

University Coal Research  
*Success* Stories

## **Computational Fluid Dynamics Model Attracts Private Sector Development**

Two private organization, **Exxon Research and Engineering Company** and **Air Products and Chemicals, Inc.**, have expressed interest in the scale up and operation of Slurry Bubble Column Reactors (SBCR) through the use of Computational Fluid Dynamics (CFD).

The CFD model was first developed under a UCR grant at **Washington University** in 1995. Under another UCR grant in 1998, the CFD model was adapted to simulate methanol synthesis in gas-liquid slurry bubble column reactors (SBCR) at the **Illinois Institute of technology (IIT)**. At this stage, **Universal Oil Products, Inc.**, **Energy International, Inc.**, and **Akron University** collaborated with IIT in this effort. The end result was a predictive, 3 phase hydrodynamic models for gas-liquid-solid catalyst reactors using a combination of computational, experimental, and theoretical studies with a feedback mechanism to correct for model deficiencies. The model's predictions of slurry height, gas hold up, and rate of methanol production agreed with pilot plant reactor data obtained from DOE's Alternative Fuels Development Unit (AFDU) in LaPorte, Texas.

The most recent effort involved another collaborative project between Washington University, **Ohio State University** and Air Products and Chemicals to advance the knowledge and understanding of the hydrodynamics of SBCRs at Fischer-Tropsch synthesis conditions. Financial support for three years was provided through an **International Consortium** and the **DOE's Office of Fossil Energy**. This research effort is to characterize all fluid dynamic parameters using advanced diagnostic techniques and to generate a new fundamental approach for scale up, design, and operation of SBCRs. The end goal is to be able to use the model to optimize indirect coal liquefaction, a technology developed by DOE and an industrial consortium.