Boulder Fluid Dynamics Seminar Series

Tuesday, February 4, 2014
3:30pm-4:30pm (refreshments at 3:15pm)
Bechtel Collaboratory in the Discovery Learning Center (DLC)
University of Colorado at Boulder

Hybrid CFD/DSMC and Big Science (Subtitle: Chemists Don't Know Much about Fluids)

John W. Daily and Qi Guan, *University of Colorado at Boulder*

We collaborate with a bunch of chemists to study pyrolysis reactions of large oxygenated biomolecules of importance in biomass gasification chemistry. The experiments are carried out in small tubular reactors and the products analyzed using Photoionization Mass Spectrometry (PIMS) and Matrix Isolation/IR spectroscopy. For many of the PIMS experiments, we utilize photons from the Lawrence Berkeley National Laboratory Advanced Light Source, hence Big Science. To recover kinetic information from the data requires knowing the residence time distributions and temperature time histories for the reactants. As a result, we have to rely on flow simulations. Because of the small diameters, 0.5 to 1 mm, it is extremely difficult to make measurements of flow field properties other than mass flow rate (controlled), inlet and outlet pressures and wall temperature. The complicating factor is that the diagnostics require high vacuum, and thus the reactor flow exits into a chamber at about 10^{-4} torr. Depending on the boundary conditions the flow in the reactor can range from mostly continuum to transitional, with the exhaust forming either a supersonic jet that rapidly transitions to free molecular flow or an effusive flow. For most of the data taken to date the downstream portion of the reactor seems to display slip at the walls even at the highest mass flow rate we can run. Therefore, we have been working on developing a coupled CFD/DSMC code. The CFD code is a 2D multi-block structured finite volume code for compressible flow with Roe flux scheme and LU-SGS time marching method. The DSMC code is based on the methods of Bird with 2D multi-block data structure and VHS collision model. The hybrid codes are coupled using a state-based method. In the seminar we will give an overview of the biomass project and present some simulation results.

Computational modeling of dilute biomass slurries

Michael Sprague, *National Renewable Energy Laboratory*

The biochemical conversion of lignocellulosic biomass to liquid transportation fuels involves a multitude of physical and chemical transformations that occur in several distinct processing steps (e.g., pretreatment, enzymatic hydrolysis, and fermentation). In this work we focus on development of a computational fluid dynamics model of a dilute biomass slurry, which is a highly viscous particle-laden fluid that can exhibit yield-stress behavior. Here, we model the biomass slurry as a generalized Newtonian fluid that accommodates biomass transport due to settling and biomass-concentration-dependent viscosity. Within a typical mixing vessel, viscosity can vary over several orders of magnitude. We solve the model with the Nek5000 spectral-finite-element solver in a simple vane mixer, and validate against experimental results. This work is directed towards our goal of a fully coupled computational model of fluid dynamics and reaction kinetics for the enzymatic hydrolysis of lignocellulosic biomass.