PRF #56386-DNI9

Pore-Resolving Simulations of Coal Char Gasification Using Micro-CT Imaging

PI: Simcha Singer, Marquette University

Introduction

The goal of this research is to understand the impact of realistic char particle morphology on gas transport and heterogeneous reaction during coal gasification. Because char particles contain a wide range of pore sizes, with the largest pores/voids often approaching the scale of the particles themselves, modeling char particles as effective porous media (an effective-continuum) is not appropriate. To understand the influence of realistic pore morphology on the transport-reaction coupling during gasification, a pore-resolving CFD simulation approach based on micro-CT developed during Year 1. During the Year 2, the CFD simulation was refined and analysis of the results yielded fundamental insight on the impact of realistic pore structures on transport/chemistry interactions. Additionally, during the second year of work, smaller, industrially-relevant pulverized coal char particles were pyrolyzed at higher heating rates and imaged using a high-resolution micro-CT, and statistical analysis of many coal char particles was performed.

Simulation Results and Analysis

To study the impact of void morphology on coal char gasification, the two transient CFD models described in the Year #1 report were employed: a three-dimensional, pore-resolving simulation based on micro-CT imaging and a corresponding classical, spherically-symmetric, effective-continuum model. Velocity fields (due to Stefan flow) within and around the respective particles are shown in Fig. 1, illustrating that the irregular morphology of real particles induces asymmetric and irregular flow patterns, with local maxima observed within the voids due to channeling.

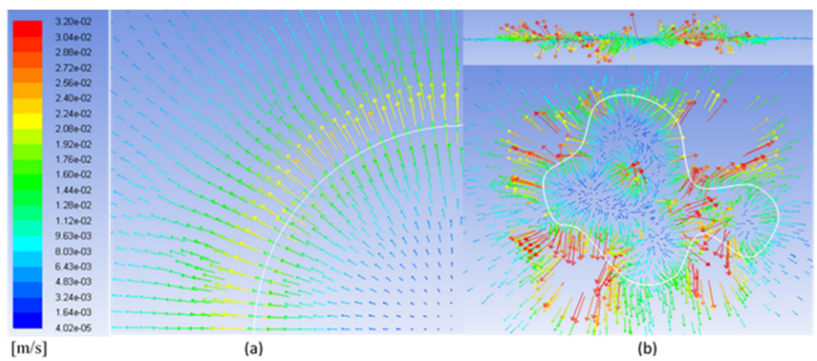

Figure 1. Velocity vector field at 25 ms: (a) effective-continuum model, and (b) pore-resolving model, with a second view in a plane orthogonal to the first (top inset).

Reactant (H_2O) mole fraction is plotted as a function of nominal particle radius in Fig. 2. For the spherically-symmetric, effective-continuum model, the data was simply taken along the particle's axis, while radial profiles for the three-dimensional, pore-resolving model were obtained by averaging over azimuthal and polar directions at every radial position. Figure 2 shows that the pore-resolving model's reactant mole fractions ("3D") were always higher throughout the particle than effective-continuum predictions ("2D). This is partially because the resolved voids serve as channels that enhance reactant transport throughout the particle. Furthermore, the enhanced reactant concentration within the voids acts to decrease the characteristic length-scale for diffusion within the microporous solid grains. Whereas the characteristic length for diffusion in an effective-continuum representation is the radius of the entire particle, the true characteristic length for diffusion is closer to the local thickness of a microporous char grain, which separates voids containing reactant at concentrations not dissimilar from the particle exterior. The contribution of this second, less-obvious mechanism is demonstrated by comparing profiles averaged over all regions ("3D") with those averaged only within the microporous solid regions ("3DMPS"). Even within the microporous solid regions of the pore-resolving model, the reactant concentrations are significantly higher than effective-continuum predictions, even though the microporous grains

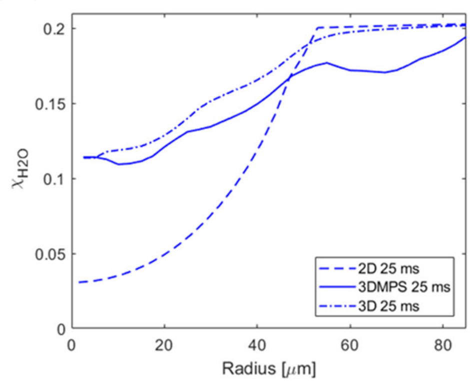

Figure 2. Polar and azimuthally-averaged H_2O mole fractions as a function of radius for the effective-continuum model (2D), the pore-resolving model averaged only over the microporous solid regions (3DMPS), and the pore-resolving model averaged over the resolved voids and microporous solid (3D).

have lower porosity, and thus lower effective diffusivity, than the porous char in the effective-continuum model. This establishes the fundamental importance of the reduced characteristic length for diffusion in realistic coal char.

Higher Resolution Imaging

Pulverized-sized Illinois #6 bituminous coal was pyrolyzed in an electrically heated furnace to produce char particles (~100-150 µm post-pyrolysis). The higher-resolution micro-CT employed in Year 2 was able to resolve the internal and external structure of individual particles (an example is shown in Fig. 3(a)) with resolution better than 2 µm. Image processing and segmentation of the particles revealed pores and voids (blue), microporous char (red) and mineral inclusions (orange), shown in Fig. 3(b).

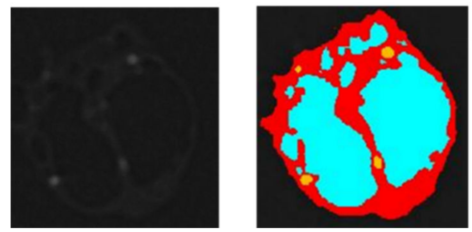

Figure 3. (a) 2-D section of a reconstructed coal char particle (~150 µm) from micro-CT, (b) segmented into microporous char (red), pores (blue) and mineral inclusions (orange).

Morphological Analysis

Three-dimensional morphological analysis based on high-resolution micro-CT was performed for an ensemble of coal char particles for the first time, with the goal of determining whether parameters affecting the interplay of transport and reaction exhibit similarities across a range of particles. Fifty coal char particles with resolved (macro-)pore volumes ranging from 10-60% were analyzed. The distribution of each particle's macro-porosity as a function of radius is shown in Fig. 3, with the total volume of each particle (including pores and solid) normalized to correspond to that of a sphere of radius 50 µm and the total macro-porosity normalized to be identical for each particle. It is observed that the distribution of normalized macro-porosity nearly collapses to a single line, especially between radii of 20–60 µm, where most particle volume is contained.

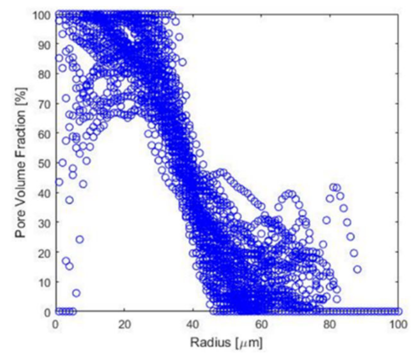

Figure 4. Distribution of normalized macro-porosity with radius.

The thickness of the microporous char regions within realistic particles was also examined using image analysis software, given the importance of the char grain thickness inferred from Fig. 2. For each particle, char "wall" thickness was measured by sampling eighteen two-dimensional slices from a three-dimensional rendering, with six from each unique plane. Each slice then takes measurements of particle wall thickness in eight directions extending from the particle's center of mass and returns the average char thickness (because multiple char regions may be encountered along each line). The mean and standard deviation was determined based on all sampled directions for each particle. Figure 5 shows the average wall thickness as a function of the particle's macro-porosity, as well as a statistical regression line. The linear regression falls within a majority of the particle's confidence intervals, leading to the conclusion that average thickness of char regions in a particle varies nearly linearly with macro-porosity for this coal char.

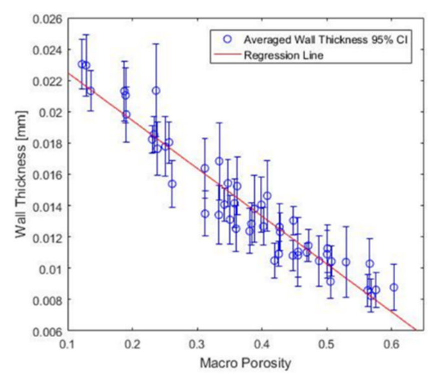

Figure 5. Average char grain ("wall") thickness as a function of particle macro-porosity.

Impact of research

A journal article describing the micro-CT-based pore-resolving simulation approach and analysis was published in *Fuel* in 2018. A conference paper was written and presented at the 2018 Central States Section meeting of the Combustion Institute, and a poster was presented at the International Combustion Symposium in 2018. A journal article is being prepared describing the morphological analysis outlined above and its connection to the interplay of transport and heterogeneous reaction.

The research funding provided by the ACS Petroleum Research Fund enabled the PI to pursue a research approach with promise for a variety of solid fuel applications. The funding also enabled the PI to increase the size of his research group and was used to support graduate students during both years of the project. Both students became proficient in CFD and image analysis. The first student obtained a Master's degree in 2017 and the second is expected to graduate in 2019. The research formed the basis of the preliminary work for the PI's recently submitted NSF CAREER proposal.