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

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Overview

Timeline

Start date	End date	Project
June 1st, 2018	May 31st, 2020	2.7% complete

Budget

	FY 18 Costs	FY 19 Costs	FY 20 Costs	Total Planned Funding
DOE Funded	–	466,268	387,771	854,039
Project Cost Share	–	116,569	97,443	214,012

Barriers

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

Team

- Iowa State University Bioeconomy Institute (Brown, Mba-Wright)
- Center for Multiphase Flow Research and Education at Iowa State University - CoMFRE (Passalacqua, Subramaniam)

Project objectives

Formulate chemical kinetic model for autothermal biomass pyrolysis

- Identify and verify biomass devolatilization model
- Identify and verify suitable char combustion model
- Identify gas-phase kinetic scheme starting from CREK mechanism for biomass

Develop homogeneous model of autothermal biomass pyrolysis

- Plug-flow reactor
- Partially stirred reactor
- Inform CFD about the role of mixing and of the controlling aspect (transport or kinetics)

Develop reacting multiphase flow model for autothermal biomass pyrolysis

- Extend the existing multi-fluid solver to incorporate kinetic theory models for polydisperse granular phases and validation against literature cases
- Implement the chemical kinetic scheme for autothermal biomass pyrolysis in the CFD code

Perform experiments to generate data for model validation

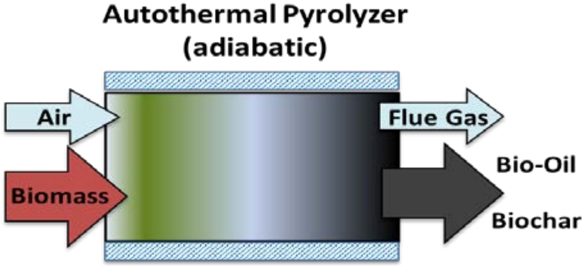
- Generate data to evaluate chemical kinetics of low temperature combustion
- Generate data to validate the complete CFD model of the fluidized bed pyrolizer

Generate reduced-order model of autothermal biomass pyrolizer

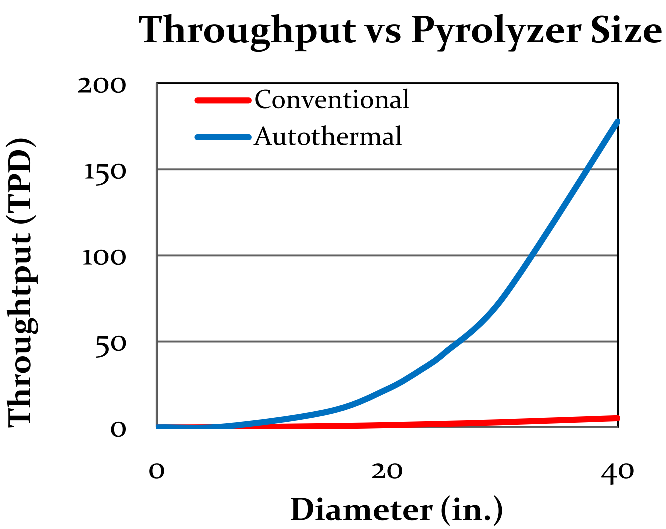
- Use the detailed CFD model to generate data to formulate the reduced-order model
- Implement the reduced-order model in DWSIM
- Demonstrate the reduced-order model to scale-up an autothermal biomass pyrolizer

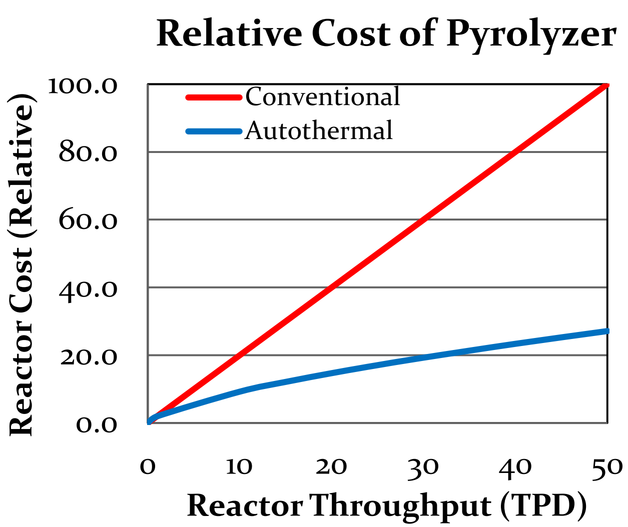
Technical innovation [1]

- 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



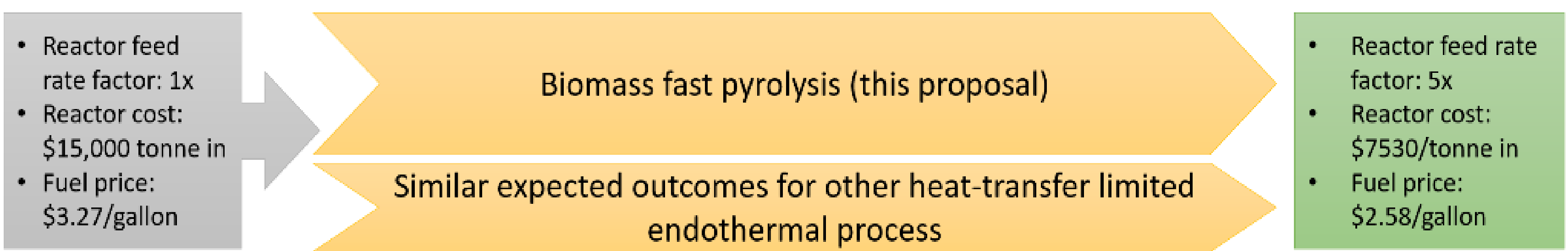
- Heat transfer only scales as **square of reactor diameter** while the energy demand for pyrolysis scales as the **cube of reactor diameter**
- Providing enthalpy of pyrolysis through partial oxidation of products (autothermal pyrolysis) **reduces size and cost of pyrolizer** compared to a heat transfer-limited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

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CoMFRE Multiphase Flow Research

Results and accomplishments

- Project started on June 1st, 2018
- Tasks to be completed
  - Year 1 (June 1st, 2018 – May 30th, 2019):
    - Kinetic modeling
      - Q1: Formulate biomass devolatilization model
      - Q3: Validate Langmuir kinetics for char combustion
      - Q4: Identify gas-phase kinetic mechanism capable of reproducing experimental measurements in autothermal biomass pyrolizer
    - Homogeneous modeling
      - Q2: Establish adequacy of plug-flow reactor model for autothermal pyrolysis
      - Q4: Establish adequacy of partially stirred reactor model for autothermal pyrolysis
    - CFD modeling
      - Q2: Extend kinetic theory model in OpenFOAM to accommodate polydisperse granular systems
      - Q3: Validate the implementation of the kinetic theory model
      - Q4: Implementation of the chemical kinetic model into the CFD model and validation against experiments (15-20% error accepted)
    - Experimental measurements
      - Q1: Modification of experimental setup
      - Q4: Produce data for validation of chemical kinetic and CFD models
  - Year 2 (June 1st, 2019 – May 30th, 2020):
    - Generation of the reduced-order model
      - Q1: Complete first batch of CFD simulations to perform
      - Q2: Implement Kringin reduced-order model (computational time of the order of seconds)
      - Q3: Implement Python reduced-order model (computational time of the order of minutes)
      - Q4: Implement CAPE-OPEN model in DWSIM (reproduces CFD results
      - Q4: Complete scale-up study of autothermal biomass pyrolizer

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)
  - Easy Energy Systems commercializes autothermal pyrolysis with plans to build a 50 tpd system

Questions