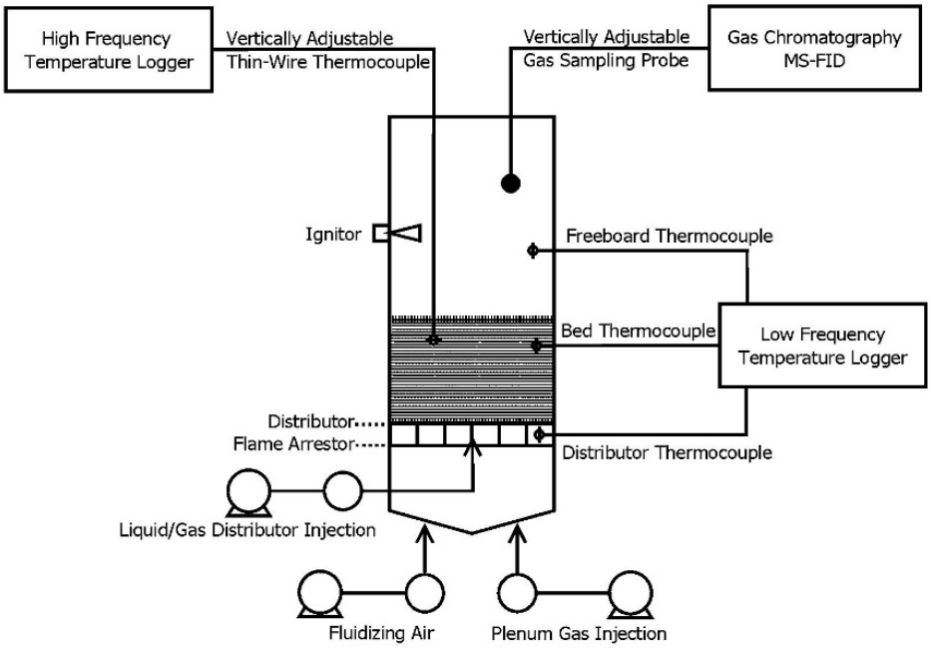
U.S. DEPARTMENT OF ENERGY

Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

An Open-Source Framework for the Computational Analysis and Design of Autothermal Chemical Processes



Schematic of gas fluidized reactor to be used to validate reaction rates for devolatilization species.

Graphic image courtesy of Iowa State University.

Chemical manufacturing and fuel refining account for a considerable portion of all U.S. manufacturing energy consumption. Providing thermal energy to these processes is often the bottleneck to reactor throughput even when chemical reactions and mass transfer are very fast. Numerous strategies have been studied to enhance heat transfer in reactors but come with significant drawbacks. These drawbacks include economic viability via increased capital cost, economy of scale for reactors, and constrained throughput. A promising way to overcome this heat transfer bottleneck is autothermal chemical processing, which balances the energy demand of endothermic chemical reactions with energy supply from exothermic chemical reactions within an adiabatic chemical reactor. There is increasing demand for advancing these processes, particularly in non-equilibrium conditions.

This project will develop software tools for simulating non-equilibrium autothermal chemical processes, seeking to improve the prospects for identifying and designing such systems. These tools will be developed and validated in simulating autothermal pyrolysis, a process recently developed at an in-house pilot-scale plant. The project will begin by formulating and developing the chemical kinetic model for a specific application; in this case, autothermal biomass pyrolysis in chemical reactors. These results will be used to develop a reacting multi-phase flow model, and experiments will be performed to assist with model validation. The team will then generate a reduced-order model for an autothermal biomass pyrolyzer.

Benefits for Our Industry and Our Nation

The computational tools for autothermal chemical processes under development are expected to have significant impacts in sectors requiring extensive process heating, particularly chemical and fuel production. Using state-of-the-art computational tools for autothermal pyrolysis are expected to have numerous benefits in chemical and fuel manufacturing, including:

- Increased product feed rate up to a factor of 5 in autothermal biomass fast pyrolysis which corresponds to a reduction of the reactor, operation costs, and fuel production costs
- Rational design pathways for other autothermal chemical processes, based on a priori knowledge of the conditions under which autothermal operation achieves the desired outcomes

Applications in Our Nation's Industry

The computational tools for autothermal chemical processes are expected to have multiple benefits to chemical and fuel manufacturing industries. These computational tools will provide an open-source framework to analyze and design autothermal chemical processes, while emphasizing biomass pyrolysis as an example. This framework will enable future developments in investigating significant advancements in other autothermal processing of gas-solid reactions, and multi-phase processes.

Project Description

The project objective is to formulate, develop, and validate computational tools for autothermal chemical processes in a pilot-scale reactor. This project aims to determine and experimentally validate a reduced-order model by first developing three different models to investigate autothermal biomass pyrolysis: a kinetic model for biomass devolatilization, char combustion and gas-phase kinetics;

a homogeneous model for mixing in plug-flow, and partially stirred reactors; and a reactive multi-phase model using computational fluid dynamics (CFD). The project outcomes address the heat transfer and reactor economy of scale challenges by generating a reduced-order model for developing future autothermal biomass pyrolyzers.

Barriers

- Formulating a chemical kinetic mechanism for biomass autothermal pyrolysis
- Reducing the computational cost and associated time to perform scale-up calculations from days to minutes

Pathways

The project is structured to address the key barriers and minimize risk. The ultimate goal is to develop a reduced-order model that supports the scale up of an autothermal biomass pyrolyzer for chemical and fuel production.

The first project pathway will formulate and develop three separate models for autothermal biomass pyrolysis processes. The first model is a chemical kinetics model, which identifies and verifies suitable conditions for biomass devolatilization, char combustion, and gas-phase kinetics of biomass. The second is a homogeneous model for a plug-flow reactor and partially stirred reactor to determine appropriate mixing conditions and subsequent control. These two models inform the third model, which is a CFD-based reacting multi-phase flow model, to incorporate chemical kinetic theories for multi-fluid solvers. This is then used to implement a chemical kinetic scheme for autothermal pyrolysis in the CFD code.

The second pathway includes the conduct of experiments to generate data for model validation. A pilot-scale fluidized bed pyrolyzer will be used to generate the required data for model validation. This data will be used to evaluate chemical kinetics of low temperature combustion, and validate the completed CFD model of the pilot-scale reactor. The pilot-scale reactor was previously assembled onsite to be utilized for these experiments.

The third pathway will generate the final computational tool using the pilot-scale reactor: a reduced-order model for autothermal pyrolysis. The CFD model will be used to generate the data needed to formulate the reduced-order model, given the multi-phase model and the experimental results. The reduced-order model will then be implemented and validated to support the scale-up of an autothermal biomass pyrolyzer.

Milestones

This three-year project began in June 2018.

- Chemical kinetic model is sufficient to describe autothermal biomass fast pyrolysis and perform the CFD simulations required to formulate the reduced-order model (Completed)
- Reduced order model is validated, enabling the completion of the autothermal biomass pyrolyzer scale-up study (2020)

Technology Transition

Iowa State University will utilize two internal entities to support this project; the Iowa State University Bioeconomy Institute will collaborate with the Iowa State Center for Multiphase Flow Research and Education (CoMFRE) to develop software tools for simulating non-equilibrium autothermal processes. Following successful development, the project team plans to implement the model's source code into a leading open-source package for numerical simulation known as OpenFOAM. The team plans to distribute the customized source code, along with providing longer-term contribution to OpenFOAM version maintenance, via the GitHub online hosting repository. Iowa State anticipates further development of the model by promoting it to companies developing computational tools, and assisting the commercialization of autothermal processes. To support the latter, the team also plans to work with Easy Energy Systems, a company that has previously licensed technology from Iowa State, to advance commercial development.

Project Partners

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