Application of computational multiphase flow to fossil fuel industry

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The following are some of the challenges to overcome to achieve the goal of this workshop:

Speed of computations: The detailed physics based models take much computational time. For example, a detailed gasifier model based on a gas-solids continuum model may require up to a week of computational time. There is a need for better computational algorithms, parallelization techniques, and model reduction strategies to reduce the computational time. Perhaps a desirable goal is to have the capability to do such detailed calculations in a few hours of computational time. For being able to use the information from such models in process simulation, it is necessary to further reduce the computational time to several minutes.

Accuracy of the models: There are issues with the accuracy of the physical models and the numerical techniques. For the physical models it is desirable to have a good way to characterize the drag and granular stresses in a polydispersed gas-solids system. The standard drag formulas have 5-20% error, which makes their use in detailed models undesirable. It appears that there is no way to obtain an accurate, universal drag law. A possible path would be to develop custom drag formulas for a given coal powder from either standard experiments or detailed simulations (discrete element or lattice Boltzmann) or a combination of both. It is desirable to develop the ability to transfer information from detailed models (e.g., discrete element) to averaged models (e.g., continuum) in an automatic manner. Also we need standard experimental methodology for determining the gasification/combustion kinetics for different coal powders. We also need ways for correcting drag and heat transfer formulas to account for the effect of mass transfer due to coal devolatilization, gasification and combustion.

There is a need to develop stable and accurate high resolution discretization techniques for multiphase flows. It is desirable to develop estimates for the error in detailed calculations and to develop the means to assure that the solutions obtained are truly grid-independent. It is necessary to develop an exhaustive test suite to verify and validate detailed computational codes.

Postprocessing of output: Detailed models already generate massive amounts of data. By 2015 the amount of data generated will be even much more. Postprocessing techniques should be developed to enable the computational engineers to digest the data, extract useful features from the data, and communicate that information to design engineers.

Outreach to design engineers: For the computational tools to ultimately make an impact on the design of future powerplants, it is essential that the information from the models is conveyed in a manner useful to the design engineers. Many of the current generation of the design engineers are not well versed in the use of detailed computational models. Likewise many of the computational scientists work without much knowledge of the needs of the design engineers. The future engineers must be trained so that there is no communication problem between design engineers and computational engineers. The computational engineers should work on making the information from detailed simulations accessible by design engineers. There should be an effort to make industrial users aware of the use of computational models for their design applications.