Eleventh International Conference on CFD in the Minerals and Process Industries
CSIRO, Melbourne, Australia
7-9 December 2015

THE NETL MFIX SUITE OF MULTIPHASE FLOW MODELS: APPLICATIONS TO FOSSIL ENERGY TECHNOLOGIES

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ABSTRACT

The Multiphase Flow Science (MFS) Team at the National Energy Technology Laboratory combines multiphase fluid dynamic (CFD) software development and application with multiphase experimentation to support U.S. Department of Energy Fossil Energy Research and Development programs. The MFiX Suite of multiphase CFD software underpins this program (https://mfix.netl.doe.gov/). The MFiX Suite includes the following approaches to multiphase simulation: MFiX-TFM, a two-fluid (Eulerian-Eulerian) model; MFiX-DEM, an Eulerian fluid with a Lagrangian Discrete Element Model for the solids phase; and MFiX-PIC, Eulerian fluid with Lagranian particle 'parcels' representing particle groups. These models are undergoing development and application, with verification, validation, and uncertainty quantification (VV&UQ) as integrated activities.

We will highlight three recent accomplishments in the application of the MFiX Suite of codes to fossil energy technology development. First, recent progress in the verification, validation and uncertainty quantification (VV&UQ) of predictive multiphase flow simulations will be described. Second, recent application of MFiX to the pilot-scale KBR TRIG™ Transport Gasifier located at DOE's National Carbon Capture Center (NCCC) will be described. Gasifier performance over a range of operating conditions has been modeled and compared to NCCC operational data to validate the ability of the model to predict parametric behavior. Third, comparison of code predictions at a detailed fundamental scale will be presented for solids sorbents designed for the post-combustion capture of CO_2 from flue gas. NETL experiments designed for model validation are being used for validation of hydrodynamics and chemical kinetics for the sorbent-based carbon capture process.

NOMENCLATURE

D	diameter of fixed/fluidized bed
ΔP	pressure drop across CFB riser
G_s	solids circulation rate
H_B	fixed/packed bed height
LMZ	lower mixing zone in CFB gasifier
p-box	probability box
QoI	uncertainty quantity of interest
T_B	local fluidized bed temperature
u_D	experimental data uncertainty
u_{input}	model input uncertainty
U_{mf}	minimum fluidization velocity
u_{num}	numerical uncertainty
u_{val}	validation uncertainty
U_g	superficial gas velocity
z	vertical position in fixed/fluidized bed

INTRODUCTION

Reacting multiphase flows are important processes found in the power generation, minerals and chemical process industries. The U.S. Department of Energy's National Energy Technology Laboratory (NETL) supports research and development into many advanced fossil energy technologies using multiphase flow process components, including sorbent-based CO_2 capture, fluidized bed coal gasification, fluidized bed coal combustion, and chemical looping combustion and gasification (NETL, 2015). The mission of NETL's Multiphase Flow Science team is the continuing development, validation, and application of multiphase computational fluid dynamics tools.

MODEL DESCRIPTION

MFiX Suite of Multiphase Flow Models

The MFiX (Multiphase Flow with Interphase eXchanges) Suite is a general-purpose set of multiphase CFD models for describing the hydrodynamics, heat transfer, and chemical reactions in dilute and dense multiphase flows. MFiX is a tool for design, optimization, and scale-up of reacting multiphase systems. (Syamlal et al. 2016). Typical NETL fossil energy applications include coal and biomass gasification, carbon capture devices, and chemical looping reactors for combustion of gaseous fuels and combustion and gasification of solid fuels. MFiX development has been ongoing at NETL for over two decades, beginning with a multi-particle (Syamlal, 1985) version of the Eulerian-Eulerian code of Gidaspow and Ettehadieh (1983) based on the Eulerian-Eulerian approach

The MFiX Suite of open-source models consist of the following tools:

- MFiX-TFM - two-fluid model, Eulerian carrier phase and Eulerian dispersed phase (Syamlal et al., 2016);
- MFiX-DEM - discrete element model, Eulerian carrier phase and discrete dispersed phase (Boyalakuntla, 2003);
- MFiX-PIC - multiphase particle-in-cell with Eulerian carrier phase and a particle-in-cell discrete representation of the dispersed phase (Garg and Dietiker, 2013);

- MFiX-Hybrid – combination of the TFM and DEM approach, with an Eulerian carrier phase with Eulerian and discrete dispersed phases.

The work reported here is based on the use of the MFiX-TFM. Governing equations and constitutive laws for MFiX-TFM are described in detail in Benyahia et al. (2012) and the upcoming Syamlal et al. (2016).

Verification, Validation, Uncertainty Quantification

Verification ensures that the model is accurately implemented and validation checks the accuracy of the model relative to the physical system. Simply stated, verification determines if we are writing the code correctly whereas validation determines if we are writing the correct code. General verification techniques include good coding practice, adhering to code convention and management of the development process – all of which comprise software quality assurance. Dynamic verification will test the code at various scales, i.e. testing small piece or modules (unit tests) up through integrated pieces. MFiX and its components are tested daily using an automated test harness. The test harness will report when a capability may have been 'broken' during the development process and it then informs the development team for their attention. Techniques for CFD-specific verification can include comparison of the solution with known accurate solutions generated by other codes or comparison with analytical solutions for simplified problems. Analytical solutions for multiphase CFD problems are rare, so an alternative technique we use for verification is the method of manufactured solutions (MMS). In MMS (Oberkampf and Roy, 2010), source terms are added to the governing equations so that the equations can be analytically solved. The resultant analytical solutions, which typically are not physically realistic, are used to determine the observed order of accuracy of the discretization schemes in both space and time. Comparing these observed orders of accuracy with what we would expect from the formal discretization scheme will point out coding errors and algorithm inconsistencies. Choudhary et al. (2014) have used the MMS approach for verifying MFiX-TFM. This approach is being extended for the other codes in the MFiX Suite.

CFD code is validated by comparing simulation results with experimental data from physical models closely related to the code application. Complete model validation requires comparisons of model results with experiments at multiple levels of complexity. No single lab-scale experiment captures all the complexities of a real-world multiphase reactor. Detailed data are usually not available from the more complex pilot-scale experiments. The MFS program uses a validation hierarchy where multiple scales of experimentation provide data specifically designed for validation. One example is the NETL Carbon Capture Simulation Initiative (CCSI), which is developing computational tools for enabling the rapid scale up of carbon capture technologies (Miller et al. 2014). CCSI's validation hierarchy includes simulation cases, ranging from simple to complex multiphase CO_2 reactors as shown in Figure 1 (Ryan et al. 2012).

Validation Uncertainty

Acceptable agreement between simulation results and experimental data obtained from the validation process is still not sufficient justification for use of the model for predictive simulations. To be truly predictive, the uncertainty in the simulation results used for comparison to experimental data should be known. ASME's *Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer* (ASME V&V standard 20-2009) calls this the validation uncertainty, u_{val}, defined by:

$$u_{val} = \sqrt{u_{num}^2 + u_{input}^2 + u_D^2} \quad (1)$$

where the simulation uncertainties come from three sources: the numerical solution, (u_{num}), the model inputs (u_{input}), and the experimental data (u_D). An example of validation uncertainty quantification for a multiphase CFD application is presented in the next section.

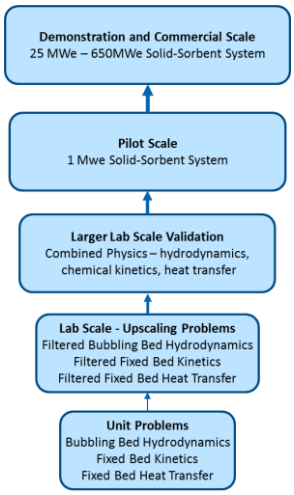

Figure 1: The computational-fluid-dynamics (CFD) validation hierarchy, illustrating the various unit problems and the levels of validation that lead up to a quantitative confidence on the predictions for the full-scale devices (adapted from Ryan et al. 2012).

Uncertainty quantification in predictive simulations

MFS team members, Gel et al. (2013), have applied the method of Roy and Oberkampf (2011) to validate the MFiX-TFM model of a circulating fluidized bed (CFB). Cold flow CFB data generated at NETL and reported by Shadle et al. (2011) was used for the validation. The general methodology is described below and illustrated with examples from Gel et al. (2013).

As the first step, Gel et al. (2013) chose the pressure drop across the CFB riser (ΔP) as the Quantity of Interest (QoI) for scale up. The following sources of validation uncertainty were identified for quantification:

- Input parameter uncertainty;
- Surrogate model uncertainty;
- Model form uncertainty;
- Experimental data;
- Spatial discretization;
- Time Averaging.

To address input parameter uncertainty, the sources of input uncertainty are identified and characterized for the critical model input parameters. A list of all the uncertain model input parameters is created by polling modeling experts who can also assess their criticality. The critical parameters could also be determined with the help of sensitivity

analysis, noting what input parameters have the greatest effect on the QoI.

Gel et al. (2013) identified the gas superficial velocity (U_g) and the solids circulation rate (G_s) as the critical input variables affecting ΔP from a field of 8 major sources of input uncertainty. In this application, Gel et al. (2013) characterized the uncertainty in U_g as a truncated normal distribution with a mean of 7.2 m/s and standard deviation of 0.04 m/s, and uncertainty in G_s as a truncated normal distribution with a mean of 14.0 kg/s and standard deviation of 0.34 kg/s.

The next step is to propagate the input uncertainty through the model. This involves running the MFiX CFB model for many values of U_g and G_s that would be sampled from their distributions. However, the computational cost of running MFiX-TFM for this application is too large (2-4 weeks of computational time on available resources) to get a statistically significant number of simulations – 100,000 in this case. Therefore, a surrogate model based on a smaller, representative set of MFiX-TFM simulations was created.

Gel et al. (2013) developed a surrogate model by expressing the ΔP as a polynomial in U_g and G_s using a set of 13 MFiX-TFM simulations. A central composite design sampling method was used to identify the simulations required for developing the surrogate model. The input uncertainty was then propagated by drawing 100,000 samples from the distributions of U_g and G_s and conducting a Monte Carlo simulation with the surrogate model.

The use of the surrogate model in place of the MFiX-TFM simulator introduces additional uncertainty. Gel et al. (2013) assumed this surrogate model uncertainty to be the maximum difference between MFiX-TFM results and the surrogate model predictions.

Roy and Oberkampf (2011) define model form uncertainty as the minimum area between the cumulative distribution functions of experimental data and the simulation results. This incorporates the experimental uncertainty as well.

Uncertainty from spatial discretization was estimated using the variation of ΔP over a range of mesh sizes. Comparison of results for coarsest and finest mesh sizes yields the value for uncertainty (Roy and Oberkampf, 2011).

Time averaging uncertainty results from the process to average the transient ΔP value over the simulation time. The uncertainty in ΔP over a given time interval is defined as the ratio of the standard deviation of ΔP values over the interval divided by the time average value of ΔP over the interval. This uncertainty decreased as the time interval for time averaging increased, as expected. To keep computational costs manageable, a time interval of 40 seconds was used for the time averaging interval for all of the MFiX-TFM simulations in Gel et al. (2013).

The total uncertainty in the predictions can now be found by combining the contributions from model form, input, surrogate model, discretization and time averaging as determined in the process described above. The result is the cumulative probability for ΔP as seen in Figure 2. The plot is called a p-box (probability box) bounded by the two S-shaped curves. The different colored regions within the p-box reflect the contributions from the various sources of uncertainty. The blue curve at the center arises from the uncertainty in the input parameters. The other uncertainties (surrogate, model form, discretization and time averaging) are added to this curve because we only know their interval values. The addition of these uncertainties converts the single curve into the p-box shape. The greatest uncertainty arises from the discretization (17.9%) with the next highest uncertainty being the model form uncertainty (5.2%).

Given the results shown in Figure 2, we will now consider what the uncertainty analysis adds to the traditional validation test which compares a predicted value to a measured value. In this application, the error between measured ΔP (20 kPa) and predicted ΔP (~19 kPa) is about 5%. However, given the uncertainty in predicted ΔP as described by the p-box, we cannot assume there will be a single value for the predicted ΔP or a single error bar for the prediction. For example, for a predicted ΔP = 24.2 kPa, the probability range is [0.8, 1.0] (from Figure 2); i.e., there is at least 80% probability that the ΔP could not exceed 24.2 kPa.

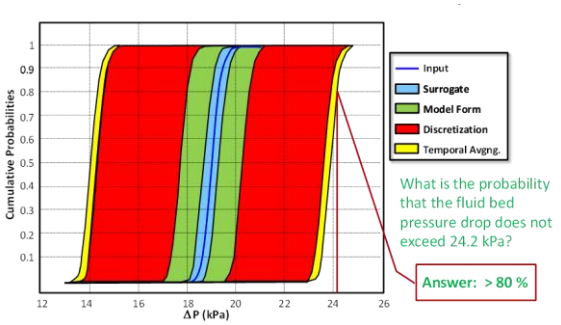

Figure 2: The p-box summarizes all the uncertainties considered in a predictive simulation. The box is colored to show the contributions from various sources in a multiphase application. (adapted from Gel et al. 2013).

What is the value in making such a nondeterministic prediction of ΔP? Suppose that the design specifications require ΔP≤ 24.2 kPa. Figure 2 says that it is 80% certain that ΔP≤ 24.2 kPa when the simulated device is built and operated. If 80% certainty in design performance is sufficient, then the design will be acceptable. If a greater degree of certainty (say 95%) in the predicted ΔP is desired, the design engineer has the options of either revising the design to operate at a higher ΔP or working to reduce the uncertainty in the predictive simulation. If the latter, there is no guarantee that even with reduced uncertainty the original design specification will be met with this present design.

MODEL APPLICATIONS AND VALIDATION

Simulation of a Pilot Scale TRIG™ Transport Gasifier

NETL and Southern Company Services (SCS) have established and operated the Power Systems Development Facility (PSDF) in Wilsonville, AL to study advanced coal-based power system technologies. The PSDF includes a KBR Transport Gasifier (TRIG™) to demonstrate gasification technologies for various coal types. The PSDF has performed tests for a variety of low rank coals as feedstock, studying TRIG™ performance over a broad range of operating conditions. These tests provide an excellent source of large scale gasifier performance data that can be used for gasifier model evaluation and

validation for pilot scale applications. Simulations of the TRIG™ gasifier using high moisture Mississippi (MS) lignite as the feedstock were performed with MFiX-TFM for comparison with SCS test program data (Li, et al., 2014).

NETL has previously modeled PSDF TRIG™ gasifier performance for Powder River Basin coals and comparison with SCS data has been very good (Li, et al. 2013). This work builds on these efforts and uses enhanced MFiX-TFM capabilities and the new NETL-based supercomputing facility to create more detailed models to more accurately model TRIG™ performance. With the enhanced meshing capability for dealing with complex flow geometry, detailed feed distributions in the gasification process are fully accounted for in the model to allow investigation of their impact on gasifier performance. The new coal chemistry enhancement to MFiX-TFM, called Carbonaceous Chemistry for Computational Modeling (C3M), leverages the kinetic models from leading coal kinetic packages to provide the detailed reaction kinetics in the gasification process for the MFiX gasifier model. Gasifier performance over a range of operating conditions has been modeled to verify the ability of the model to predict parametric behavior. The model outcome can be used to help the industrial designers and operators improve the process efficiency and reduce risks in design and operation.

The TRIG^{TM} gasifier design is based on fluidized catalytic cracking designs for gasoline refinery operation and consists of the basic components illustrated in Figure 3, namely riser, cyclone, loop-seal, standpipe and J-leg. This unit has been operated under a broad range of conditions for many coal types, but is well-suited for low-rank coals due to low operating temperatures and high recirculation rate (Ariyapadi, et al. 2008).

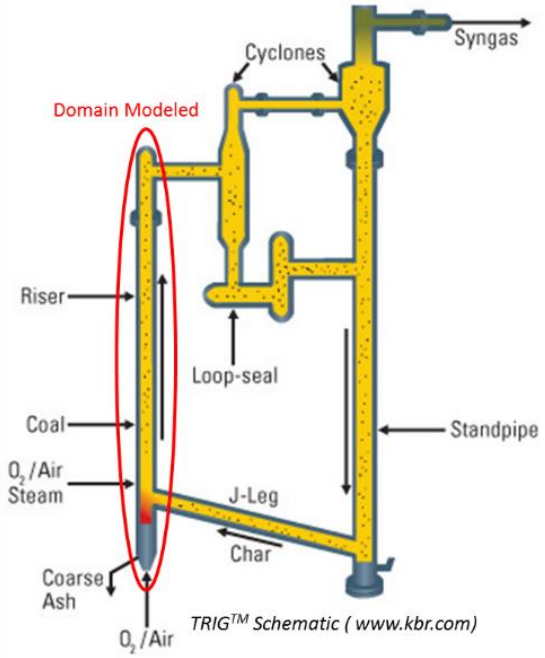

Figure 3: TRIG^{TM} Schematic and domain being modeled

This work studied gasifier performance while using MS lignite as the feedstock (Yongue and Laird, 2010). Eleven simulations were performed over a range of operating conditions representing a parametric test campaign that was conducted in August 2008 (Southern Company Services, Inc., 2009) for pre-dried MS lignite under air-blown operation. The riser operating conditions are shown on Table 1.

Run	Riser Outlet Temperature (K)	Riser Outlet Pressure (kPa)	Total Air flow (kg/s)	Total Steam Flow (kg/s)	Coal Flow (kg/s)
1	1177	1420	1.53	0.026	0.545
2	1183	1420	1.56	0.012	0.546
3	1217	1455	1.60	0.012	0.504
4	1226	1455	1.59	0.02	0.494
5	1224	1455	1.63	0.023	0.501
6	1240	1455	1.63	0.002	0.509
7	1243	1455	1.67	0.001	0.516
8	1164	1448	1.41	0.021	0.467
9	1171	1324	1.45	0.077	0.441
10	1206	1448	1.54	0.067	0.451
11	1215	1448	1.64	0.047	0.529

Table 1: Gasifier Operating Conditions that were studied

Operating conditions describing composition, temperature, pressure, and flow rate for the various inlet flows were taken from the test data (Southern Company Services, Inc., 2009). The MS lignite analysis used for the simulations is shown in Table 2 and represents the composition as-fed to the riser, after the lignite was dried.

The computational model considers only the riser section of the gasifier consisting of the lower mixing zone below the J-Leg inlet, the upper mixing zone above the J-Leg inlet, coal injection, and riser section. The computational domain is shown in Figure 4. A computational mesh consisting of 400,000 computational cells was used, with major inlets and outlets being well-resolved using the cut-cell method (NETL, 2015b). Secondary injection points are represented as point sources (NETL, 2015b).

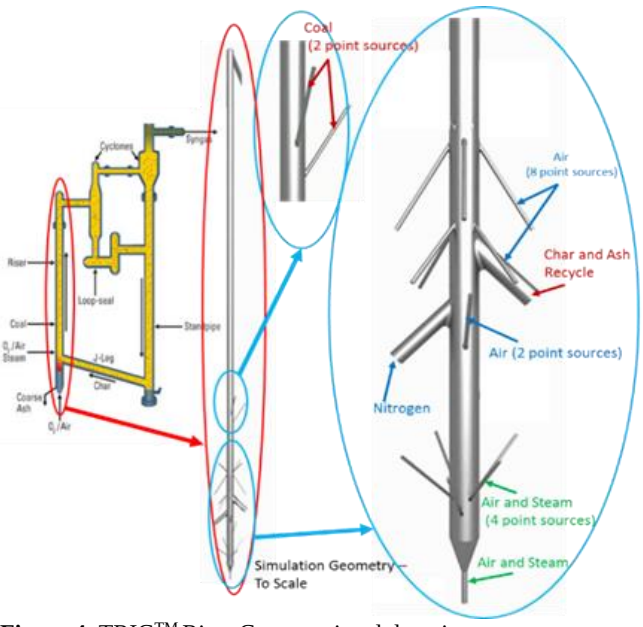

Figure 4: TRIG^{TM} Riser Computational domain

Proximate Analysis (%)		Ultimate Analysis (%)	
Fixed Carbon	31.0	Carbon	46.0
Volatiles	37.1	Hydrogen	3.5
Moisture	17.1	Oxygen	17.1
Ash	14.8	Nitrogen	1.0
		Sulfur	0.6

Table 2: MS Lignite, as-fed, post drying

Gasifier chemistry was modeled using a combination of heterogeneous coal reactions and homogeneous chemical reactions for gaseous products. The heterogeneous coal chemical reactions include devolatilization, char gasification, and char combustion. Heterogeneous reaction rates were obtained using the NETL chemistry management software C3M exercising PC Coal Lab (PCCL) software (Niksa, 2008). Details of the process can be found in Li et al., 2013. Gas phase species considered in the chemistry scheme include O_2, CO, CO_2, CH_4, H_2, H_2O, N_2, Tar, Soot, PAH, Oil, H_2S, C_3H_6, HCN, C_2H_4, C_2H_6, and SO_3. Solid phase species considered include "char", "volatiles", "moisture", and "ash". Char combustion was modeled using the shrinking core model of Syamlal and Bissett (1992) as implemented in MFiX-TFM (NETL 2015b). Gas phase combustion used the global reaction mechanisms and reaction rates of Westbrook and Dryer (1981). A catalytic water-gas shift reaction, catalyzed by the presence of coal ash, was included from the work of Wen, et al. (1992). Homogeneous phase water-gas shift was modeled with mechanism and rate information from Gomez and Leckner (2010) and Biba, et al., (1978).

MFiX-TFM simulations of the riser were performed for approximately 50-60 seconds of simulated riser time. Figure 5 compares model (black line) and experimental (red diamond) results for time-averaged riser temperature as a function of riser height.

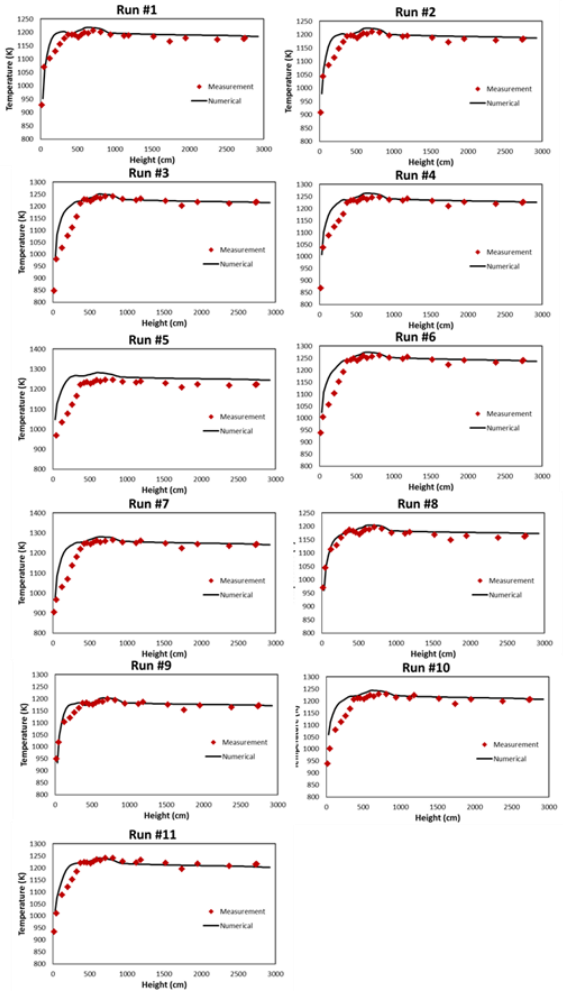

Figure 5: Time-averaged temperature as a function of riser height

The model predictions in Figure 5 reflect the riser centerline gas-phase temperature averaged over the final 30 seconds of simulated riser time. Model temperature data points correspond to the locations of wall thermocouples in the riser.

Excellent agreement between measured and experimental data is noted for the simulations, with most of the discrepancy coming in the bottommost section of the riser in the region called the lower mixing zone (LMZ). The model over predicts temperature in the LMZ by 10-15% of the experimental values. This is due to the fact that the model under predicts the solids concentration in the LMZ, allowing for more carbon from recycle char to reach the LMZ and oxidize.

Figure 6 compares time-averaged major gas-phase species composition at the riser exit from the model (red) to experimental measurement near the same location (blue). Model data is obtained by a mass-flow weighted average of gas composition at the riser exit plane. Predicted exit syngas compositions are in good agreement with measurements over the full range of operating conditions studied. Most discrepancies were less than 20% of the experimental values.

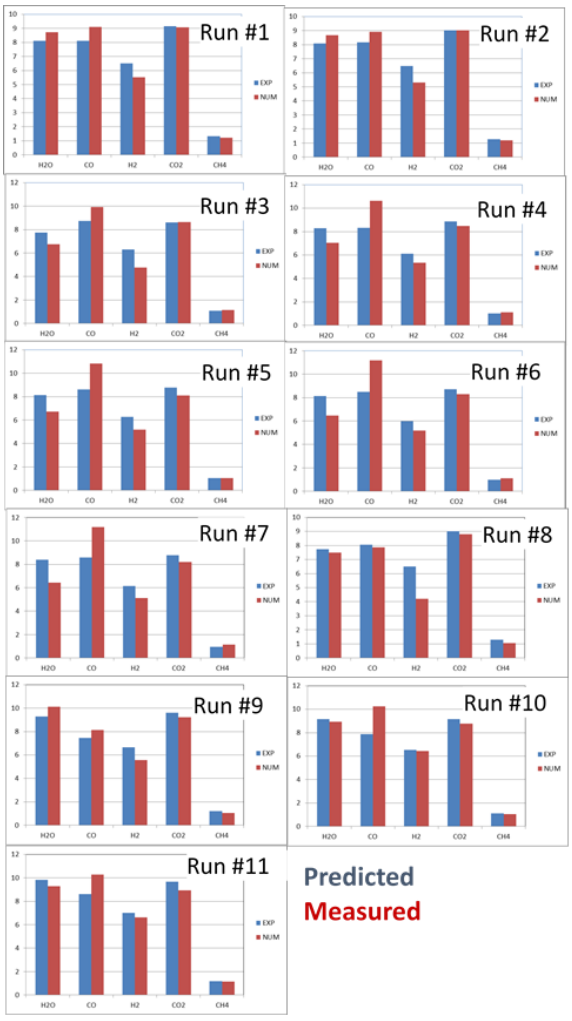

Figure 6: Time-averaged gas composition at the riser exit in per cent by volume.

Simulation of CO2 capture with solid sorbents

According to EPA (2013), carbon dioxide is the main greenhouse gas emitted through human activities – with CO_2 accounting for approximately 82% of all U.S. greenhouse gas emissions from human activities. The main source of this CO_2 is fossil fuel combustion for power generation and transportation. NETL is involved in extensive research and development efforts studying carbon capture technologies to address climate change without drastically disrupting energy systems in the short term.

One key candidate technology is the use of solid, granular, CO_2 sorbent material to separate CO_2 from flue gas streams for possible sequestration. The sorbent is used in a multiple fluidized bed system based on a pressure or temperature swing process. One aspect of NETL's Carbon Capture Simulation Initiative (Miller et al., 2014) is the development and demonstration of multiphase flow models for solid sorbent applications in post-combustion capture of CO_2. As part of this effort, the NETL Multiphase Flow Science Team have performed small-scale, fixed bed and fluidized bed experiments and simulations designed to validate hydrodynamics and chemical kinetics for solid CO_2 sorbent application (Li et al., 2014a), (Rabha, et al., 2015).

Figure 7 shows a schematic of the 0.1m diameter by 1.8m height bed used for the NETL experiments. The bed is instrumented with thermocouples and pressure transmitters at multiple heights, with control of inlet flow rate, gas composition, inlet temperature, and inlet humidity. (Rabha, et al., 2015) The inlet gas is a mixture of N_2 and CO_2 which can be passed through a bubbler for humidification. The sorbent that was tested and reported here is NETL-32D, which is branched polyethyleneimine (PEI) with N-[3-(trimethoxysilyl)propyl] supported in silica gel (Mebane et al., 2011) with a nominal amine concentration of 20% by volume. Sorbent material properties are shown in Table 3.

Sauter mean particle diameter (μm)	92
Sphericity (-)	0.89
Particle density (kg/m^3)	520
Particle Skeletal Density (kg/m^3)	1500
Bulk density (kg/m^3)	280
Particle porosity (-)	0.71
Void fraction (-)	0.45
Minimum fluidization velocity (m/s)	0.002

Table 3: Material properties of the NETL-32D sorbent

Figure 8 presents an example of fixed bed experimental data showing the bed temperature along the centerline at multiple heights as a function of simulation time for a humidified inlet gas volumetric analysis of 79.2% N_2, 19.8% O_2, and 1% H_2O. The gray lines in Figure 8 represent the estimated error bars in the data. As the sorbent is consumed in the exothermic adsorption process, an elevated temperature "front" moves upward though the bed. The dashed vertical line in Figure 8 denotes the point in time when CO_2 breaks through the fixed bed. The rate at which the temperature front moves through the bed and the peak temperature values can be used to validate model predictions in the absence of solids phase hydrodynamics.

In an effort to validate the chemical kinetic scheme used to model the adsorption process, fixed bed simulations were performed using the MFiX two-fluid model. The kinetic scheme used for the simulation is described in Bhat et al., 2012.

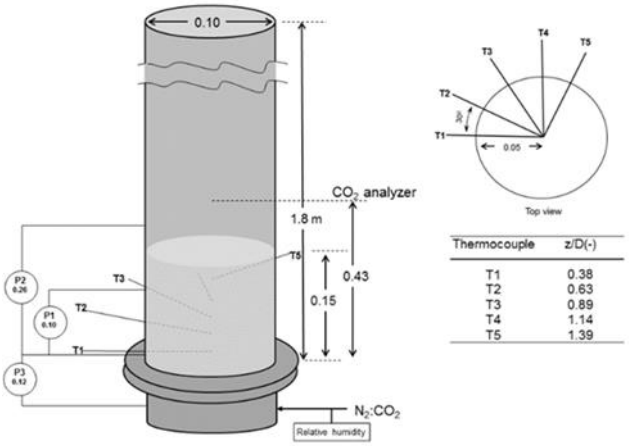

Figure 7: Schematic of the carbon sorbent fixed bed experimental setup showing thermocouple and pressure drop measurement locations (adapted from Rabha, et al., 2015)

Kinetic rate parameters were determined using data from thermogravimetric analysis of sorbent performance. A two-dimensional axisymmetric mesh with used, with the mesh size being approximately ten times the measured Sauter mean diameter. Figure 9 illustrates a comparison of

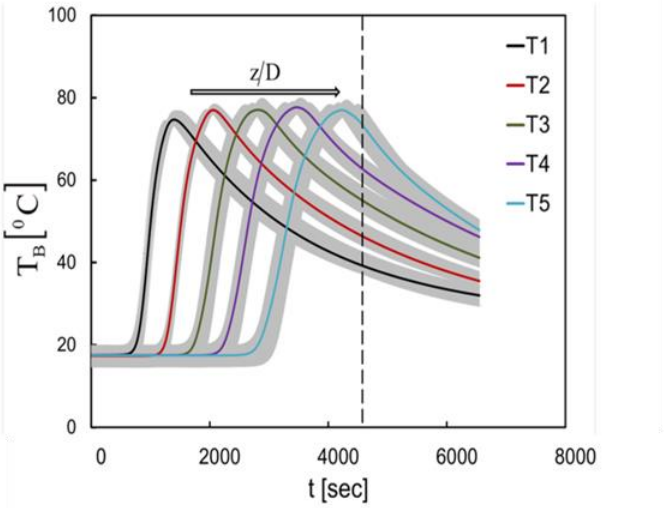

Figure 8: Measured local fixed bed temperature at the centerline at $0.39 \le z/D \le 1.39$ for a gas with volumetric analysis of 79.2% N_2, 19.8% O_2, 1% H_2O at $U_g/U_{mf} = 0.9$ and with $H_B = 0.15\,m$ (adapted from Rabha, et al., 2015)

the measured and simulated temperature values along the fixed bed centerline for a gas with volumetric analysis of 80% N_2, 20% CO_2 at U_g/U_{mf} = 0.9 and with fixed bed height, H_B = 0.15m. Experimental error for this set of tests is estimated to be +/- 2C, so Figure 9 illustrates that very good agreement between data and model results was obtained for this set of conditions. In addition to the kinetic

parameters used for the CO_2 absorption chemistry, the values for amine concentration, solid phase specific heat and solid phase thermal conductivity can affect the peak temperature value reached at each location. Future work will include additional fixed bed simulations with heated N_2 (no CO_2) to verify assumed values for solid phase specific heat and thermal conductivity and validate the heat transfer model. These will include fixed and fluidized bed tests.

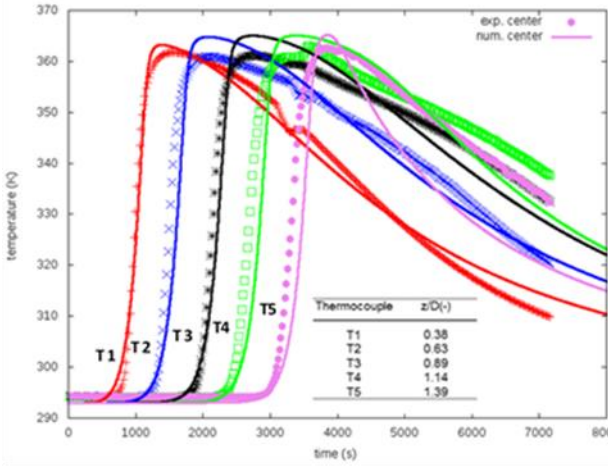

Figure 9: Comparison of measured and simulated temperature values at the bed centerline for a gas with volumetric analysis of 80% N_2, 20% CO_2 at $U_g/U_{mf} = 0.9$ and with $H_B = 0.15\,m$

CONCLUSION

We have demonstrated the following three recent advances in the application of the NETL MFiX Suite of multiphase CFD codes for fossil energy technology development:

- Recent progress in the verification, validation, and uncertainty quantification of predictive multiphase flow simulations;
- Application of MFiX-TFM to the pilot-scale KBR TRIG™ Transport Gasifier located at DOE's National Carbon Capture Center and comparison to operating data for lignite feedstock;
- And comparison of MFiX-TFM predictions to experimental data at a detailed, fundamental scale for solid CO_2 sorbents designed for the post-combustion capture of CO_2 from flue gas.

These results help to demonstrate the increased emphasis on verification and validation of the MFiX Suite of codes at small scale and industrial scales. A Method of Manufactured Solutions capability has been developed for verification of the MFiX-TFM code and this has been made an integral part of the ongoing verification program. Efforts are also underway to create a comprehensive collection of verification and validation problems – single and multiphase, applicable to all the MFiX versions for our V&V program. All of this is being documented in a V&V manual for public access.

A discussion has been presented describing the ongoing work to develop and demonstrate uncertainty quantification techniques for predictive multiphase simulations. A specific application of the predictive UQ method proposed by Roy and Oberkampf (2011) to a circulating fluidized bed application (Gel et al. 2013) was discussed in detail, illustrating where the various sources of uncertainty arise in a predictive application and how they can be quantified.

Recent MFiX-TFM validation efforts were reported at two extremes of time and length scale. First, large, complex simulations of a pilot-scale gasifier riser were performed over a broad range of operating conditions. Comparison with data showed excellent agreement while model parameters were fixed for all conditions modeled. Additional work is underway to improve solids holdup predictions to better match experimental data.

Finally, progress was reported on an ongoing program of detailed lab-scale models and experiments studying the hydrodynamics and chemical kinetics of solid CO2 sorbents for validation of MFiX-TFM and MFiX-DEM models. This work is part of a hierarchical validation process where small-scale validation experiments are providing high quality, detailed data for validation of hydrodynamics, heat transfer, and chemical kinetics models.

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