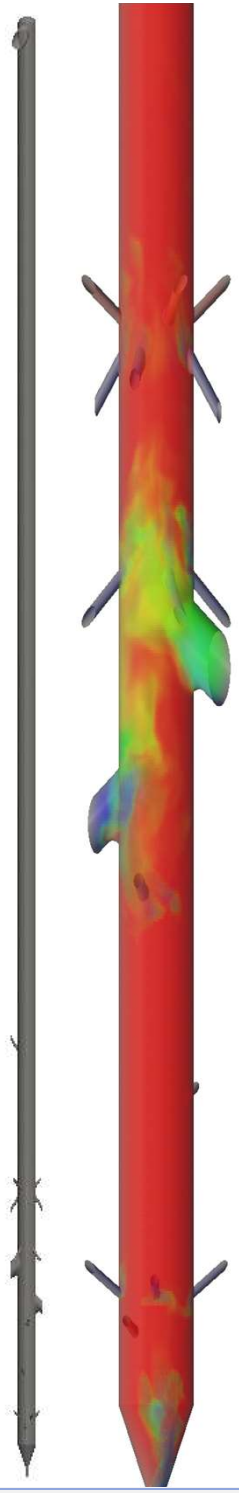

MFiX Multiphase Flow with Interphase eXchanges

Open source multiphase flow modeling for real-world applications

NETL's computational fluid dynamics (CFD) code, MFIX is central to the laboratory's multiphase flow reactor modeling efforts. This open-source software has over two decades of development history and more than 3,500 registered users worldwide. MFIX has become the standard for comparing, implementing, and evaluating multiphase flow constitutive models and has been applied to an extremely diverse range of multiphase flows applications. The successes achieved in modeling complex multiphase flow systems have led to new and improved key attributes such as drag, polydispersity, attrition, and agglomeration.

MFiX TFM is an Eulerian-Eulerian model which supports a broad range of capabilities for dense, reacting, multiphase flows by representing the fluid and solids as interpenetrating continua. This is the most mature MFIX model and is capable of modeling multiphase reactors ranging in size from benchtop to industry-scale. Approximation of the solid phase as a continuum typically allows for faster simulation time than Lagrangian techniques, however it also introduces the need for accurate mathematical models to capture realistic solids phase behavior. This includes transport properties, heterogeneous reaction kinetics, and constitutive relations for interaction between fluid and solid phases, e.g., solids phase drag and interphase heat transfer.

MFiX DEM is an Eulerian-Lagrangian model that treats the fluid phase as a continuum and models the individual particles of the solid phase. This is a relatively new variation on MFIX. While the treatment of individual particles can provide higher fidelity over a broad range of flow regimes (from dilute to packed), it also very challenging when dealing with very large numbers of particles for large-scale simulations. These large-scale applications will require high performance computing (HPC) resources and large amounts of computer time. Code optimization and speed up are critical research fronts to support industrial scale applications.

MFiX PIC is another Eulerian-Lagrangian model that represents the fluid as a continuum while using "parcels" to represent groups of real particles with similar physical characteristics. The MFIX-PIC approach offers reduced computational cost over MFIX-DEM as there are typically few parcels to track and parcel collisions are not resolved. However, the added modeling approximations impact the overall accuracy of the method. Development, validation, and optimization of modeling approximations are critical research fronts.

MFiX Hybrid is blend of MFIX-TFM and MFIX-DEM that represents the fluid as a continuum and models solids as either a continuous phase (TFM) or discrete particles (DEM). This technique is presently restricted to solving only the momentum equations to yield hydrodynamic predictions. This model is still in its infancy and has seen only limited testing.

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Images from an MFIX-TFM simulation of a reacting transport gasifier colored by CO_2 mass fraction. Nearly 2.4 million active grid cells used to capture the 100ft tall geometry. Momentum, thermal energy, and species and mass conservations equations were solved for three distinct phases (two solids, and a gas mixture). Simulation results provided by Tingwen Li, URS.