Multiphase Flow Science at NETL

Multiphase Models to Advance Energy Technologies

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NETL Multiphase Flow Science – 30 years of R&D

- Development, Validation, Application and Support of Practical Multiphase Flow Simulation Tools
  - Tools to guide the design, operation, and troubleshooting of multiphase flow devices
  - Emphasis on Fossil Fuel Technologies (e.g., coal gasifiers, CO₂ capture devices, Chemical Looping)

- 30+ Engineers and Scientists on the team
  - Open-source Software Tools
    - **MFiX Suite** of Multiphase CFD Software
    - **C3M** Multiphase Chemistry Management Software
    - Multiphase experimentation for model development and validation
      - High quality data made available to the public
    - Funded research with universities and industry
      - University and Industrial stakeholders help to guide MFS program
      - Access to university capability
      - Access to industrial applications

MFiX Suite - managing the tradeoff between accuracy and time-to-solution

Direct Numerical Simulation: Very fine scale, accurate simulations for very limited size domain

Discrete Element Method: Track individual particles and resolve collisions

Hybrid: Continuum and discrete solids coexist

Two-Fluid Model: Gas and solids form an interpenetrating continuum

Particle-in-Cell: Track parcels of particles and approximate collisions

Reduced Order Models: Simplified models with limited application

Model Uncertainty

Development VV&UQ
MFiX Suite

- MFiX Suite – State of Development
  - Goal is to have all codes with full set of capabilities

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<th>MFiX TFM</th>
<th>MFiX DEM</th>
<th>MFiX PIC</th>
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<td>Energy Equations</td>
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- ● – implemented and fully tested
- ○ – implemented with limited testing
- □ – not tested or status unknown
MFiX Suite – Open Source Toolset

- MFiX Suite of software has a large (>3500) user base

**FY14 new registrations**
- University: 175
- Industry: 29
- National Labs: 11
- Others: 14

**Total MFiX registrations**
- University: 2506
- Industry: 559
- National Labs: 163
- Other: 285
What Does C3M Bring to the User?

- Easy, Intuitive, Reliable, and Graphical User Interface
- Comprehensive interface between reliable sources of kinetic data and reacting, multi-phase CFD models
- “Virtual Kinetic Laboratory” for quickly assessing the validity of a chemical equation sets before going to full scale, expensive models
- Seamless formatting and units management for code specific implementation
- Advanced Chemistry Analysis and Development Tools
- Open source for collaboration and development

136+ User Downloads
96+ Version 4.0 Downloads (300% increase)
Version 5.0 Coming Soon!
Recent Developments in C3M

Virtual Experimental Capability (TGA/Drop Tube)

1) Select Species
2) Define Chemistry

Neural Network Surrogates

Unlimited Domain Scale Information
Unlimited Local Information
Reaction Rates

User Defined Modules
MFiX Graphical User Interface

Makes MFiX Easy to Use
- Providing intuitive tools to create, compile, run, and post process MFiX models.
- Cross platform, binaries available (Windows, Linux).
- Written in Python.
- Integration with MFiX website (download mfix).

Download Today: mfix.netl.doe.gov

Tutorials on YouTube

Next Release: Workflow - Automating Design of Experiments

The GUI

Internal Console

Plot

Text Editor

Documentation Viewer

Grid Editor
MFS support of the Gasification Program

- **Development of Reacting Multiphase Models for Advanced Gasification Processes**
  - Model Development and Optimization
  - Verification, Validation, and Uncertainty Quantification Tools and Processes for Multiphase Flow
  - Physical Sub-Models, Pre- and Post-Processing Tools for Model Enhancement
  - Model Application And Validation

- **Experimentation for Model Development and Validation**
  - Operation of Small-Scale Fixed, Bubbling, and Circulating Fluidized Beds for Validation
MFS support of the Gasification Program
Model Development and Optimization

- Speed and accuracy improvements to MFiX-TFM for industrial scale gasification application
- Enhancement to MFiX-DEM for large-scale reacting flows
  - Efficiency
  - Improved parallel performance
- Enhancement to MFiX-PIC for industrial scale gasification application
  - Reacting flow capability
  - Complex geometry
- Optimization of all codes for new supercomputer architectures
MFS support of the Gasification Program
Verification, Validation, Uncertainty Quantification

• Implementation of “Method of Manufactured Solutions” for MFiX Verification
• Verification “Test Harness” executed daily to monitor code development process and ensure code quality
• Multiphase Flow Validation Problem Set
  – Validation Hierarchy
• Develop and Demonstrate Methodologies to Quantify Uncertainty in Model Predictions
  – Develop and distribute a UQ Toolset
• Multiphase Flow CFD “Best Practices”

Sources of Uncertainty in Model Predictions
• Input parameter
• Surrogate model
• Model form
• Experimental data;
• Spatial discretization
• Time Averaging
MFS support of the Gasification Program
Physical Sub-Models, Pre- and Post-Processing Tools

- Enhance C3M Capabilities
- Enhance MFiX GUI Capabilities
- “Filters” for capturing small-scale effects for more accurate scale-up
- Particle size distribution
- Cohesion/Agglomeration
- Improve heterogeneous chemistry
- Improve radiative heat transfer modeling
- Bring all codes in the MFiX Suite to same level of capability
MFS support of the Gasification Program
Model Application and Validation

- Application to TRIG™ Gasifier Riser and Validation with Plant Data for Mississippi Lignite feedstock

Comparison of Model and Operating Data
- Time-averaged pressure drop values - parity plots comparing prediction to measurement

Comparison of Model and Operating Data
- Time-averaged syngas composition at riser exit

* Temperature profiles are in good agreement with measurements
* Lower mixing zone temperatures from the model are slightly higher than data
* Model overpredicts carbon and hydrogen concentration in LPG

* Predicted exit syngas compositions are in good agreement with measurements, with most discrepancies within 20%
MFS support of the Gasification Program
Model Application and Validation

- Application to TRIG™ Gasifier and Validation with Data for Mississippi Lignite feedstock
MFS support of the Gasification Program
Model Application and Validation

• **Application to Integrated Waste Treatment Unit Gasifiers – Idaho National Lab**
  - Develop and validate MFiX-TFM models of the Denitration Mineralization Reformer (DMR) and Carbon Reduction Reformer (CRR).
    - Validate with DMR (mock up) pressure data for cold flow conditions
    - Validate with CRR gas composition data for reacting conditions
  - Provide model-based information to better understand chemistry and hydrodynamics of the vessels

36 orifices for sparger ring
44 orifices for the distributor rails
30 nozzles for the 2 distributor rails
18 nozzles on side walls
• Validate with DMR pressure data for cold flow conditions

Effect of Bed Height on Bubble Behavior

Pressure Drop in Experimental Mock-up

Pressure Drop Comparison
MFiX:
Avg. = 1.56 psi
Std. Dev. = 0.14 psi
Experiment:
Avg. = 1.52 psi
Std. Dev. = 0.23 psi
MFS support of the Gasification Program
Model Application and Validation

- Validate with CRR gas composition data for reacting conditions

  - Composition
    - 10 gas species (Soot, O₂, CO, CO₂, CH₄, H₂, H₂O, N₂, HCN, C₂H₆)
    - 2 solids phases: coal (C, volatile matter, moisture, ash) and Bauxite
    - Total of 30 transport equations (continuity, momentum, energy, species)

- Heterogeneous chemical reactions:
  - Coal moisture release: \( H₂O(\ell) → H₂O(\varphi) \)
  - Pyrolysis: \( VM → 1.3788CO + 0.48148CH₄ + 2.8737₃H₂ + 0.12861₅HCN + 0.01284₉G₂H₆ \)
  - Steam gasification: \( C + H₂O ↔ CO + H₂ \)
  - CO₂ gasification: \( C + CO₂ ↔ 2CO \)
  - H₂ gasification: \( C + 2H₂ ↔ CH₄ \)
  - Char combustion: \( C + O₂ ↔ CO₂ \)

- Homogeneous chemical reactions:
  - Water gas shift: \( CO + H₂O ↔ CO₂ + H₂ \)
  - CO combustion: \( CO + \frac{1}{2}O₂ ↔ CO₂ \)
  - H₂ combustion: \( H₂ + \frac{1}{2}O₂ ↔ H₂O \)
  - CH₄ combustion: \( CH₄ + 2O₂ ↔ CO₂ + 2H₂O \)

Kinetics implemented with C3M
MFS support of the Gasification Program

- Experimentation for Model Development and Validation
  - Operation of Small-Scale Fixed, Bubbling, and Circulating Fluidized Beds for Validation
    - Small Fixed Bed for heat transfer, kinetics (1in Dx 6 in H)
    - Bubbling Fluidized Bed (4in D x 72in H)
    - Rectangular 2-D bed (2in x 0.125in x 18in H)
    - Small Scale Circulating Bed (1in D x 48in H)
  - Pilot-Scale Cold Flow Circulating Bed (12in D x 60 ft H)
  - Flow control, measurement, diagnostics
    - High Speed PIV
    - LDV
    - Low and High Speed Pressure
    - High Speed video
    - Image analysis
    - Tracer gas
• Small-Scale Bubbling Bed experiments performed with NETL CO₂ Sorbent Particles to validate MFiX-TFM
  – excellent agreement with fixed bed tests
- 2-D bed being used for detailed measurements for validation data
• High Speed PIV for local particle velocity, solids concentration

FCC at $U = 2U_{mf}$  

Frame = 400-600
Radically Engineered Modular Systems (REMS)
Use CFD Simulation-Based Optimization for Reactor Design

**Build on Existing Techniques**

- **Use of CFD-Based Optimization is growing for single phase applications**
  - Proven technique in many engineering applications - chemical process, aerospace, turbomachinery, automotive
  - Optimization of airfoil shape for lift and drag
  - Optimization of heat exchanger tube shape, size, location
  - Optimal combustor design

- **REMS will develop, validate, and apply a Multiphase CFD-based Optimization Toolset**
  - Multiphase CFD brings new challenges to the optimization process
    - Complex multiphase physics require accurate submodels for flow, heat transfer, chemical kinetics, coupling between phases
    - Very computationally intensive
    - Potential for huge datasets resulting from pilot and industrial scale applications
  - The new software capability will be based on the NETL MFiX Suite of multiphase flow CFD software
User Interface and Toolset to Manage the Optimization Process

- Design and develop GUI-based, Multi-objective Optimization software framework
  - Code infrastructure for managing the optimization process
  - Methodologies and code to create and manage reactor models created using MFIX Suite of multiphase flow software

- The modeling tools will become part of the publicly available, Open Source MFIX Suite of codes (https://mfix.netl.doe.gov)
Use CFD Simulation-Based Optimization for Reactor Design

- Optimization process will investigate radically different reactor geometries
  - Allow for precise manipulation of different coal and biomass particles
    - Segregation of low ash melting particles in a lower temperature part of the reactor
    - Continuous removal of ash or volatiles as they are created,
    - Segregation of char to a higher temperature part of the reactor
    - Segregation of catalysts and reactive particles types for more efficient conversion
    - Use of neutral/reactive particle addition and removal
  - Optimize reactant and product gas flow
    - Improve particle-gas contacting to better control carbon conversion and product composition
    - Control heat addition/removal, etc.
Summary

- Multiphase Flow Science at NETL has a long and successful history of R&D
- Our emphasis is on Multiphase CFD for dense, reacting flow
  - MFiX Suite of open source, multiphase CFD software
    - Development, VV&UQ, Application and Support
- Experiments designed for model validation are critical to our program
- Gasification is a key focus for code capability development
- The goal is a practical and useful toolset for industry
It’s All About a Clean, Affordable Energy Future

For More Information, Contact NETL

the ENERGY lab
Delivering Yesterday and Preparing for Tomorrow