



## Carbonaceous Chemistry for Computational Modeling

### Opportunity

The Department of Energy's National Energy Technology Laboratory (NETL) has developed a software platform entitled Carbonaceous Chemistry for Computational Modeling (C3M) that is used to access a variety of kinetic processes and reaction mechanisms typically found in coal gasification, gas clean-up, and carbon capture processes. This unique software provides the user the ability to conduct virtual kinetic experiments using leading kinetic packages and available experimental data to evaluate kinetic predictions as a function of fuel and sorbent type and/or operating conditions. A Patent Cooperation Treaty application was filed in June 2008.

NETL is seeking non-exclusive licensing partners interested in implementing this software into their current systems and/or marketing this commercial software to industry.

### Overview

The coal gasification industry is now at the forefront of a worldwide clean energy initiative. Industry experts agree that the markets for advanced technologies for gasification, gas clean-up and carbon capture are growing, with worldwide gasification capacity projected to increase along with stringent regulations for trace contaminant removal and aggressive targets for CO<sub>2</sub> capture.

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### Patent Details

U.S. non-provisional patent application titled "The Coal Chemistry Module" was filed on 12/10/09.

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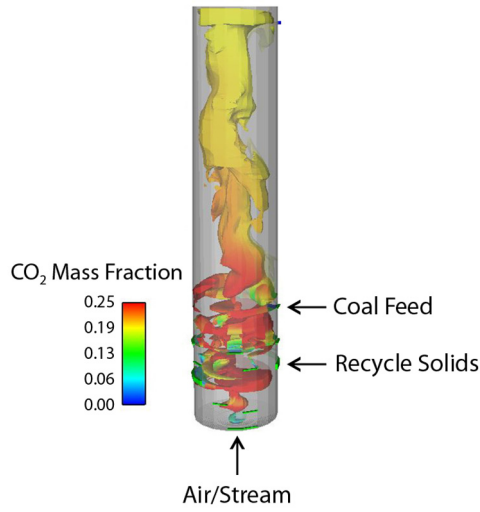
**C3M**™  
Carbonaceous Chemistry for  
Computational Modeling

### Significance

- This program has been tested, verified, and implemented into a variety of industrial relevant applications.
- By using C3M as an add-on to a CFD program, designers can quickly develop reacting multiphase models which can predict and visualize fluid flow within a gasifier.
- C3M is applicable to any carbonaceous feedstock.
- The program addresses the need for a single source of kinetic information that modelers can use and couple to their computational fluid dynamic models.
- The ability to understand and evaluate kinetic dependencies on fuel and operating conditions is essential to the development and application of a reacting multiphase model.
- The model can be used to determine operating conditions that optimize throughput, thermal efficiency, and carbon conversion.

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Designing advanced gasification processes and devices requires an understanding of the physical transformations that fuel and sorbent particles undergo when exposed to hot, multiphase environments; the chemical reactions responsible for conversion of the solid material to gaseous species; the mechanisms responsible for a sorbent particle to remove pollutants from a gas stream must also be realized.



*Solids volume fraction isosurfaces colored by CO<sub>2</sub> mass fraction. Results of a C3M /MFIx simulation of a pilot-scale gasifier.*

The C3M augments existing computational fluid dynamic (CFD) software by helping researchers to model the complex interactions between gas and solid phases in a reacting environment. This software, coupled with a multiphase CFD model, allows a modeler to choose a kinetic process of interest (e.g., pyrolysis, gasification, sorbent based CO<sub>2</sub> capture etc.) and evaluate it as a function of fuel and/or operating conditions. Furthermore, the user can select the appropriate set of kinetic expressions for his or her application and conditions and then couple that choice into industry standard multiphase CFD models.

