

**U. S. DEPARTMENT OF ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY**

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“CONTINUUM CHEMISTRY MODULE FOR HYDROGASIFICATION (CCMH)”

Some advanced energy technologies combine flowing solids and gases with high-temperature chemical reactions to convert solid fuels such as coal or biomass into energy. For example, coal, a complex solid chemical mixture, can be reacted with gas-phase steam, air and other gases at high temperatures and pressures to produce a gaseous fuel. This process is called “gasification.” The gas produced can be used as a substitute for natural gas or converted to a liquid fuel to replace gasoline. Thus, developing a reliable, low-cost coal gasification process could help to solve much of the United States’ energy supply problems by relying on our most abundant natural resource—coal.

In order to achieve this, however, scientists and engineers must first understand the fundamental mechanisms of the gasification process in more detail. Traditional design approaches to these processes have used a repetitive and expensive build-and-test cycle to scale up new technologies. Now, advanced computing systems with sophisticated mathematical models can simulate coal gasification processes to better understand their inner workings and eliminate these costly traditional procedures. But, even with the most advanced computers and models available, the simulations are challenging. The behavior of the flowing solids and gases and the chemical reactions that occur between them in these systems are inextricably linked; mathematical models cannot address these phenomena separately but must solve the flow and reaction chemistry equations simultaneously. Understanding these complex interactions requires new, more sophisticated, mathematical models.

The National Energy Technology Laboratory (NETL), with industry partners, is leading the way to a new generation of simulation software capable of integrated solutions to this technology challenge, starting with the Continuum Chemistry Module for Hydrogasification (CCMH). Hydrogasification is a process in which hydrogen reacts with coal to form methane, or Substitute Natural Gas (SNG). In developing CCMH, NETL researchers have simplified the mathematical computations by combining the flow of gases and solids into a single continuous medium (hence “continuum chemistry”). Through a cost-shared cooperative technology transfer agreement with NETL, Arizona Public Service (APS) is using CCHM to develop the Advanced Hydrogasification Process (AHP). To facilitate the technology transfer, NETL’s Office of Research and Development (ORD) conducted extensive simulations with CCMH to assist with reactor design, especially hydrogen nozzle design. Test operations with a bench-scale reactor are scheduled for fall 2008 to validate the design information provided by the simulations. Once pilot reactor studies are completed, design of a full-scale hydrogasification process will be initiated, again using these modeling tools. CCMH is also being applied under a cooperative research agreement between NETL and University of California-Riverside. The goal of this project is to produce synthetic fuels from coal using a bubbling bed operating in a steam-rich environment under relatively low pressures and temperatures.