Accelerating the Industrial Application of Energy-Efficient Chemical Separation

Deborah J. Bard, NERSC

[Collaborators: David J. C. Constable (ACS GCI), Robert Giraud (ACS GCI ChMRT), Peter Nugent (LBNL)  Nathan Mahynski (NIST), Vincent Shen (NIST)]

Need
Fluid separations at the heart of chemical processes accounts for approximately 10% of the total U.S. energy consumption.

- Virtually all separation processes rely on an energy separating agent, i.e. distillation. Reducing this energy footprint is essential to assure the sustainability and global competitiveness of the U.S.-based chemical enterprise.
- The NIST Material Measurement Laboratory (MML) Chemical Sciences Division and the American Chemical Society Green Chemistry Institute Chemical Manufacturers Roundtable are collaborating to accelerate the industrial application of energy-efficient alternatives to distillation.
- Porous membranes and adsorbants can replace distillation at a fraction of the energy cost, but the profound changes in technology infrastructure required must be driven by collaboration between government and industry.
- Through HPC, this project will kick-start the fundamental understanding of separations that rely on porous materials.

Approach
In this work, we use advanced molecular simulation techniques to systematically study the thermodynamic behavior of fluid mixtures confined in pores – and the resulting efficiency of molecular adsorption.

- Large numbers of parameters are needed to describe the complex behavior of fluids in the confining pore.
- These parameters include the size/shape of the pore, intra- and intermolecular fluid interactions, and fluid-wall interactions.
- We need 300,000 simulations to sample 7 parameters, which in total requires 150M CPU-hours.

As well as access to HPC resources, NERSC provides unique expertise in:
- Optimizing the simulation code for Intel’s Xeon Phi architecture.
- Orchestrating and automating the suites of simulations to run on supercomputing resources.
- Aggregating and tracking the provenance of the output datasets.

Benefits
Experimental design of porous materials-based processes for chemical separation requires iterative trial and error that can take years in practice. The physical experiments required to establish technical and economic viability are expensive, labor intensive, and time consuming.

Outcomes:
- Thermodynamic data over an array of confined fluid mixtures will be made publicly available to researchers.
- The ensuing design framework is expected to significantly cut the time needed to match porous materials to industrial separation needs.
- The theoretical framework for physics-based design of porous materials and the separation processes that rely on them will be transformed.

This research was supported by the High-Performance Computing for Manufacturing Project Program (HPC4Mfg), managed by the U.S. Department of Energy Advanced Manufacturing Office within the Energy Efficiency and Renewable Energy Office. It was performed under the auspices of the US Department of Energy by the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

Relative energy use by chemical separation process

The energy used in separation by membranes is 5-10 times less than that used by distillation processes.