

Motivation

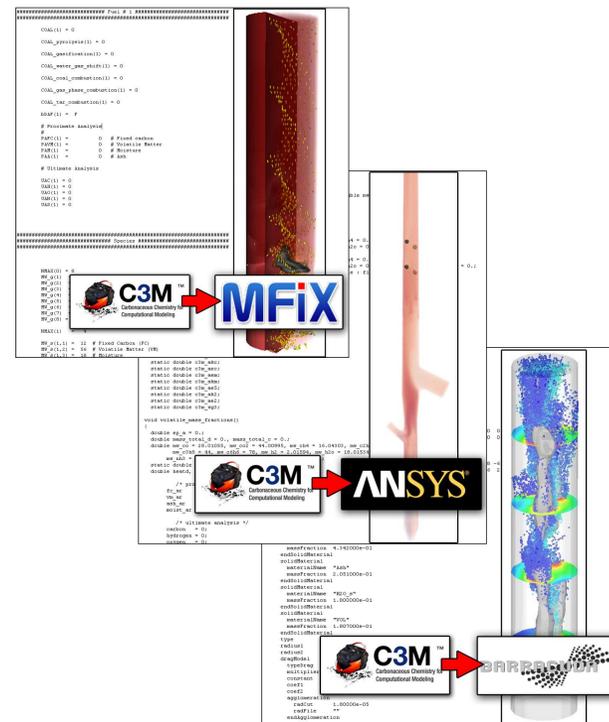
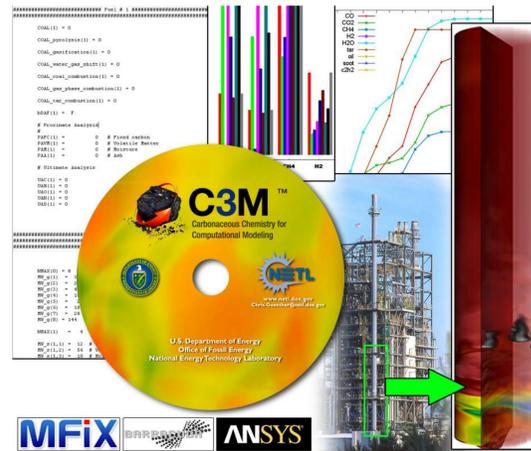
One of the most complex, time consuming and expensive parts of reactive computational modeling is appropriately handling kinetics. Inputting chemistry into computational modeling is tedious, error prone, and difficult to debug. C3M greatly improves this process, reducing time and expense

Technology Overview

- C3M provides validated and verified kinetics for reacting CFD models of energy related systems
- C3M contains a “Virtual Kinetic Laboratory” which provides user friendly, rapid methods to analyze complex chemical kinetic equations sets before getting to time consuming and expensive CFD models
- The C3M software has a user friendly graphical user interface designed with rapid work flow in mind, taking just minutes to set up a full kinetic model for reacting CFD
- C3M directly exports formatted input files to leading CFD codes such as ANSYS FLUENT, CPFD BARRACUDA, and NETL’s MFiX

Industry Significance

- Can cut thousands of man hours and hundreds of computational hours off of the development and implementation of reacting CFD Models
- Currently contains a full kinetic set for gasification but will contain kinetics from other areas of research at NETL such as sulfur removal, mercury capture, and oxy-combustion
- Will contain methods to do uncertainty quantification and response surface modeling
- Will contain methods to directly compare computational models with experimental systems like drop tubes and high speed TGA’s
- Will contain the ability for user defined kinetic module implementation



Benefits to Partner

- Reduced time to CFD solution
- Reduced expense in R&D
- Ability to quickly obtain multi-scale design data from CFD
- Increased certainty in CFD solutions
- Reduction in staff requirements
- Provides kinetics for coal/biomass co-feeding, an industry first

Opportunity

- Seeking company/institution to license the innovation
- Seeking partner to develop, test, and validate new chemical kinetic models for energy related processes

Development Status

- U.S. non-provisional patent application number 12/663,944
- Releasing comprehensive gasification model in version 2.5 in late November, 2012
- Work has begun on advanced features

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