

NETL Multiphase Flow Research Overview

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Jack Halow's Computational Science Team Circa 1999



A world class capability for addressing Fossil Energy's key priorities

3 Decades of development history

5,000+ registered users

5 Fold return on investment*

* Not including the value of knowledge disseminated to universities & industry

175+ downloads per month 400+

citations per year



MFiX with new capabilities released

MFiX 19.1 April 2019

Particle in Cell (PIC) model puts simulation of industrial scale multi-phase flow reactors within our grasp!



50 kW Chemical Looping reactor



MFiX 19.2 July 2019

- Text editor in GUI
- Keyword search
- Advanced pane for user-defined keywords
- Material database to import particle diameter and density

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Tracker 19.1 released (July 2019)



Particle tracking velocimetry application





Added template matching, calibration tool, and efficiency improvements

Weber J, Bobek MM, Rowan SL, Yang JJ, Breault R. Tracker, An Opensource Particle Tracking Velocimetry (Ptv) Application Applied To Multiphase Flow Reactors. AJKFLUIDS2019-5181, Proceedings of the ASME-JSME-KSME 2019 Joint Fluids Engineering Conference, July 28-August 1, 2019, San Francisco, CA, USA



Nodeworks 19.1 released (April 2019)



Enables optimization and uncertainty quantification workflows

uncertainty

5 sensitivity

analysis methods





methods

MFiX + Nodeworks used to optimize cyclone NE NATIONAL

100 MFiX PIC simulations, varying 5 geometric parameters





- 11X lower pressure drop
- 2.3X lower mass loss

Weber J, Fullmer W, Gel A, Musser J. Optimization of a cyclone using multiphase flow computational fluid dynamics. AJKFLUIDS2019-5182, Proceedings of the ASME-JSME-KSME 2019 Joint Fluids Engineering Conference, July 28-August 1, 2019, San Francisco, CA, USA



VVUQ framework demonstrated



Parity plot

A Verification, Validation, and Uncertainty Quantification framework for granular and multiphase flows was developed and demonstrated



Response surface

Gel A, Vaidheeswaran A, Musser J, Tong CH. Toward the Development of a Verification, Validation, and Uncertainty Quantification Framework for Granular and Multiphase Flows—Part 1: Screening Study and Sensitivity Analysis. J. Verif. Valid. Uncert.. 2019; 3(3)



Accelerating CFD with machine learning and TensorFlow





Buchheit K, Owoyele O, Jordan T, Van Essendelft D. The Stabilized Explicit Variable-Load Solver with Machine Learning Acceleration for the Rapid Solution of Stiff Chemical kinetics. <u>https://arxiv.org/abs/1905.09395</u>



40K cells/node: 120X faster than LSODA serial 20X faster than LSODA MPI 2M cells/node: 300X faster than LSODA serial



Micro-Encapsulated Carbon Solvent (MECS)



CFD Model developed:¹

- High CO₂ capacity and selectivity of liquid solvents
- Enabling very viscous or precipitating solvents
- High surface area of solid sorbents



1) Finn J, Galvin J. Int J of Greenhouse Gas Control, Vol 74 (2018) pp. 191-205

CFD model validation with benchscale experimental data²



2) Finn J, Galvin J, Hornbostel K, CFD investigation of CO₂ absorption/desorption by a fluidized bed of microencapsulated solvents, submitted to CES, June 2019. Experiments and model predictions demonstrate that modest compressive forces can lead to significant water loss³



3) Finn J, Galvin J, Panday R, Ashfaq H. Deformation and water loss from solvent filled microcapsules under compressive loads, submitted to AIChE J., Jan. 2019.



NATIONAL Validation of a biomass pyrolyser model based on MFiX-CGDEM ENERGY TECHNOLOGY LABORATORY



Biomass cumulative mass at inlet







Optimize part-load operation of power plants

CFD model





Proxy Model Using Deep Neural Net



Gas temperature in the combustion rig

Next Steps: Apply methodology to the Tri-State/ Escalante 285 MW Boiler under turn-down operations.

Ansari A, Mohaghegh SD, Shahnam M, Dietiker JF. Modeling Average Pressure and Volume Fraction of a Fluidized Bed Using Data-Driven Smart Proxy. *Fluids* **2019**, *4*, 123.





Drag model developed for sand-biomass co-fluidization



Hybrid drag model:

57.2mm

25.4mm

Distributor

3.33 Umf,

4.44 Umf

5.55 Umf

Syamlal-O'Brien drag model for sand Gidaspow model with Ganser correction for biomass



Lu L, Gao X, Shahnam M, Rogers WA. Coarse Grained CFD-DEM Simulation of Sands and Biomass Fluidization with a Hybrid Drag Model. Submitted to AIChE Journal 2019.

Hybrid drag model has the least error in the predicted pressure drop, based on data from six locations, and different biomass loads and fluidization velocities.





Energy Efficiency & Renewable Energy

BIOENERGY TECHNOLOGIES OFFICE



14.1

- Vapor-phase upgrading (VPU) reactor model validated and used to predict residence time distribution (RTD)
- Model coupled with VPU kinetics to predict reactor performance
- The model will be used for process integration and scale up

Gao X, Li T, Rogers WA. CFD simulation of hydrodynamics, RTD, heat transfer and chemical reaction in a pilot-scale biomass pyrolysis vapor-phase upgrading (VPU) reactor. ACS Spring 2019 National Meeting & Exposition. Orlando, April 2019.









reactor at NREL

MFiX-Exa: mesh refinement and porting to GPUs

Development of CFD-DEM and MP-PIC tools for the exascale

- Added local mesh refinement and pruning for complex reactor geometries
- Migrated particle kernels from the CPU to GPU and to multiple MPI tasks
- MFIX-Exa, a seed project until FY19, \bullet was selected to be a full project extending to FY23.

8X speedup in the particle time step for 8 MPI tasks sharing one GPU (Summit) relative to single KNL node (Cori)

Examples of mesh pruning for a simple loop system (left) and near-wall mesh refinement, also with corner pruning, for internal pipe flow (right).















