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The National Energy Technology Laboratory Wins the FLC Mid-Atlantic Region Technology Transfer Award for Coal Chemistry Module Software

The Mid-Atlantic Region of the Federal Laboratory Consortium this year presented the Regional Excellence in Technology Transfer Honorable Mention Award to Dr. Chris Guenther and Dr. Madhava Syamlal of the DOE National Energy Technology Laboratory for work on "Coal Chemistry Module Software."

The researchers developed the Coal Chemistry Module (CCM) software as a means to incorporate coal chemical reactions into physics-based models of multiphase reactors to solve scale-up problems for advanced power plants using coal gasification, such as Integrated Gasification Combined Cycle (IGCC) plants. Advanced power plant technologies combine the technology of multiphase reactors with high-temperature chemical reactions for processing fossil fuels; for example, coal, a complex solid chemical mixture, is reacted with gas-phase steam and air in a gasifier at high temperatures and pressures. The chemical reactions in these systems are inextricably linked with the multiphase flows, i.e. mathematical models cannot address these phenomena separately but must solve the reaction chemistry and multi-phase flow equations in a coupled or integrated manner. NETL is leading the way, with industry partners, to a new generation of simulation software capable of integrated solutions to this technology challenge. NETL's effort has resulted in the development of CCM, which has been incorporated in the NETL open-source multi-phase flow code MFI (Multiphase Flow with Interphase eXchanges) (winner of a 2007 R&D 100 Award), and has been used in collaborative projects with end users. CCM is also being incorporated into a future version of the well-known commercial FLUENT computational fluid dynamics software. These developments have positively impacted not only the primary target, the fossil fuel industry, but also coal conversion R&D at universities and national labs.

A collaborative project between NETL and gasifier developers has resulted in CCM being used with MFI for advanced gasifier design. NETL researchers have been using CCM to simulate the coal chemistry as part of an overall MFI simulation of the transport gasifier at the Power Systems Development Facility, Wilsonville, Alabama, operated by Southern Company and Kellogg Brown & Root (KBR). The advanced transport gasifier is a promising process for use in high efficiency, low emission IGCC systems that can capture carbon for sequestration. The simulations convincingly showed the gasifier developers that the model does not merely reproduce what is already known, but provides insight into unobserved phenomena, which they could later experimentally verify. Also, CCM was used with MFI to predict the expected gasifier behavior almost a year before certain design modifications were completed. KBR design engineers are using similar simulations to help in the design of a commercial-scale Clean Coal Power Initiative (CCPI) transport gasifier at Orlando, Florida. Technology transfer of CCM is also being done under a CRADA in collaboration with Fluent, a leading vendor of simulation software, leading to incorporation of CCM in the well-known (commercial) computational fluid dynamics code FLUENT.

One of the most coveted awards in the field of technology transfer, FLC awards for Excellence in Technology Transfer recognize laboratory employees who have accomplished outstanding work in the process of transferring Federally-developed

technology to the marketplace. The award was made on September 21 at the region's annual meeting.

The Federal Laboratory Consortium is comprised of the technology transfer offices of all of the Federal laboratories throughout the country while its Mid-Atlantic Region focuses on the 70 Federal laboratories in DC, DE, MD, PA, VA and WV.

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