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The NETL MFiX Suite of multiphase flow models: A brief review and recent applications of MFiX-TFM to fossil energy technologies

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HIGHLIGHTS

- High level overview of MFiX suite of multiphase computational fluid dynamics codes.
- Emphasis on verification, validation, and uncertainty quantification for predictive simulations.
- Recent accomplishments in application of MFiX-TFM to fossil energy technology development.

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ABSTRACT

The MFiX suite of multiphase computational fluid dynamics (CFD) codes is being developed at U.S. Department of Energy's National Energy Technology Laboratory (NETL). It includes several different approaches to multiphase simulation: MFiX-TFM, a two-fluid (Eulerian–Eulerian) model; MFiX-DEM, an Eulerian fluid model with a Lagrangian Discrete Element Model for the solids phase; and MFiX-PIC, Eulerian fluid model with Lagrangian particle 'parcels' representing particle groups. These models are undergoing continuous development and application, with verification, validation, and uncertainty quantification (VV&UQ) as integrated activities. After a brief summary of recent progress in the verification, validation and uncertainty quantification (VV&UQ), this article highlights two recent accomplishments in the application of MFiX-TFM to fossil energy technology development. First, recent application of MFiX to the pilot-scale KBR TRIG™ Transport Gasifier located at DOE's National Carbon Capture Center (NCCC) is described. Gasifier performance over a range of operating conditions was modeled and compared to NCCC operational data to validate the ability of the model to predict parametric behavior. Second, comparison of code predictions at a detailed fundamental scale is presented studying solid sorbents for the post-combustion capture of CO_2 from flue gas. Specifically designed NETL experiments are being used to validate hydrodynamics and chemical kinetics for the sorbent-based carbon capture process.

1. Introduction

Reacting multiphase flows are encountered in many important processes in the power generation, minerals and chemical process industries. Fundamental understanding of these flows is critical for development of novel processes or for optimizing and trouble-shooting existing technologies. Computational Fluid Dynamic (CFD) modeling has become a valuable tool to simulate multiphase flow in these devices, providing detailed flow hydrodynamics, chemical reaction, and heat transfer data. This detailed performance data and the ability to model commercial scale up means that validated multiphase CFD models are becoming critical tools for cost effective design and optimization.

The U.S. Department of Energy's National Energy Technology Laboratory (NETL) supports research and development of advanced fossil energy technologies using multiphase flow process components. These technologies include sorbent-based CO_2 capture, fluidized bed coal gasification, fluidized bed coal combustion, and chemical looping combustion and gasification (NETL, 2015a).

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