Theoretical Prediction of Material Properties

Mature carbon capture technologies are currently projected to increase the price of energy up to 80%. There are an almost infinite number of possible materials that could be explored as alternative carbon capture materials. Given the properties of a carbon capture material (and dependencies on conditions such as gas loadings, temperature and pressure), the CCSI toolset makes possible optimization of the carbon capture process. However, synthesis, characterization and testing of new materials are expensive and time consuming. We are building the capabilities to predict these properties, via computational methods (ab initio calculations, molecular dynamics and Monte Carlo simulations), not only for existing materials but for hypothetical materials. By linking computational properties prediction to process optimization, not only screening but reverse engineering is possible.

Non-reactive crystalline solid materials: MOFs, 2IFs, COFs, zeolites, etc.

Non-reactive (physical) solvents: Selecox®, Rectisolv®, hybrid PDMS, weakly-interacting ILs, etc.

Recent computational work serves both to validate our simulation methods as well as highlight the features of a promising physical solvent. NETL CRD has created a hybrid polyethylene glycol diethy ether (PEGDME) polydimethylsiloxane (PDMS) carbon capture solvent that combines the desired carbon capture properties of PEGDME with the hydrophobicity of PDMS.

Accuracy of the theoretical prediction for the properties can be further improved by adding more terms or refining parameters of the classical force field, which could be obtained from ab initio calculations

In-house Monte Carlo and molecular dynamics code

Atomic molecular simulation tools for the calculation of:
- full gas absorption isotherms for both pure and mixed gases
- gas absorption Henry’s law constants
- heat of absorption
- excess molar entropy, excess molar volume, partial molar volume
- surface tension
- viscosity
- heat capacity
- gas diffusivity
- gas permeability
- thermal conductivity

The linkage of high throughput computationally predicted material properties with the CCSI toolset will create an "atoms-to-process" multiscale approach that considers materials performance in the context of a tailored carbon capture process.

Experimental Validation Of Material Performance

- High throughput experimental tools are being conceived and developed as material screening tools and to provide verification of material properties predictions
- For example, high throughput gas sorption analyzer (HTGSA) will measure CO$_2$ and N$_2$ sorption into reactive and non-reactive solvents
- Modular, expandable design with automated experiment and data collection via LabVIEW, allowing rapid and simple solubility screening of pure or mixed solvents
- A five-cell unit is planned for construction at NETL within the next few months