MFiX - Multiphase Flow with Interphase Exchanges

Software tools and expertise to address multiphase flow challenges in research, design, and optimization

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LRST

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Project Description and Objectives

CARD: CFD for Advanced Reactor Design

• Develop, enhance, and apply NETL’s suite of MFiX software tools that are used for design and analysis of novel reactors and devices for fossil energy (FE) applications.

• Enable science-based models as viable tools to reduce the risk, cost, and time required for development of novel FE reactors.

• Open-source codes are developed, validated, and supported in-house by NETL’s software development and application specialists.

• Support the following FE pillars of research:
  • Modernization of existing coal fleet
  • Development of coal plants of the future
  • Reduction of the cost of carbon capture, utilization, and storage (CCUS)

• Unique NETL competencies:
  • Multiphase flow modeling expertise
  • Joule 2.0 Supercomputer
  • MFAL: high fidelity data that measures key performance parameters across a broad range of flow conditions—including fixed bed, bubbling, turbulent, entrained flow, and CFBs
Task 2: MFiX Development, Validation, and Enhancements

• Graphical user interface (GUI)
  • Increase usability of the code
  • Minimize error in setup, execution, and post processing.

• Additional Models/physics required for challenging FE applications:
  • Particle in Cell
  • Coarse Grain Discrete Element Method
  • Non-spherical particles
  • Polydispersity
  • Acceleration of the flow solver

• Quality Assurance (QA) Program
  • Validation
  • Verification
  • Improved documentation, user guides, and validation experiments.

• Outreach capabilities through the MFiX web portal to better serve FE and NETL stakeholders.
MFiX Suite of Multiphase CFD Software

Capabilities and Benefits

• **Versatile toolset** (hydrodynamics, heat transfer, chemical reactions)

• **Gas/solids flows**
  - Gas: transport equations (continuity, momentum energy species)
  - Solids: transport equations or particle tracking

• **Open source**
  - Developed at NETL, in-house expertise
  - Runs on large HPC systems

• **Accelerate development and reduce cost**

• **Optimizes performance**

• **Reduces design risks**

MFiX-TFM (Two-Fluid Model)
MFiX-DEM (Discrete Element Model)
MFiX-PIC (Multiphase Particle-In-Cell)
MFiX-CGDEM (Coarse Grain DEM)

MFiX Exa (Exascale) – under development
C3M multiphase chemistry management software
Nodeworks: Optimization and UQ Toolsets
Tracker: Object tracking in videos/image stack

MFS Software Portfolio
MFiX Suite of Multiphase CFD Software

Managing the tradeoff between accuracy and time to solution

- **DNS** (Direct Numerical Simulation): fine scale, accurate simulations for limited size domain
- **Discrete Element Method (DEM)**: track individual particles and resolve collisions
- **Two-Fluid Model (TFM)**: gas and solids form an interpenetrating continuum

- **Exascale (Ex)**: new code for new generation of computers
- **Particle-in-Cell (PIC)**: track parcels of particles and approximate collisions
- **Reduced Order Models (ROM)**: simplified models with limited application

**Model Uncertainty**
MFiX-TFM: Two Fluid Model

Continuous and disperse phases (e.g., gas and solids) are treated as coexisting continua.

Highlights

- Long track record of successfully supporting DOE-FE priorities
- Computationally efficient
- Historical workhorse for large-scale FE applications

Technical limitations

- Unable to efficiently model phenomena like particle size distributions
- Relies on complex constitutive relations to approximate solid stresses
- Ad hoc extension to multiple solids phases

\[ \frac{\partial}{\partial t} (\varepsilon_g \rho_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{u}_g) = S_g \]

\[ \frac{\partial}{\partial t} (\varepsilon_g \rho_g \mathbf{u}_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{u}_g \mathbf{u}_g) = -\varepsilon_g \nabla p_g + \nabla \cdot \tau_g + \varepsilon_g \rho_g \mathbf{g} + \sum_m g_{g,m} \]

\[ \frac{\partial}{\partial t} (\varepsilon_m \rho_m) + \nabla \cdot (\varepsilon_m \rho_m \mathbf{u}_m) = S_m \]

\[ \frac{\partial}{\partial t} (\varepsilon_m \rho_m \mathbf{u}_m) + \nabla \cdot (\varepsilon_m \rho_m \mathbf{u}_m \mathbf{u}_m) = -\nabla p_m + \nabla \cdot \tau_m + \varepsilon_m \rho_m \mathbf{g} - g_{g,m} \]

Solver time: Fluid Solid (one solids phase)
MFiX-DEM : Discrete Element Model

Fluid is a continuum and particles are individually tracked, resolving particle-particle-wall collisions

Advantages

- Uses first principles to account for particle interactions, reducing model complexity.
- Fewer complex closures results in less overall model uncertainty.
- Only open-source, fully coupled CFD-DEM code designed for reacting flows.

Technical limitations

- Computationally expensive, limiting the size of systems that can be modeled.
- Fluid-particle interaction is closed using drag models.

Fluid continuity equation:

\[ \frac{\partial}{\partial t} (\varepsilon_g \rho_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{u}_g) = S_g \]

Fluid momentum equation:

\[ \frac{\partial}{\partial t} (\varepsilon_g \rho_g \mathbf{u}_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{u}_g \mathbf{u}_g) = -\varepsilon_g \nabla p_g + \nabla \cdot \mathbf{r}_g + \varepsilon_g \rho_g \mathbf{g} + \sum_p \mathbf{j}_{g,p} \]

Particle continuity equation:

\[ \frac{\partial}{\partial t} (m_p) = S_p \]

Particle momentum equations:

\[ m_p \frac{\partial \mathbf{u}_p}{\partial t} = m \mathbf{g} + F_{\text{coll}} - \mathbf{j}_{g,p} \]

\[ l_p \frac{\partial \mathbf{\omega}_p}{\partial t} = \mathbf{T} \]
**MFiX-DEM : Discrete Element Model**

Fluid is a continuum and particles are individually tracked, resolving particle-particle-wall collisions

**Advantages**
- Uses first principles to account for particle interactions, reducing model complexity.
- Fewer complex closures results in less overall model uncertainty.
- Only open-source, fully coupled CFD-DEM code designed for reacting flows.

**Technical limitations**
- Computationally expensive, limiting the size of systems that can be modeled.
- Fluid-particle interaction is closed using drag models.

**Fluid continuity equation:**
\[
\frac{\partial}{\partial t} (\varepsilon_g \rho_g) + \nabla \cdot \left( \varepsilon_g \rho_g \mathbf{u}_g \right) = S_g
\]

**Fluid momentum equation:**
\[
\frac{\partial}{\partial t} (\varepsilon_g \rho_g \mathbf{u}_g) + \nabla \cdot \left( \varepsilon_g \rho_g \mathbf{u}_g \mathbf{u}_g \right) \\
= -\varepsilon_g \nabla p_g + \nabla \cdot \mathbf{\tau}_g + \varepsilon_g \rho_g \mathbf{g} + \sum_p \mathbf{j}_{g,p}
\]

**Particle continuity equation:**
\[
\frac{\partial}{\partial t} (m_p) = S_p
\]

**Particle momentum equations:**
\[
m_p \frac{\partial \mathbf{u}_p}{\partial t} = m \mathbf{g} + F_{coll} - \mathbf{j}_{g,p} \\
l_p \frac{\partial \omega_p}{\partial t} = \mathbf{T}
\]

**P-P and P-W collisions are resolved (soft sphere)**
MFiX-CGDEM : Coarse Grain Discrete Element Model

Fluid is a continuum, particles are grouped into larger particles (CGP). CGP are individually tracked, resolving collisions.

Advantages
- Same formulation as DEM
- Runs faster than DEM

Technical limitations
- Loss of accuracy for large statistical weights

Fluid continuity equation:
\[ \frac{\partial}{\partial t} (\varepsilon_g \rho_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{u}_g) = \mathcal{S}_g \]

Fluid momentum equation:
\[ \frac{\partial}{\partial t} (\varepsilon_g \rho_g \mathbf{u}_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{u}_g \mathbf{u}_g) = -\varepsilon_g \nabla p_g + \nabla \cdot \mathbf{\tau}_g + \varepsilon_g \rho_g \mathbf{g} + \sum_p \mathcal{J}_{g,p} \]

Particle continuity equation:
\[ \frac{\partial}{\partial t} (m_p) = \mathcal{S}_p \]

Particle momentum equations:
\[ m_p \frac{\partial \mathbf{u}_p}{\partial t} = m \mathbf{g} + F_{coll} - \mathcal{J}_{g,p} \]
\[ I_p \frac{\partial \omega_p}{\partial t} = \mathcal{I} \]

Drag force is based on real particle size

Solver time: Fluid        Solid
MFIX-PIC: (Multiphase) Particle-in-Cell

Fluid is a continuum and particles are tracked as parcels, solid-stress model approximates collisions

Advantages
- Computationally efficient
- Able to track particle-scale phenomena like time-histories and size distributions
- Only open-source, PIC model

Technical limitations
- Relies on a continuum stress model to approximate particle-particle interactions
- Strong dependence on implementation

Formally released: April, 2019

Fluid continuity equation:
\[
\frac{\partial}{\partial t} (\varepsilon_g \rho_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{u}_g) = S_g
\]

Fluid momentum equation:
\[
\frac{\partial}{\partial t} (\varepsilon_g \rho_g \mathbf{u}_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{u}_g \mathbf{u}_g) = -\varepsilon_g \nabla p_g + \nabla \cdot \mathbf{\tau}_g + \varepsilon_g \rho_g \mathbf{g} + \sum_p \mathbf{j}_{g,p}
\]

Parcel continuity equation:
\[
\frac{\partial}{\partial t} (m_p) = S_p
\]

Parcel momentum equation:
\[
m_p \frac{\partial \mathbf{u}_p}{\partial t} = m \mathbf{g} + \nabla \mathbf{\tau}_p - \mathbf{j}_{g,p}
\]
What can be modeled with 1 Million particles?

100 μm

200 μm

500 μm

1,000 μm
Enabling large Scale simulations

DEM example

Height = 0.68 m
Particle diameter = 800 microns
Particle count = 500,000 particles
Enabling large Scale simulations

Height = 4.0 m  (x6)
Particle count = 650 Millions (x1,300)
- DEM
- PIC, Parcel counts = 13 Millions

Height = 0.68 m
Particle count = 500,000
- DEM
### Multi-Phase Particle In Cell (MP-PIC)

**Use MP-PIC for computational speed and averaged accuracy**

<table>
<thead>
<tr>
<th>Parcel</th>
<th>Solid Stress Gradient</th>
<th>Momentum Conservation</th>
<th>Collision Resolved</th>
<th>CGPM</th>
<th>CGHS</th>
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<tbody>
<tr>
<td>CGPM</td>
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<td></td>
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<td>Coarse Grained Particle Method</td>
<td>Coarse Grained Hard Sphere</td>
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<td>Event Driven/ Time Driven Hard Sphere</td>
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<td>Tsuji et al., 1993</td>
<td></td>
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<td></td>
<td>Ouyang and Li, 1999</td>
<td></td>
</tr>
</tbody>
</table>

**MP-PIC**

- Multi-Phase Particle In Cell
- Andrews and O’Rourke, 1996

- REDUCED ACCURACY

- SOLIDS REPRESENTATION

- INCREASED COMPUTATIONAL SPEED

MP-PIC can significantly reduce computational effort, and in the right type of application, maintain accuracy.
Multiphase Particle In Cell (MP-PIC)

Simulation of industrial scale multi-phase flow devices is within MFiX’s grasp!
MFiX-PIC couples the MFiX Eulerian fluid solver with new Lagrangian solids stress model.

- ~4 meters tall
- 650 million particles
- 13 million PIC parcels
- 200 cores on Joule 2
- 15 seconds/day
MFiX Development

Recent developments

• 20.4  • Coarse Grain DEM
  • PIC collision damping

• 21.1  • 2x fluid solver speedup
  • Procedural STL
  • 6 new drag laws, 3 new Nusselt number correlations

• 21.2  • CGDEM specify statistical weight per phase
  • Force chain visualization
  • Reaction rate output
  • Filtering of particle_input.dat/partile_output.dat

• 21.3  • Guo-Boyce friction model
  • Residence time output
  • Create animation from GUI

• 21.4  • Polydispersity for PIC

• 22.1  • DEM Rolling friction
MFiX Development

20.4 – Coarse Grain DEM

- Particles are lumped together to create a CG particle
- CG particles collide with each other
- Heat transfer, chemical reactions
- MFiX-CGDEM formal release: 12/31/2020

Coarse Grain DEM – **10 to 100x speedup** compared with DEM

Original system with \( N \) particles
(color stands for different species fraction and temperature, vector stands for velocity)
MFiX Development
CG-DEM Simulation of 2-inch Fluidized Bed Pyrolysis Reactor

1. Sands & 130 microns Biomass
2. Coarse Grained DEM Simulation
3. Hybrid drag model
4. DNS calibrated heat transfer & reaction kinetics
21.1 PIC Collision Damping

- Update parcel velocity (regular PIC algorithm)

- Compute mean velocity
  \[ \bar{V}_i = \frac{\int \int m v_i d m d v_i}{\int \int m d m d v_i} \]

- Compute std.dev
  \[ \sigma = \left( \frac{\int \int (v_i - \bar{V}_i)^2 m d m d v_i}{\int \int m d m d v_i} \right)^{1/2} \]

- Compute Sauter mean radius
  \[ r_{32} = \frac{\int \int r^3 m d m d v_i}{\int \int r^2 m d m d v_i} \]

- Compute radial dist. function
  \[ g_0(\theta) = \frac{\theta_{cp}}{\theta_{cp} - \theta} \]
  \[ \frac{1}{\tau_D} \rightarrow \frac{16}{\sqrt{3\pi r_{32}}} g_0\theta(1-\eta) \]

- Compute collision frequency

- If collision frequency is not zero: replace regular PIC velocity with
  \[ \nu_{p}^{n+1} = \frac{\nu_{p}^{n} + (\delta t / 2 \tau_D) \bar{V}_i}{1 + (\delta t / 2 \tau_D)} \]

- Restitution coefficient \( e_p \) controls amount of damping
  \[ \eta = \frac{1 + e_p}{2} \]

- Setting \( e_p = 1 \) turns off damping

- Introduced a new keyword `pic_cd_e` instead of reusing `mppic_coeff_en1`

- If collision frequency is very large, we “replace” parcel velocity with the average velocity
Test case: Jet collision

- Collision of gas–solid jets
- 2 jets colliding
- Solids fraction = 0.1, velocity = 20m/s
- No energy loss at walls ($e_w = 1$)
- Statistical weight = 1
- Without collision damping, the two jets do not interact
- Polydisperse system, particle diameter:
  - Mean=650 μm, σ=25 μm, clipped at mean±2σ
  - Mean=350 μm, σ=25 μm, clipped at mean±2σ

Fig. 5. Channel geometry used for the calculations of two impinging gas-particle jets.
MFiX Development

Mean=650 μm, σ=25 μm, clipped at mean±2σ

Time: 0.0002 s

No damping

With damping, ep=0.8
MFiX Development

Mean=650 μm, σ=25 μm, clipped at mean±2σ

No damping

With damping, ep=0.8

Barracuda (Paper)

MFiX
MFiX Development

Mean=350 μm, σ=25 μm, clipped at mean±2σ

With damping, ep=0.8
With damping, ep=0.9

Barracuda (Paper)
MFiX Development

21.1 Fluid solver 2x speedup

• Single Phase benchmarks
  • SQUARE PIPE: Steady State
  • BLUFF BODY
  • SQUARE PIPE DYNAMIC: Unsteady, transient inlet BC
• MFiX tutorials
  • FLD VORTEX SHEDDING
  • TFM HOPPER 3D
  • TFM HOPPER 2D
  • DEM CYCLONE
  • PIC LOOPSEAL

• Timing based on 1 to 3 repeats, manually launched on a dedicated node on Joule
• 21.1 Milestone: Accelerate fluid solver by a factor of 2
MFiX Development

21.1 Fluid solver 2x speedup

- Reference: MFiX 20.4, “-O2”, Line PC, ppg_den=10, epp_den=10
- Dev: Feb 2021 develop version:
  - Code change: SS convergence criteria: only affects Steady State simulations
  - Regular vs Optimized Thomas algorithm: only affects simulation with Line PC (Charles Waldman)
  - New control for PPG and EPP residual scaling (ppg_den, epp_den): loosen convergence when norm_g=0, norm_s=0; default values: ppg_den=10, epp_den=10
- Optimization flag: “-O2” (default) vs “-march=native -O3”
- Line PC: On vs OFF

- REF (20.4)
- Dev (-O2)
- Dev (Native -O3)
- Dev (-O2) + Thomas
- Dev (Native -O3) + Thomas
- Dev (-O2), No PC
- Dev (Native -O3) + ppg_den=1
- Dev (Native -O3) + ppg_den=1, NoPC
21.1 Fluid solver 2x speedup

Speedup: Higher is better
21.1 Fluid solver 2x speedup

- New convergence criteria for Steady State: ~ 4x speedup
- “march=native –O3”: 3 to 14% faster
- Optimized Thomas algorithm: 3 to 11% faster
- Lowering ppg_den from 10 to 1: up to 25% faster (helps when ppg is dominant residual)
- Turning off the PC:
  - ~ 2x speedup (fluid solver)
  - May fail to converge if DT=cst with bad initial conditions (need to set adaptive DT)
- Best combination: No PC, “march=native –O3” flag, ppg_den=1

Better to start with small DT

Faster than real time!!
MFiX Development

21.2 – Force chain visualization
Ability to visualize force chain
Between particles (DEM)
MFiX Development

21.3 – Guo-Boyce friction model (TFM)

- This model was graciously provided by researchers from Columbia University, NY.
- Allows to correctly predict bubble pattern in a pulsating fluidized bed.

Qiang Guo, Yuxuan Zhang, Azin Padash, Kenan Xi, Thomas M. Kovar, Christopher M. Boyce, "Dynamically structured bubbling in vibrated gas-fluidized granular materials", Proceedings of the National Academy of Sciences Aug 2021, 118 (35) e2108647118; DOI: 10.1073/pnas.2108647118

Time = 5.00 s
MFiX Development

21.4 Polydispersity for PIC

- Extension of DEM polydispersity
- Normal distributions
- log-normal distributions
- Custom distributions
- Boundary condition and initial condition
MFiX Development

22.1 DEM Rolling friction
22.1 DEM Rolling friction

**Test case 2**: Formation of a stagnant zone

- Particles initially in the top half
- Particle sizes = 6 mm and 10 mm
- Particles collect at the bottom once the ends are opened.
- A stagnant zone at the midplane is formed whose characteristics depend on the value of the rolling friction coefficient
- As the value is increased, more particles accumulate in the stagnant zone. In our case, we obtain reasonable results while using $\mu_r = 1.0E^{-4}$ m.
- Good qualitative comparison of final particle locations between MFiX-DEM predictions and the work of Zhou et al.

Non-spherical particles (SuperDEM)

• Superquadrics are a family of geometric shapes defined as

\[
\left(\frac{x}{a_1}\right)^{\frac{2}{\varepsilon_2}} + \left(\frac{y}{a_2}\right)^{\frac{2}{\varepsilon_1}} + \left(\frac{z}{a_3}\right)^{\frac{2}{\varepsilon_1}} = 1
\]

• Can represent ~ 80% of all shapes by varying five parameters

\[
[a_1, a_2, a_3, \varepsilon_1, \varepsilon_2]^T
\]

Semi-axis  roundness parameters

Superquadric particles

\(a_1=2\)  \(a_2=2\)  \(a_3=4\)
SuperDEM examples

M&M candy static packing
Cylinder candy static packing

Cylinder rotating drum

M&M candy discharging from a hopper
Validation experiment

The solver was parallelized using MPI.

Simulation on NETL supercomputer Joule 2 (80K cores), World Top 60, 2020

Non-spherical particles fluidization simulation, 100 million (6800 cores)
Non-spherical particles code acceleration

\[
\left( \left| \frac{x}{a} \right|^m + \left| \frac{y}{b} \right|^m \right)^{n/m} + \left| \frac{z}{c} \right|^n
\]

- Need to compute \( x^y \) for non-integer \( x \) and \( y \).
- Range \( 0 \leq x \leq 2 \) and \( y \geq 1 \).
- 70% code spent on exponentiations
- Integer powers and square roots are computationally inexpensive
- We can compute certain powers quickly, e.g. \( x^{2.5} \) is \( x \times x \times \sqrt{x} \) (not an approximation)
- Constrain \( m \) and \( n \) to be integers or dyadic rationals
- Does not guarantee that the ratio \( n/m \) is similarly nice
- Restricting values on \( m \) and \( n \) such that \( m,n \) and the ratio \( n/m \) are lead to an efficient exponent computations
Non-spherical particles code acceleration

- Prototype function xpow
- Checks for integer exponents or exponents of the form $a+b/4$
- Efficient methods based on squaring and square roots
- 6x speedup compared with built-in math library
- Overall speedup on hopper benchmark is about 2.1x
Non-spherical particle drag

Non-spherical particle drag law

- Detailed simulations of flow around prolate spheroids
- Lattice Boltzmann method (LBM).
- Reynolds numbers range $0.1 \leq Re \leq 2000$
- Incident angles $0^\circ \leq \Phi \leq 90^\circ$
- Aspect ratios $1 \leq \lambda \leq 16$.
- Accurate correlations for average drag, lift and torque coefficients are proposed.

Sathish Sanjeevi, Jean-F. Dietiker, and Johan T. Padding, “Accurate hydrodynamic force and torque correlations for prolate spheroids from Stokes regime to high Reynolds numbers “, accepted for publication,  Chemical Engineering Journal
Non-spherical particle drag

Lift and drag
Non-spherical particle drag

Non-spherical particle drag law

Lift and drag

Figure 12: Comparison of $C_D$ against $\phi$ for $\lambda = 2.5$ at (a) $Re = 100$ and (b) $Re = 2000$.

Figure 13: Comparison of $C_D$ for a particle of $\lambda = 6$ at $\phi = 45^\circ$ from different correlations with the DNS data of Jiang et al. [21, 22].
Hundredfold Speedup of MFiX-DEM using GPU

DEM solver was ported to GPU (prototype)

• 170 fold speedup with double precision, 243 fold with single precision
• Re-use CFD, interphase coupling, and chemical reaction modules in MFiX

Fluidized bed Speedup

<table>
<thead>
<tr>
<th>Method</th>
<th>COMPUTATION TIME (HR)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MFiX-CPUDDEM</td>
<td>69.52</td>
</tr>
<tr>
<td>DEM</td>
<td>76.22</td>
</tr>
<tr>
<td>CFODEM</td>
<td>76.25</td>
</tr>
<tr>
<td>TOTAL</td>
<td>6.70</td>
</tr>
</tbody>
</table>

Particle packing Speedup

<table>
<thead>
<tr>
<th>Method</th>
<th>SPEEDUP (GPU/CPUD)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle Parallel (PP)</td>
<td>120.1</td>
</tr>
<tr>
<td>Collision Pair Parallel (CPP)</td>
<td>130.2</td>
</tr>
<tr>
<td>CPP/PP</td>
<td>120.1</td>
</tr>
</tbody>
</table>

Heat transfer & chemical reactions (biomass drying)
Hundredfold Speedup of MFiX-DEM using GPU

Effect of coarse graining
Glued-sphere DEM

Irregular Shape of Particles

• Composite spheres
• Intra-particle temperature distribution
MFiX Quality Assurance

Building Confidence in Simulation Results

- **Verification**
  - Code verification – Does the code do what we expect?
  - Solution verification – Is the answer any good?
- **Validation** - How does the answer compare to the real world?
- **Uncertainty Quantification**
  - Where is the error in my solution coming from?
  - What happens to my answer when I change an input to my model?

**Accomplishments** (https://mfix.netl.doe.gov/mfix/mfix-documentation)
- MFiX Verification and Validation Manual 2nd Ed. (PDF & html)
- PIC theory guide (May 2020)
MFiX Quality Assurance

Building Confidence in Simulation Results

- PIC parameter sensitivity and calibration
  - How sensitive are PIC simulations to PIC model parameters?
  - Recommend parameter values for a given type of application

Cases selected to cover a broad range of flow conditions

- Particle Settling: $U/U_{mf} < 1.0$ ($P_0 \sim 1$) (Analytical solution)
- Bubbling Fluidized bed: $U/U_{mf} \sim 1$ ($P_0 \sim 10$)
- Circulating Fluidized bed: $U/U_{mf} >> 1.0$ ($P_0 \sim 100$)

Parcel momentum equation

$$
\frac{d\bar{V}_p}{dt} = \beta (U_g - \bar{V}_p) - \frac{1}{\rho_p} \nabla p - \frac{1}{\epsilon_p \rho_p} \nabla \tau_p + \ddot{g}
$$

$$
\tau_p = \frac{P_0 \epsilon_p^\beta}{\max (\epsilon_{cp} - \epsilon_p, \delta (1 - \epsilon_p))}
$$
C1: Particle settling

Sensitivity analysis and Deterministic calibration

- Response surface (55 samples)
- Sobol indices show:
  - main effects (first order)
  - interactive effects (second order)

Parameters obtained through deterministic calibration

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Default</th>
<th>Range</th>
<th>Calibrated</th>
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</thead>
<tbody>
<tr>
<td>t1: Pressure linear scale factor</td>
<td>100</td>
<td>[1,20]</td>
<td>14.309</td>
</tr>
<tr>
<td>t2: Vol. fraction exponential scale factor</td>
<td>3.0</td>
<td>[2.5]</td>
<td>2.165</td>
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<tr>
<td>t3: Statistical weight</td>
<td>5.0</td>
<td>[3,20]</td>
<td>12.241</td>
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<td>t4: Vol. fraction at maximum packing</td>
<td>0.42</td>
<td>[0.35,0.5]</td>
<td>0.399</td>
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<td>t5: Solid slip velocity factor</td>
<td>1.0</td>
<td>[0.5,1.0]</td>
<td>0.828</td>
</tr>
</tbody>
</table>
MFiX Development

**EY22 plans**

- **Validation and formal release of superDEM particle capability**
  - Step-change from the typical approximation of spherical particle shape
  - Code optimization for faster turn-around time on large supercomputing systems
  - These capabilities allow for accurate modeling of mixed feedstocks of large, reacting particles

- **Validation and Formal release of multiphase radiation modeling capability**
  - This work incorporates the development work performed by University of Wyoming under NETL support
  - New radiation models available for all multiphase modeling approaches (TFM, DEM, PIC)
  - Enhanced accuracy of heat transfer in high temperature FE reactors

- **Development of conjugate heat transfer capability in MFiX**
  - Accurate modeling of internal heat transfer surfaces critical to industrial scale reactors
  - Critical capability for Hydrogen production and Oxygen separation technologies

- **Continued development of the Graphical User Interface (GUI)**
  - Improved usability, reduced user setup error, faster overall workflow
  - Contributes to a larger MFiX community worldwide and better visibility of NETL’s multiphase modeling expertise

- **Continued Verification and Validation efforts**
  - Improved confidence in new implemented models
  - Documentation of parameters sensitivity and best practices for simulation setups
Comparison with other codes

MFiX – Ansys Fluent (2021)

Marchelli, F.; Di Felice, R. A Comparison of Ansys Fluent and MFiX in Performing CFD-DEM Simulations of a Spouted Bed. Fluids 2021, 6, 382. https://doi.org/10.3390/fluids6110382

“Both programs can provide acceptable qualitative predictions when employing standard settings. If the Di Felice drag model is applied, MFiX yields better results and provides a very good quantitative reproduction of the experimental particle velocity profile. Moreover, despite employing similar mesh and time steps and the same number of particles, MFiX is about 17 times faster. However, Fluent seems to respond slightly more efficiently to an increase in the particle number and appears to have better parallelisation functionalities. “
MFiX featured on Journal covers

*Investigating the rheology of fluidized and non-fluidized gas-particle beds: implications for the dynamics of geophysical flows and substrate entrainment*

*GPU accelerated MFiX-DEM simulations of granular and multiphase flows*
By L. Lu

*Using a proper orthogonal decomposition to elucidate features in granular flows*
By J. E. Higham, M. Shahnam & A. Vaidheeswaran
Resources – MFiX website

- Showcase NETL’s Multiphase Flow Science (MFS) team
  - MFS software
  - Documentation
  - Forum
  - Experimental data (Challenge pbs)
  - Publications
  - Workshop proceedings
  - News, announcements

Install MFiX

For detailed setup instructions, follow the setup guide.

Setup Guide

Windows  Linux  Mac  Source / Pip

Install Anaconda

Download and install Anaconda (link op)

Anaconda Download

Install MFiX (in new)

Open the Anaconda Prompt (installed)

Copy and paste the following command

MFiX Version 21.4 condac iore

This will create a new conda environment.

Run MFiX

MFiX Documentation

Latest Documentation

- MFiX User Manual HTML  PDF
- MFiX Verification and Validation Manual, Second Edition HTML  PDF
- MFiX PIC Theory Guide PDF
- Software Plugins

Older Documentation

- Summary of MFiX Features (2015)
- DEM documentation (2015)
- Cartesian grid user guide (2015)
- Particle swarm optimization (2012)
- Fortran compiler (2012)

Legacy Manuals

- Numerics guide (1998)

MFiX Training

- MFiX Training (2011)

https://mfix.netl.doe.gov
Resources – MFiX website

List of Publications

Sort by: Year (Newest to Oldest)  

Total: 663

Publication Year 2022


MFiX Forum

- User support
- Categories
  - Installation
  - How to
  - Bug report
  - Share
- Topics (threads)
- File attachment
- Searchable

https://mfix.netl.doe.gov/forum
MFiX User Community

7,000+ all-time MFiX registrations

Top 5 Countries

<table>
<thead>
<tr>
<th>Country</th>
<th>KPI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Canada</td>
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</tr>
<tr>
<td>Brazil</td>
<td>395</td>
</tr>
<tr>
<td>India</td>
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<tr>
<td>China</td>
<td>1,120</td>
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<tr>
<td>USA</td>
<td>1,464</td>
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</tbody>
</table>
Sorbent-based Carbon Capture - MFiX-DEM

Compare Simulations to Small-Scale, Reacting Flow Measurements

Simulation Results: MFiX-DEM

NETL CO₂ Capture Rig
Excellent comparison between modeled and measured solids holdup (pressure drop values) around the flow loop.
Decarbonization through gasification of coal, Biomass and MSW

Commercial-scale gasifier design (22MW)

Accomplishments

- Support the University of Alaska-Fairbanks Modular Gasification project
- Model validated with Sotacarbo pilot scale data
- 3D, transient simulation of prototype gasifier compares well to UAF design
- Transient response of gasifier to load variations, ramp-rate and turndown
- Gasifier performance for coal-biomass co-feed conditions to explore novel Net Zero Carbon, BECCS, and H2 production has been modeled

Impact: NETL’s model predicts gasifier performance relative to feedstocks and operating conditions

- Predicted syngas data will provide key information for design of downstream components including engines for generators
- Modeling effort will significantly de-risk the design of the $46million facility

Reactor dimensions: 3.05 m diameter x 4.5 m height
Solids inventory: >10 tons
Number of CG particles: ~130,000
Time scale (physical time): >10 hours

Advanced Reactor System – MFiX CGDEM

Plant Design Conditions (100% load)
Simulations show that the prototype gasifier is adaptable to a wide range of oxygen enriched conditions with steam and CO₂ diluents.

- This meets key requirements for candidate gasifiers for Net Zero Carbon and H₂ production.
- Oxygen-blown with steam produces higher H₂ as expected.
Biomass gasification – MFiX CGDEM

FABER (Fluidized Air Blow Experimental Gasifier Reactor)

Project Goals:
• Develop reaction kinetic for Cypress Biomass gasification
• Validate reaction kinetic for FABER
• Design and optimization of the fluidized bed reactor

Accomplishments
• Gasification of Cypress biomass in FABER was simulated.
• Gasification reaction kinetics were developed and validated against experimental results.

Reactor dimensions: ID = 0.489 m, height = 5.733 m
Number of CG particles: ~64,000
Solids inventory: Sand 234 Kg, Biomass 25 Kg
NETL and Natural Resources Canada-CanmetENERGY have teamed to study CFB combustion systems with coal-biomass co-feed with potential for carbon capture

Accomplishments:

• NETL is simulating the 50kWth pilot CFB system being operated at NRCan over a range of coal-biomass blends and oxygen-enrichment conditions
• The collaboration provides NETL with high quality, detailed data describing rig operations which is critical information for validating the model
• The model is providing NRCan with valuable insight on conditions inside the system to help guide system optimization

Impact:

• Once validated at the small pilot scale, these MFiX models running on FE’s JOULE2 Supercomputer will be used to study scale-up and performance optimization of coal-biomass CFB combustion systems designed for negative CO2 emissions
Hydrodynamics Benchmarking – Effect of Drag Model

- First step: validate hydrodynamics
- Riser-only simulations
- Fluidization is impeded by applying the filtered drag model, so more particles are retained in the lower riser
- Circulation rate is reduced, reflected in the average mass of recirculated particles in the side inlet
- Pressure drop distribution and overall pressure drop using the filtered drag model show better agreement with the experimental results ($P_p = 10$, $\gamma = 3$)

First 5s shown
Biomass particles enlarged 50x for visualization of shrinking particle due to pyrolysis and char combustion.
Thank you!