HIGH RESOLUTION SIMULATIONS OF COAL JETS IN A GASIFIER

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Summary

A continuum multiphase flow model that considers gas and solids as interpenetrating continua (in the open-source code MFIX) is used to model a coal gasifier. To be predictive, the model needs to consider the spatiotemporal variations in gas and solids volume fractions, velocities, temperatures with any associated phase change and chemical reactions. These processes occur at various time- and length-scales requiring very high spatial resolution and large number of iterations with small time-steps. We performed a high resolution simulation of the gasifier employing thousands of processors on a high performance computer, to reveal new features of the coal jet trajectory.

Keywords

Complex reacting flows; Multiphase and particulate reactors; Clean coal/heavy oil/frontier resources/biomass processing technologies; CO_2 capture, utilization and sequestration.

Introduction

Integrated Gasification Combined Cycle (IGCC) is a promising technology for meeting the growing demand for power using fossil fuel resources, while economically controlling the emission of CO_2 and other pollutants. The centerpiece of an IGCC system is the gasifier, which converts coal or other carbonaceous materials such as biomass into syngas, a mixture of CO and H_2. The syngas can be used for the production of liquid fuels and chemicals or for power generation. In an IGCC system the syngas is shift converted into a mixture of CO_2 and H_2, CO_2 is captured and stored, and H_2 is used for power generation.

A reliable gasifier is critical for the commercial viability of IGCC. The gas-solids multiphase flow such as occurring in the gasifier is known to make the design of commercial-scale units using traditional scale-up methods unreliable[1]. To address that challenge, Multiphase computational fluid dynamic (CFD) models are being developed and applied for gasifier design at National Energy Technology Laboratory (NETL).

The validation of the NETL gasifier model with data from pilot-scale facility has been reported before[2]. The results showed not only agreement with existing measurements but also unexpected physical phenomena that were validated with measurements made after the predictions. For example, the simulations showed that oxygen reached the upper region of the mixing section in a pilot-scale transport gasifier contrary to the expectation that that all the oxygen would be consumed in the lower region where the air is mixed with the hot, recycled char. This prediction was later validated with measurements of oxygen concentration.

The validated model was then used to help with the design of a Clean Coal Power Initiative (CCPI) gasifier (285 MW electric), which was scaled up from the pilot-scale gasifier (13 MW thermal), representing a factor of 50 scale-up. The multiphase CFD simulations were used to study the effect of pressure, the height to diameter ratio, coal feed rate, coal feed nozzle operation, solids circulation rate, and the effect of recycled syngas. Several sets of parametric evaluations showed an unexpected dependence of the gas species concentrations and solids temperature upon the coal jet penetration. High solids temperature could cause unwanted agglomeration and refractory degradation and have a significant impact on gasifier reliability.

This result generated interest in conducting simulations of the CCPI gasifier at greater grid resolutions. A INCITE grant from DOE Office of Science is allowing the group to conduct CCPI gasifier simulations at greater grid resolution than was previously possible. This paper describes the preliminary computational results from the high resolution simulations.

Coal Gasifier Model

Gas-solids flows such as occurring in coal gasifiers are one of the highly non-linear processes observed in natural and man-made devices. To be predictive, the simulations need to model the spatiotemporal variations in gas and solids volume fractions, velocities, temperatures with any associated phase change and corresponding chemical reactions. These processes occur at various time- and length-scales requiring very high spatial resolution and large number of iterations with small time-steps. In the continuum modeling approach used in this study the coal particles are represented as a granular phase, which co-locates with the gas phase to form a multiphase mixture, the volume fraction giving the amount of phase *m* at each spatial location. The multiphase CFD model consists of the mass, momentum, energy, and species-mass balances for each phase, gas or solids[3]. These equations are solved using a finite volume technique available in the open source code MFIX (http://mfix.netl.doe.gov).

For modeling coal gasifiers, the chemical reaction rates and heats of reaction are supplied through the module carbonaceous chemistry for computational modeling (C_3M) developed by NETL. C_3M represents the gas phase composition with eight species (O_2, CO, CO_2, CH_4, H_2, H_2O, N_2, and Tar) and the solids phase (coal/char) composition with four pseudo-species (fixed carbon, volatile matter, moisture, and ash). Ash does not take part in any reactions, moisture is released in an initial stage reaction, and the volatile matter produces several gas-phase species through devolitization. The gas phase reactions are tar decomposition, water gas shift reaction, and combustion of H_2, CH_4, CO. The heterogeneous reactions are char combustion and gasification.

The model described in the previous section was developed at NETL over last two decades and was recently ported to high performance computer (HPC) platforms. The results presented in this paper are from the simulations conducted on the HPC platform Jaguar at the National Center for Computational Sciences, currently world's fastest super computer (http://www.nccs.gov/). Extensive profiling of MFIX was conducted on HPC platforms using standard benchmark cases that scaled up to 10 million cells on 6032 cores, to determine the computational bottlenecks. For running efficiently on HPC platforms, MFIX was improved in several phases[4].

Results of High Resolution Simulation

Figure 1 shows the motion of the coal jet at a particular instant of the simulation. The plot was created by running a 60 x 450 x 90 cells simulation with high-order discretization and using as boundary condition data from the 10M cells run. Comparison of the results of low (1 million cells) and high (10 million cells) resolution simulations shows that the coal jet tends to move away from the wall to a greater extent in the high resolution case than in the low resolution case. The differences in the simulation results at the two resolutions have practical implications for the gasifier design. For example, the trajectory of the coal jet could have significant effect on the gasifier reliability. A coal jet trajectory closer to the wall could lead to greater erosion of the refractory. So the low resolution simulation would predict a shorter refractory life than the high resolution simulation. Given that it is not currently feasible to conduct high resolution simulations for all the design cases, it remains to be determined how a few high resolution simulations could be combined with a large number of low resolution simulations to help with the design.

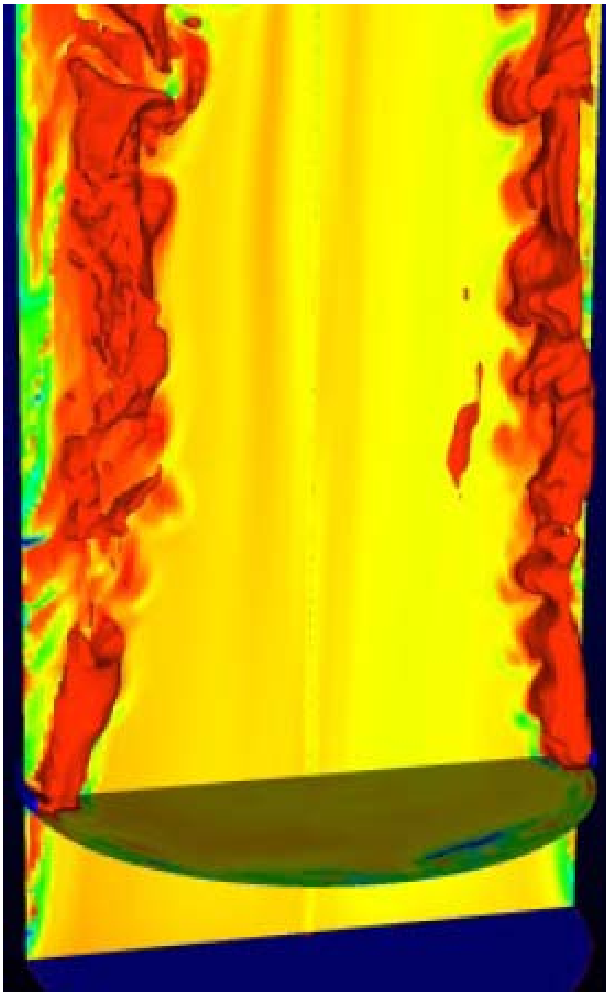

Figure 1. Highly resolved view of a coal jet, iso-surfaces show the solids volume fraction

References

(1) Report on Workshop on Multiphase Flow Research, Morgantown, WV, June 6-7, 2006, DOE/NETL-2007/1259, http://tinyurl.com/c9r7ux

(2) Guenther C, Syamlal M, Longanbach J, and Smith P, "CFD modeling of a transport gasifier Part II", Proceedings of the 20th Annual Pittsburgh Coal Conference, Pittsburgh, PA, September 15-19, 2003.

(3) Benyahia S, Syamlal M, and O'Brien T J, "Summary of MFIX Equations 2005-4," March 2006, http://www.mfix.org/documentation/MfixEquations2005-4-1.pdf.

(4) M. Syamlal, C. Guenther, A. Gel, S. Pannala, "Advanced Coal Gasifier Designs Using Large-Scale Simulations," *Journal of Physics*: Conference Series 180 (2009) 012034 doi:10.1088/1742-6596/180/1/012034.