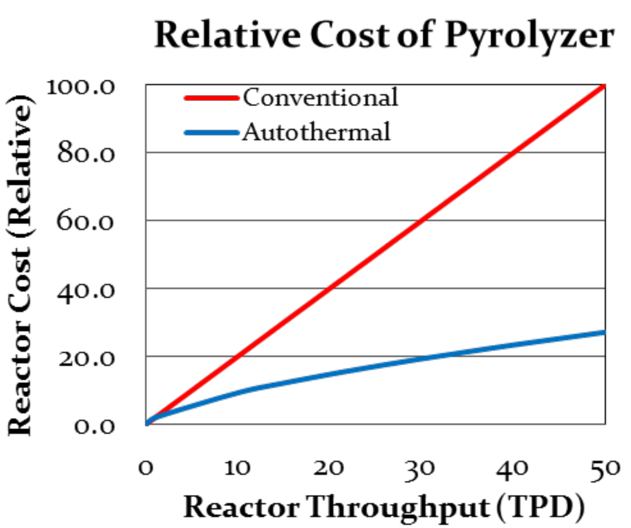
Technical innovation [1]

- Autothermal pyrolysis
  - Regular pyrolysis: heat is provided by means of heat transfer
  - **Autothermal pyrolysis**: heat is generated by an **exothermal reaction** that happens in parallel to the endothermal one



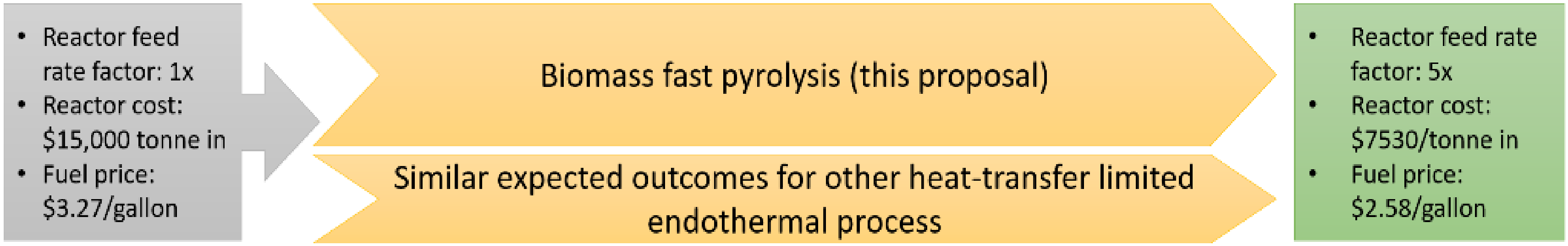
- Heat transfer only scales as **square of reactor diameter** while the energy demand for pyrolysis scales as the **cube of reactor diameter**
- Providing enthalpy of pyrolysis through partial oxidation of products (autothermal pyrolysis) **reduces size and cost of pyrolyzer** compared to a heat transfer-limited reactor





Technical innovation [2]

- Current design and scale-up heavily relies on experimental observations and empiricism
  - Difficult to explore different operating conditions
  - Complex scale-up operations
- The proposed approach will impact the design and scale-up of biomass pyrolizers
  - Systematic investigation of kinetic mechanism
  - Understanding of the role of mixing
  - Formulation of a reduced-order model for reliable scale-up, integrated in already available tools for engineering simulation (OpenFOAM, DWSIM)
  - Demonstration of the reduced-order model to scale-up an autothermal biomass pyrolizer from laboratory scale to 50-250 tpd of processed biomass
- Potential applications to other endothermic chemical processes affected by heat-transfer limitation



Technical approach [1]

- Kinetic modeling
  - Biomass devolatilization
    - Empirical model to reproduce experiments from feedstock composition
  - Char combustion
    - Verification of Langmuir kinetics
  - Gas-phase kinetics
    - Investigation of CRECK detailed mechanism to identify relevant reactions to extract a reduced mechanism for CFD
- Homogeneous modeling to investigate the role of mixing
  - PFR model (no mixing) and PaSR model (controlled mixing) with detailed chemical kinetic mechanism for the gas phase
    - Inform CFD model on the relevance of mixing modeling in the non-homogeneous model
- CFD reactive multiphase model
  - Implement polydisperse kinetic theory model for the granular phase
  - Implement reduced kinetic mechanism accounting for the relevant reactions for autothermal pyrolysis
  - Use to generate datasets to produce the reduced-order model
- Experiments to validate kinetic and CFD model
  - Evaluate kinetics of low-temperature combustion
  - Measure products obtained in a laboratory-scale pyrolizer to compare with the predictions of the CFD simulations
- Reduced order model
  - Kriging model
  - CAPE-OPEN model in DWSIM
  - Validate in scale-up of actual system to pyrolyze 50 – 250 tpd of biomass

Technical approach [2]

- ISU synergic team
  - **Alberto Passalacqua**
    - **Expertise**: development and validation of detailed Euler-Euler CFD models, uncertainty quantification and development of open-source simulation tools. Team-leader for device-scale simulation of the Center for Multiphase Flow Research and Education at ISU
    - **Role**: PI and lead of the development and application of the CFD model; contributes to the formulation of the kinetic model
  - **Shankar Subramaniam**
    - **Expertise:** particle-resolved direct numerical simulation, formulation of constitutive laws for multiphase flow, turbulence and mixing modeling. Founding and past Director of the Center for Multiphase Flow Research and Education at ISU
    - **Role**: Co-PI. Formulation of homogeneous model and investigation of mixing; contributes to the formulation of the kinetic model and identification of mixing/transport contribution
  - **Robert Brown**
    - **Expertise**: biomass pyrolysis processes and experimental techniques to collect data from these processes. Director of the ISU Bioeconomy Institute
    - **Role**: Co-PI. Experimental work to collect data for model validation; contributes to the formulation and validation of the kinetic model
  - **Mark Mba-Wright**
    - **Expertise**: formulation of reduced order-models; techno-economic analysis
    - **Role**: Co-PI. Formulation and validation of the reduced-order model

IOWA STATE UNIVERSITY
Bioeconomy Institute

Advanced Manufacturing
Energy
Sustainability & Environment
Critical Infrastructure
Health/Bio
Materials by Design
Multiphase Flow Science

CoMFRE Multiphase Flow Research

Results and accomplishments

- Project started on June 1st, 2018
- Formulated and implemented biomass kinetic model
  - Devolatilization + char combustion + gas-phase reactions
- Developed homogeneous model based on plug-flow assumption
- Extended CFD model in OpenFOAM
  - Accommodated polydisperse granular phases
  - Implemented chemical kinetics for biomass pyrolysis
- Produced experimental data for model validation
  - Devolatilization and gas-phase compositions
  - Data for comparison to CFD

Transition plan

- Source code of the model implemented into OpenFOAM will be distributed via GitHub
  - Custom repository for the project
  - Contribution to upstream version of OpenFOAM for long-term maintenance
- Models implemented in DWSIM will be
  - Released via the project GitHub repository
  - Contributed to DWSIM
- Potential for further development
  - Companies developing computational tools for engineering (CFD codes, process simulators)
  - A 50 tpd autothermal pyrolysis demonstration system is being built with private funding