

U.S. DEPARTMENT OF ENERGY  
OFFICE OF FOSSIL ENERGY  
NATIONAL ENERGY TECHNOLOGY LABORATORY



## DEVELOPMENT, VALIDATION AND APPLICATION OF CFD-BASED MODELS FOR DESCRIBING CHEMICAL LOOPING PROCESSES

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### Background

Chemical looping combustion is a new technology that uses a metal oxide (MeO) to flamelessly combust a hydrocarbon fuel to CO<sub>2</sub> and H<sub>2</sub>O with very little production of NO<sub>x</sub>. Once the water is condensed, this results in a relatively pure stream of CO<sub>2</sub> that is ready for sequestration. The reduced metal (Me) is then transported to an oxidation reactor where it is oxidized back to the metal oxide using air, producing a hot gas stream which can be used for power generation, as shown in Figure 1. The oxidized metal is then recycled. This basic combustion configuration can be modified into a reforming process and extended to allow S capture. The objective of this project is to develop computational fluid dynamic (CFD) models for chemical looping power systems. Only a few small process development CL units exist in the world. Thus, this technology will benefit greatly from development of computational fluid dynamic models that can be used to design the oxidation and reduction reactors, model the oxidation/reduction chemistry for various metal/metal oxide combinations, and simulate the operations of the oxidation/reduction reactors.

### Accomplishments

A complete collection of CLC literature has been compiled and reviewed. These include articles on carrier development, possible process configurations, and process design. Our review shows that computational fluid dynamic models for chemical looping power systems are currently unavailable. Such tools are needed to efficiently design and scale-up novel systems such as the Alstom and General Electric chemical looping power systems.

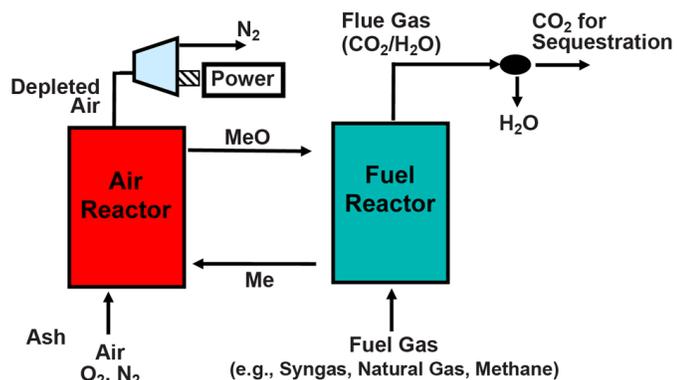


Figure 1. Simplified Diagram of Chemical Looping Combustion



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Formulation of the chemistry scheme for modeling the reduction chemistry using NiO and CH<sub>4</sub> has begun. Detailed CFD hydrodynamic simulations of the combustor unit for such a process have been performed. Results, shown in Figure 2, present a series of metal oxide volume fractions. Consistent with experimental observations, the plots show bubbles forming, rising, bursting and collapsing.

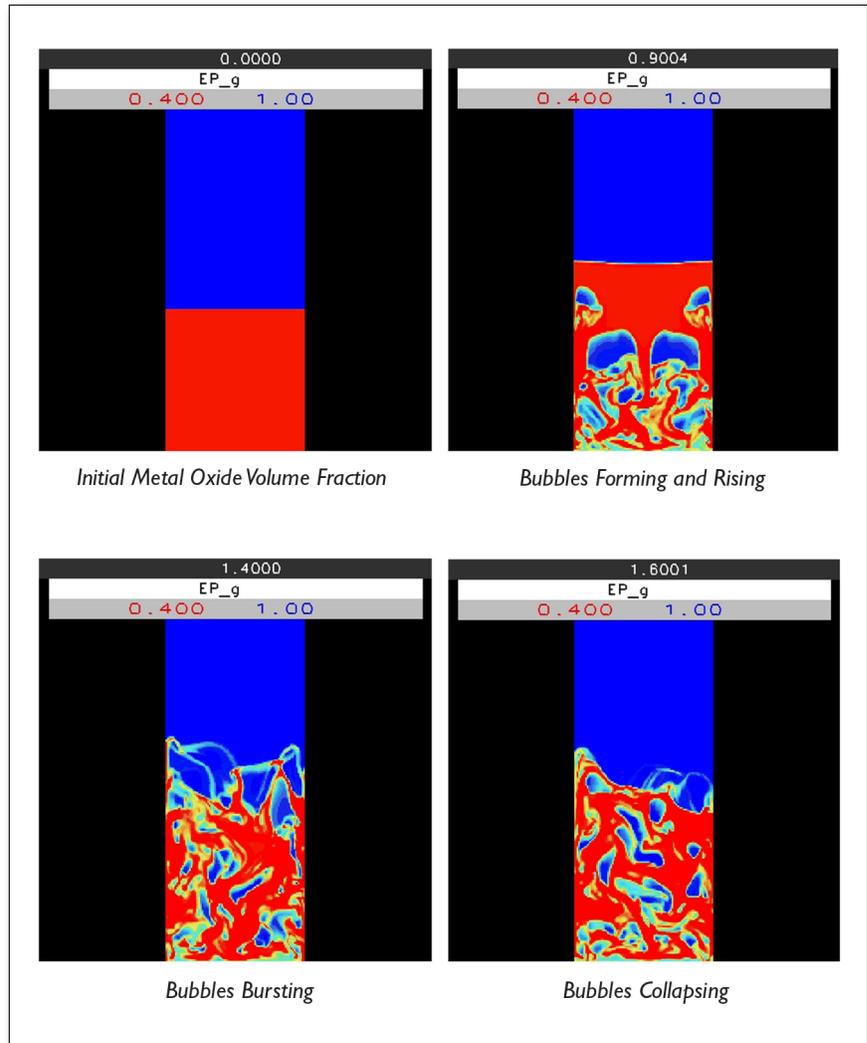


Figure 2. Series of Volume Fraction Plots Showing Bed Hydrodynamics in the Bubbling Fluidized Bed Oxidation Reactor

## Benefits

The successful integration of chemical looping technology in large CO<sub>2</sub>-free power plants depends on optimal handling of the solids flow in the oxidation and reduction systems. Dense multiphase CFD is a powerful tool for studying the performance of these systems. This work will develop the capability to model chemical looping processes, validate this capability using available data from the literature and use these techniques to help in the further development of chemical looping technology.