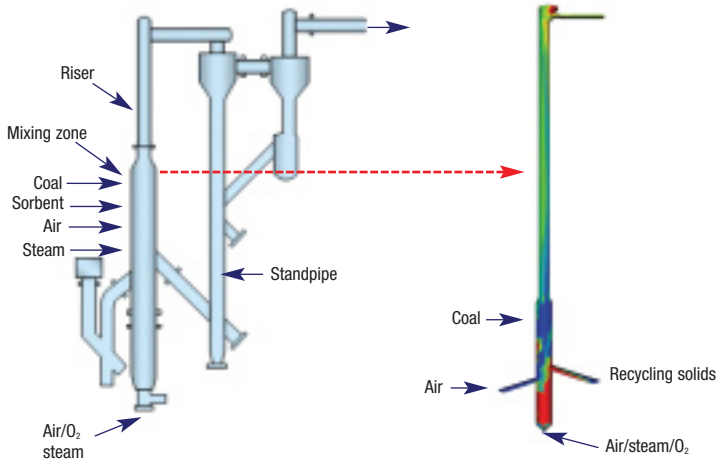
Gassing Up with Coal

A two-fluid multiphase model allows for more accurate simulation of coal gasification.

By Christopher Guenther, U.S. Department of Energy, National Energy Technology Laboratory West Virginia, U.S.A., and Shaoping Shi and Stefano Orsino, ANSYS, Inc.



PSDF gasifier schematics (left) and an exploded view of the mixing zone (right) colored by contours of CO fraction

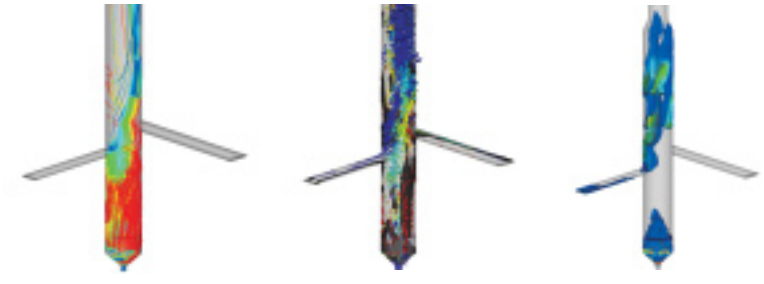
The technology of coal gasification has existed since the early 19th century. Prior to the discovery of natural gas, coal was used to produce so-called "town gas" for lighting and heat in cities across the United States and Europe. Specifically, the gasification process is used to convert any carbon-containing material into a synthesis gas, or syngas. Syngas contains mostly carbon monoxide (CO), carbon dioxide (CO_2) and hydrogen (H_2) and can be used as a fuel to generate electricity or as a basic chemical building block for a large number of applications in the petrochemical and refining industries. Gasification thus adds value to low-rank coal feedstocks by converting them into marketable fuels and products. Due to more recent technological advances, gasification offers one of the most efficient and cleanest ways to convert the energy content of coal into electricity, hydrogen, methanol and other usable forms.

Based on the mode of conveyance of the coal and the gasifying medium, gasifiers can be classified into fixed- or moving-bed, fluidized-bed, and entrained-flow reactors. Entrained-flow gasifiers are normally dilute-flow with small particle sizes and have been successfully modeled with computational fluid dynamics (CFD) using the Euler–Lagrange, or discrete phase, model approach [1]. For fluidized-bed gasifiers however, Eulerian–Eulerian (E-E), or two-fluid multiphase, model is the most appropriate approach. The E-E model treats the solid phase as a distinct interpenetrating granular "fluid" and is the most general-purpose multi-fluid model.

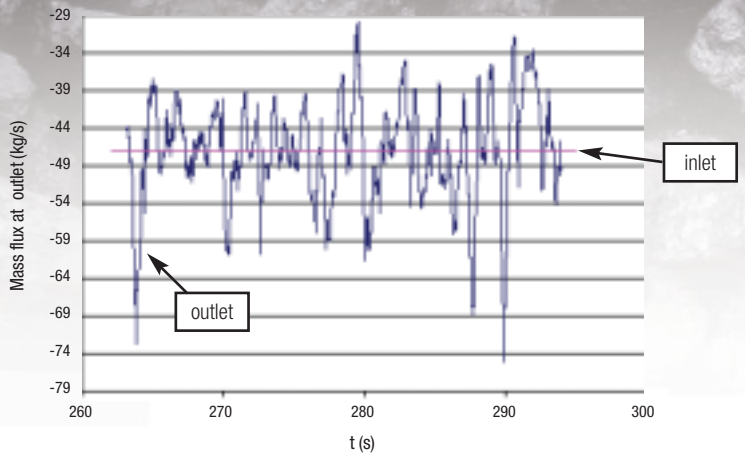
Transport gasifiers are based on circulating fluidized–bed (CFB) reactor technology and have the ability to achieve higher throughput, better mixing, and increased heat and mass transfer rates compared to other conventional technologies. CFB reactors have been an established technology in the chemical and power generation industries for years. However, new reactor designs to improve performance, reliability and safety have been slow to emerge due primarily to the lack of understanding of the complex hydrodynamics of the gas and solid phases.

The idea of describing fluidized beds and CFBs with two-fluid hydrodynamic models has existed since the early 1960s [2]. Even with today's powerful computers, numerical solutions of large-scale CFBs are rarely found in the literature, and even fewer that consider 3-D solutions [3]. Fortunately, the E-E modeling approach is one that can help researchers understand the complex interactions between the gas and solid phases and aid engineers in the design of new reactors. This approach can provide detailed 3-D transient information inside the reactor that otherwise could not be obtained through experiments due to the large scale, high pressures and high temperatures involved.

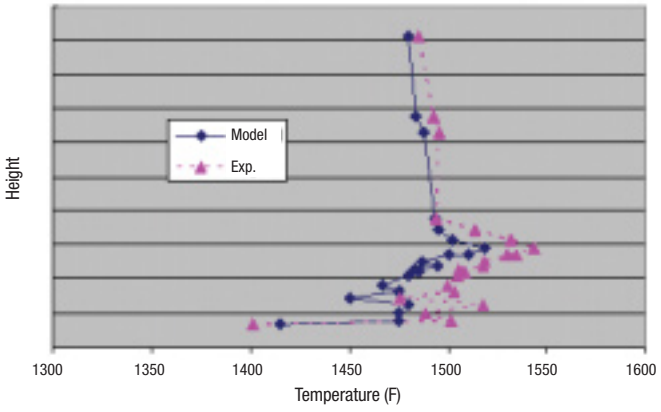
To gain more insight into the process phenomena, ANSYS teamed with the U.S. Department of Energy's National Energy Technology Laboratory (NETL) to develop different CFD models for simulating coal gasification applications.



Visualizations of the flow in the mixing zone of the PSDF gasifier for a case with air-blown and steam-enhanced lignite fuel. Included are flow pathlines colored by CO fraction (left); velocity vectors on isosurfaces of solid fraction of 0.2 and 0.3, in which the formation of particle clusters can be seen (center); and contours of carbon reaction rate (right).

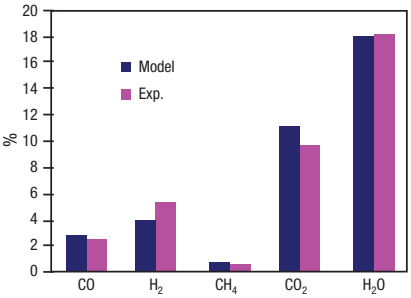


Fluctuations of the mass flux (including both solid and gas) at the gasifier outlet. The negative value represents the outgoing flow at the outlet. The magnitude of these fluctuations can deviate by as much as 70 percent around the mean of –47.12 kg/s.



Time-averaged temperature distribution along the PSDF center line as compared to experiment

Their objective was to illustrate how CFD can be used for complex large-scale geometry with detailed physics and chemistry. Using FLUENT software, the team developed a 3-D transient model of KBR, Inc.'s Power Systems Development Facility (PSDF) transport gasifier. KBR is a global engineering, construction and services company that has partnered with other companies to build a commercial transport gasification unit, based on the technology developed from the PSDF, at a 285-MW power generation facility in Florida that promises to be the cleanest coal-fueled plant in the world.



Outlet gas composition for the PSDF transport gasifier as compared to experiment

In the FLUENT simulation of the PSDF, 11 species were included in the gas phase while four species were assumed to be in the solid phase. A total of 16 reactions, both homogeneous (involving only gas phase species) and heterogeneous (involving species in both gas and solid phases), were used to model the coal gasification chemistry. The gas combustion reactions were simulated with a finite-rate combustion model. The coal reactions, including moisture releasing, devolatilization, char combustion, char gasification, tar cracking and water–gas shift reactions, were modeled with a heterogeneous reaction scheme and a set of user-defined functions. The geometry was meshed with 70,000 cells, and each simulation case was run in parallel on an eight-processor machine. Post-processing the data was done once the solution reached a pseudo-steady state, which required running the simulation until it generated physical data representing about 40 seconds of time.

The basic design of the PSDF transport gasifier included a mixing zone, which kept the recycling solids present long enough for the carbon left in the particles to react with the incoming gas (O_2, steam or CO_2). Visualizations of the system interior showed that the flow was recirculating and mixing in the mixing zone before it moved up into the riser section, and also that local conditions were very chaotic and turbulent. At the bottom of the mixing zone, combustion of the carbon present in the recycle material depleted the available O_2. Further combustion occurred as the solids moved up higher into the mixing zone. At the same time, other reactions such as CO and H_2 combustion were competing for the O_2. These exothermic reactions generated the necessary heat for the endothermic reactions, including steam gasification and CO_2 gasification of carbon.

The research team validated the overall computational results against PSDF experimental data for both bituminous and sub-bituminous coals under both air-blown and oxygen-blown conditions. The computational difference between the mass flux at the inlet and average mass flux at the outlet was only 0.1 percent, which meant that the mass was balanced well from the simulation standpoint. The team drew the same conclusion for the heat balance. For the temperature profile, the difference between the simulation and measurement was due mainly to the location of the probes relative to the center line. Despite the finding of very uneven temperature distributions at any given cross section, the overall trends of the temperature profiles were in good agreement with the measured data. ■

References

[1] Shi, S.; Zitney, S.; Shahnam, M.; Syamlal, M.; Rogers, W., Modeling Coal Gasification with CFD and the Discrete Phase Method, 4th International Conference on Computational Heat and Mass Transfer, May 2005, Paris.

[2] Davidson, J., Symposium on Fluidization — Discussion, *Trans. Inst. Chem. Eng.*, 1961, 39, pp. 230-232.

[3] Guenther, C.; Syamlal, M.; Shadle, L.; Ludlow, C., A Numerical Investigation of an Industrial Scale Gas–Solids CFB, *Circulating Fluidized Bed Technology VII*; Grace, J.; Zhu, J.; de Lasa, H., Eds.; CSCHE, Ottawa, 2002, pp. 483-488.