The Power Systems Development Facility
Wilsonville, Alabama

TRANSPORT GASIFICATION

DOE announced the Orlando project in October 2004 as part of its Clean Coal Power Initiative. They selected the Southern Company, an Atlanta-based energy company, along with Orlando Utilities Commission, to build the $557 million venture, for which DOE is contributing $235 million. Houston-based KBR and Southern Company are responsible for engineering.

The 285-megawatt plant is based on a technology called "transport gasification," invented and bench-scale tested by KBR in the early 1990s. For further development, the project team relied on a pre-commercial-scale plant — the Power Systems Development Facility (PSDF) — in Wilsonville, Alabama, built by Southern Company and DOE in the mid-1990s to evaluate and commercialize advanced coal-based power technologies. With the PSDF, engineers are able to adjust operating conditions of systems being evaluated, to learn what works and what doesn't. For the transport gasifier, to reduce the trial-and-error guesswork and gain improved understanding of the physics and reaction chemistry, PSDF engineers worked closely with a NETL computational modeling team, the Device Scale Modeling Group, led by Chris Guenther.

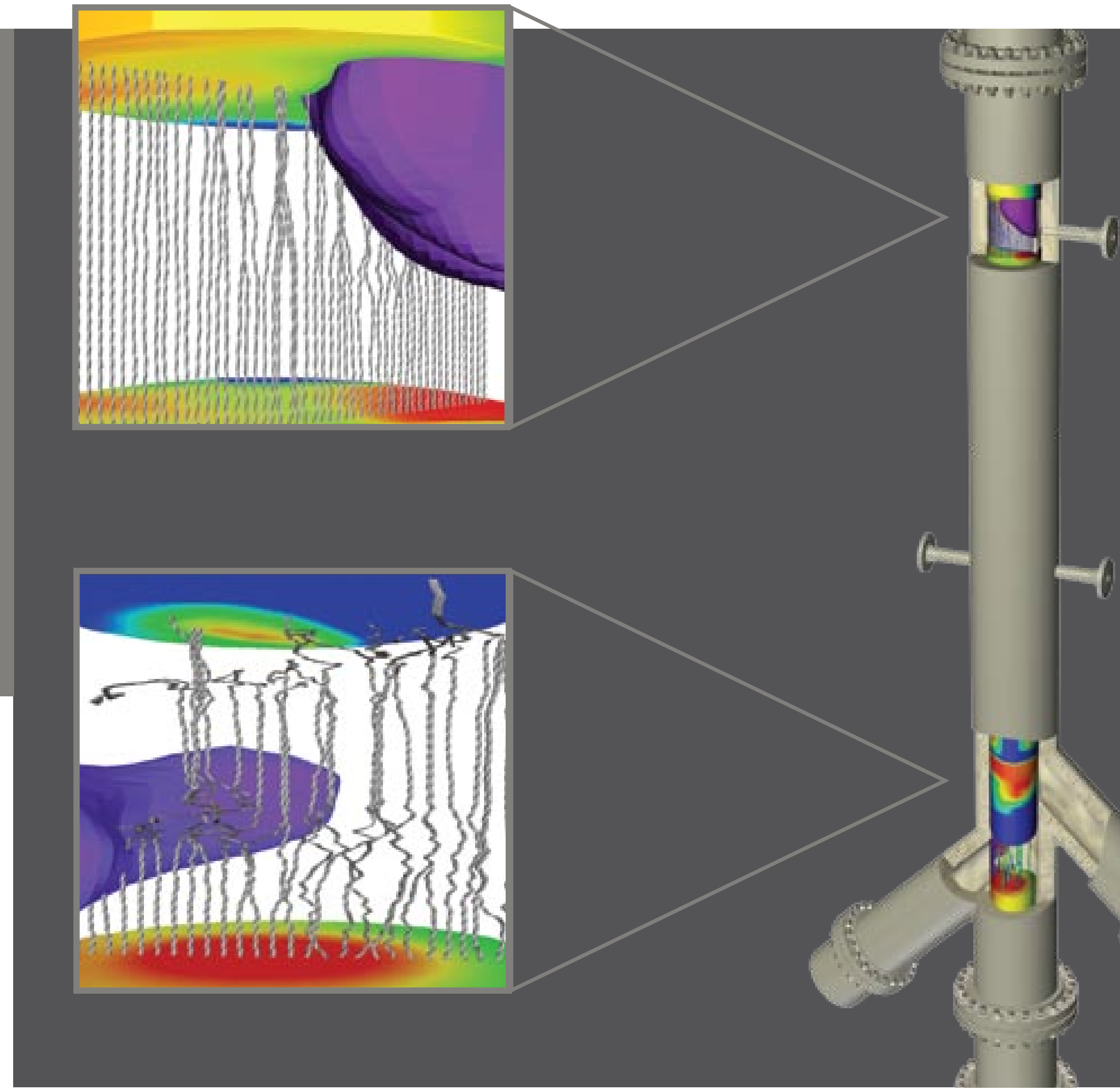
Guenther's group had a powerful tool at their disposal: MFIX (Multiphase Flow with Interphase Exchanges), software developed at NETL to reduce cost in development of clean-coal technologies. It describes the hydrodynamics, heat transfer, and chemical reactions in fluid-solid systems such as coal gasification. MFIX's ability to simulate various coal-combustion processes and its usefulness as a design tool were recognized this year by R&D Magazine, which gave MFIX an R&D 100 award as one of the top 100 technologies of the year.

Using LeMieux over the past five years, Guenther's team validated MFIX's ability to accurately predict conditions at the PSDF. Via this process they developed a patent-pending coal-chemistry module to be used with MFIX. "LeMieux's speed allowed us to quickly make whatever changes we wanted in the virtual world and then tell the plant engineers at PSDF what to expect if they changed this or that variable," says Guenther. "With LeMieux we had the CPU power, and the basic physics-based equations were there in the software."

They used from 16 to 64 of LeMieux's processors. "The support staff at PSC often gave us a high priority," says Guenther, "which was really critical for our work. Sometimes MFIX was running absolutely continuously around the clock at PSC for every bit of an entire work week or longer."

PSC scientific-visualization specialist Kent Eschenberg created a software routine to take data from the LeMieux runs and translate it into a format Guenther could use directly with advanced 3D visualization software, so he could see and analyze the results quickly.

When the PSDF work began, however, the MFIX team lacked solid information on crucial "reaction rate" parameters involved in gasification, and it required iterative, careful work over time — with many simulations on LeMieux — to improve the software's predictive ability, work which led eventually to some surprising findings.



Transport Coal Gasification

Simulation results from MFIX with PSC's LeMieux system. The upper graphic shows a result from simulating coal as it enters the upper region of the gasifier (purple). Minimal impact on the vertical flow pattern of the gas (grey streamlines) implies poor coal penetration into the gasifier, which can lead to lower conversion of the coal and elevate discharge of soot and carbon-dioxide from the gasifier.

The lower graphic shows a result from simulating burner air entering the gasifier (purple) and the complex flow pattern (grey streamlines) it creates. Complex flow in this region of the gasifier is critical for sufficient mixing and to maximize contact between the gas and solid particles.

KEYING ON KINETICS

MFIX has modeled many gas-solids reaction processes, but it had not before been used to model a transport gasifier — so-called because the hot gas and unburnt solids travel upward through the long, pipe-like reactor. In this environment, coal particles react with steam, air, and other chemicals in many reactions that lead ultimately to a mixture of carbon monoxide, hydrogen, and other gas species called "syngas" — short for "synthesis gas." Unreacted coal particles recirculate from the "riser" — a vertical tube at the top — back to the reactor's "mixing zone." Eventually, all the coal particles transform into syngas, and the coal is gasified.

THE XT3 OPENS UNPRECEDENTED ABILITY TO DO LOCALIZED PREDICTIONS FOR THE REACTOR AT VERY HIGH RESOLUTION

A critical variable in this environment where multiple reactions take place simultaneously is "kinetics" — how fast the reactions proceed. "This transport gasifier was a fairly new piece of technology," says Guenther, "and when we began there were no reaction rates in the open literature that covered our conditions. The kinetics for detailed gas-phase combustion is out there, but detailed reaction mechanisms for devolitization, tar cracking, and gasification under transport conditions are not readily available."

By adjusting the kinetics in the MFIX code incrementally through a series of simulations, Guenther and his colleagues began to get results that matched what was happening in the PSDF. It was a back-and-forth process. The engineers in Alabama would make a gasification run, and the NETL researchers would run the MFIX model on LeMieux to simulate the same conditions.

They knew they were getting it right when they pointed out a potential problem to the PSDF engineers. Simulations showed "oxygen breakthrough" — a stream of oxygen that did not react with the recirculated coal, but reacted instead with fresh coal higher up in the riser. This could cause the coal to combust rather than gasify, resulting in higher temperatures and elevated levels of CO_2. "We made some predictions that at first the plant engineers found hard to believe,' says Guenther, "but later accepted."

Another leap occurred when the PSDF was shut down eight months for modifications and NETL ran simulations to see what effect the modifications would have. "When they were back up and running they were getting numbers like we predicted," says Guenther. "That was a milestone for us in showing that MFIX running on LeMieux is a valuable tool for commercial-scale design."

The Orlando project's partners agree. "Previously we had to rely on pilot-plant data and theoretical models that had a limited range of applicability," says Nicola Salazar, director of coal monetization at KBR. "But with this cutting-edge tool, we are able to predict the effects more quickly and with greater confidence. Ultimately, the tool will help us to develop safe, reliable, and energy-efficient designs for our commercial gasifiers."

MFIX is currently running on PSC's Cray XT3 to continue the scale-up that will lead to start-up of the Orlando plant in 2010. "What's the best ratio of the length of the reactor to its diameter?" says Guenther. "Is it better to use 100-micron-diameter coal particles or 300-micron-diameter coal particles? These are the kind of "what if" scenarios we can investigate."

With the XT3, Guenther can run MFIX efficiently on up to 1,024 processors, which opens unprecedented ability to do localized predictions in specific areas of the reactor at very high resolution. "For localized predictions, we are using 12-million computational cells, seven times more resolution than we did with LeMieux. To my knowledge, commercial-scale simulations at this fine a resolution have never been done before, and it means we can answer much more in-depth questions about reactor performance."

The Orlando plant will be the world's first commercial-scale plant that incorporates a transport gasifier with integrated gasification combined cycle technology. Syngas from the transport gasifier will pass through a gas turbine to generate electricity, then heat water for a steam turbine that generates more electricity. Along with more electricity per ton of coal, there are essentially no emissions of sulfur dioxide and particulates, appreciably lower oxides of nitrogen, and 25-percent less carbon dioxide. With help from supercomputing, Florida energy consumers will soon begin to reap the benefit. (TP)

MORE INFORMATION:
www.psc.edu/science/2007/coal.html