



## DEVICE SCALE MODEL DEVELOPMENT FOR TRANSPORT REACTOR

### Background

Coal gasification is an efficient and environmentally acceptable technology that can utilize the vast coal reserves in the United States to produce clean affordable power and reduce dependence on foreign oil. Coal and other carbon containing materials can be gasified to produce a synthesis gas. This syngas can be fed to a turbine to produce electricity or used in a number of petrochemical applications to produce fuels, chemicals, fertilizers, or other industrial gases. Given the tremendous potential of coal gasification, understanding the process is a critical need, which is being addressed by the Power Systems Development Facility (PSDF) in Wilsonville, Alabama. The PSDF is a joint project of the U.S. Department of Energy, Southern Company, Kellogg Brown & Root (KBR) and others to demonstrate advanced coal-fueled power systems and key components at sufficient scale to provide data for commercial scale-up. The center piece of this project is the development of the transport gasifier. The transport gasifier has higher throughput, better mixing, and increased heat and mass transfer rates compared to other conventional technologies.

To better understand the complex interactions between the gas and solids inside the transport gasifier and to optimize the process and design, National Energy Technology Laboratory (NETL) has been actively involved in developing and applying physics-based computer simulations of the gasifier. To accomplish this, researchers at NETL have been using the MFIx (Multiphase Flow with Interphase eXchanges) code. MFIx was developed at NETL and is internationally recognized as one of the premier multiphase codes available to researchers. NETL researchers have been applying the MFIx model to the transport gasifier at PSDF and have validated the model for both bituminous and sub-bituminous coals under air and oxygen blown conditions.

### Accomplishments

Recently, two unexpected phenomena were observed in the MFIx predictions that were subsequently verified experimentally. One, the simulations showed that oxygen reached the upper region of the mixing section. The gasifier developers had expected that all the oxygen would be consumed by the recycled char in the lower region of the mixing section. This prediction was later verified with experimental measurements. Two, the calculations showed high concentration of CO and solids in the upper part of the riser, above the exit. This prediction was also later confirmed with experimental measurements. These convincingly showed the gasifier developers that the model does not merely reproduce what is already known, but provides information on unobserved phenomena.

NETL researchers recently completed simulations of the transport gasifier based on certain design modifications. The implementation of the design changes in the reactor has taken nearly a year to complete the construction. NETL researchers completed the simulations in a fraction of that time and presented the results to engineers at PSDF. The results show a significant increase in CO mole fraction in the exit syngas because of changes in the hydrodynamics inside the reactor. Engineers

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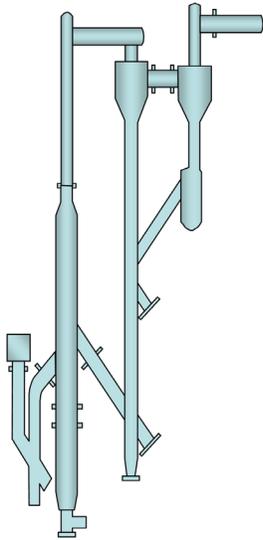
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Schematic of a Transport Gasifier

at PSDF were delighted to see these predictions because the design modifications were specifically made to achieve higher CO mole fractions in the syngas. The calculations have already shown that their expectation would be realized when construction of the modified reactor is completed.

A variety of other simulations of the PSDF transport gasifier have been completed using MFIX. Simulations were performed to understand the effect exit configuration has on syngas composition. A parametric study has also been completed to study the impact increasing the height of the reactor has on syngas composition. The model has also been employed to simulate the recent design modifications of the PSDF reactor at both 250 and 465 psig showing increased levels of methane in the syngas as pressure increases. In an effort to promote technology transfer between NETL and their industrial partners, the Fluent code has been modified to include all the chemistry sub-models for coal gasification and combustion that are currently in MFIX. These Fluent modifications were verified against MFIX simulations of air and oxygen blown gasification of a Powder River coal and a Hiawatha coal.

## Benefits

Engineers at PSDF are using the model to understand the impact the exit has on syngas composition and the effect reactor height has on CO production. They are using the model to understand how the coal enters the reactor and how gas temperature varies inside the reactor. The model has been used to study the effect of increasing the pressure. These high pressure simulations are being conducted in anticipation of scaling-up the transport reactor to a commercial scale. Scale-up is a difficult issue especially when there are large changes in the scale or operating parameters. To aid in the scale-up of the PSDF transport gasifier, MFIX simulations at scale are being conducted. These simulations are providing engineers with detailed information of various commercial designs that would otherwise be unavailable.

Successful completion of this project will allow NETL to accurately predict the product composition from a transport gasifier over a wide range of input fuels and operating conditions. This project will enable designers to foresee and solve problems, optimize designs independent of scale, and complete parametric studies resulting in significant reduction in time and cost to commercialization.

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