Fossil Energy with Carbon Capture

MFIX-EXA: Performance Prediction of Multiphase Energy Conversion Device

Carbon capture and storage (CCS) technologies such as oxy-fuel combustion, chemical looping combustion, and post-combustion capture systems offer the most promising approaches for reducing CO_2 emissions from fossil fuel power plants. Large-scale commercial deployment of CO_2 capture technologies requires an understanding of how to scale laboratory designs of multiphase flow reactors to industrial sizes. However, the direct scale-up of such reactors is known to be unreliable, and the current approach requires building and testing physical systems at increasingly larger intermediate scales. The cost in both dollars and development time of having to build and extensively test systems at multiple intermediate scales is prohibitive. High-fidelity computational tools that use exascale computing power can be used to model emerging CCS technologies to enable the design and optimization of these systems, which are critical to controlling costs and reducing the risk of designs failing to meet performance standards.

This work specifically targets scale-up of chemical looping reactors (CLRs) through the creation of MFIX-Exa, a scalable computational fluid dynamics–discrete element model (CFD-DEM) code, which is the next generation of the highly successful NETL-based MFIX code. CFD-DEM is an approach that allows for tracking of individual particles (DEM portion) within a continuum fluid phase (i.e., CFD portion). To date, the focus of existing MFIX CFD-DEM efforts has been on validation and development of physical models in the context of a relatively basic computational framework. MFIX-Exa will integrate expertise in HPC directly with expertise in multiphase modeling and will outperform the existing MFIX by orders of magnitude.

The challenge problem requires representing the full-loop CLR geometry, covering various gas-solids flow regimes occurring in the CLR (bubbling bed, riser, cyclone, standpipe, and L-valve), and including chemical reactions and interphase mass, momentum, and energy transfer. Without the capabilities of MFiX-Exa at exascale, it is not possible to resolve the distribution in particle-scale properties (size, density, chemical conversion) in simulations of gas-solids reactors as large as NETL's CLR.

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Progress to date

- Enabled dynamic load-balancing strategies that account for particle density and a dual-grid approach that allows different domain decompositions for the mesh data and particle data.
- Replaced the SIMPLE algorithm for fluid flow with a modern projection method and explored two spatial discretization alternatives. The new projection formulation demonstrates a factor of four speed-up relative to the SIMPLE method in a weak scaling study from 1 to 4,096 cores.
- Implemented AMReX embedded boundary capability and local mesh refinement at and near solid boundaries and successfully demonstrated coupled fluid-particle flows in basic nonrectangular geometries

Using NETL's 50 kW CLR as an exemplar, MFIX-Exa is developing an exascale application that can be used in the design process of emerging carbon capture reactors to reduce technology development costs and ensure that scaled-up reactors meet performance targets.