CCSI™

Carbon Capture Simulation Initiative

Center for Gas Separations Relevant to Clean Energy Technologies

Integrating the Carbon Capture Materials Database with the process simulation tools of the Carbon Capture Simulation Initiative

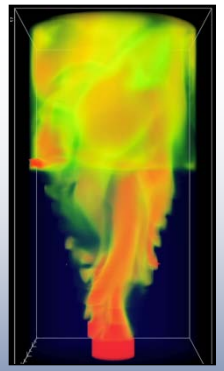
Hosoo Kim[1], Maciej Haranczyk[2], Tom Epperly[3], Mahmoud Abouelnasr[4], David Mebane[5], Berend Smit[4], Joel Kress[6], and David C. Miller[1]

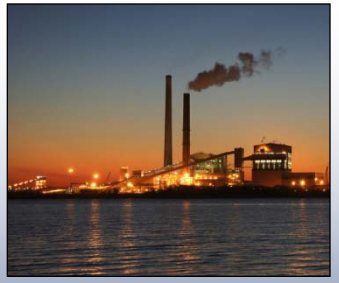
[1]National Energy Technology Laboratory, [2]Lawrence Berkeley National Laboratory, [3]Lawrence Livermore National Laboratory, [4]University of California - Berkeley, [5]West Virginia University, [6]Los Alamos National Laboratory

NETL Berkeley Lab Lawrence Livermore National Laboratory Los Alamos National Laboratory Pacific Northwest National Laboratory U.S. Department of Energy

CCSI: Computational Tools to Accelerate Technology Development





Identify promising concepts → **Reduce the time for design & troubleshooting** → **Quantify the technical risk, to enable reaching larger scales, earlier** → **Stabilize the cost during commercial deployment**

National Labs

- Berkeley Lab
- Pacific Northwest National Laboratory
- NETL
- Los Alamos National Laboratory
- Lawrence Livermore National Laboratory

Academia

- Carnegie Mellon
- Princeton University
- West Virginia University
- Boston University
- Institute for Clean and Secure Energy, The University of Utah

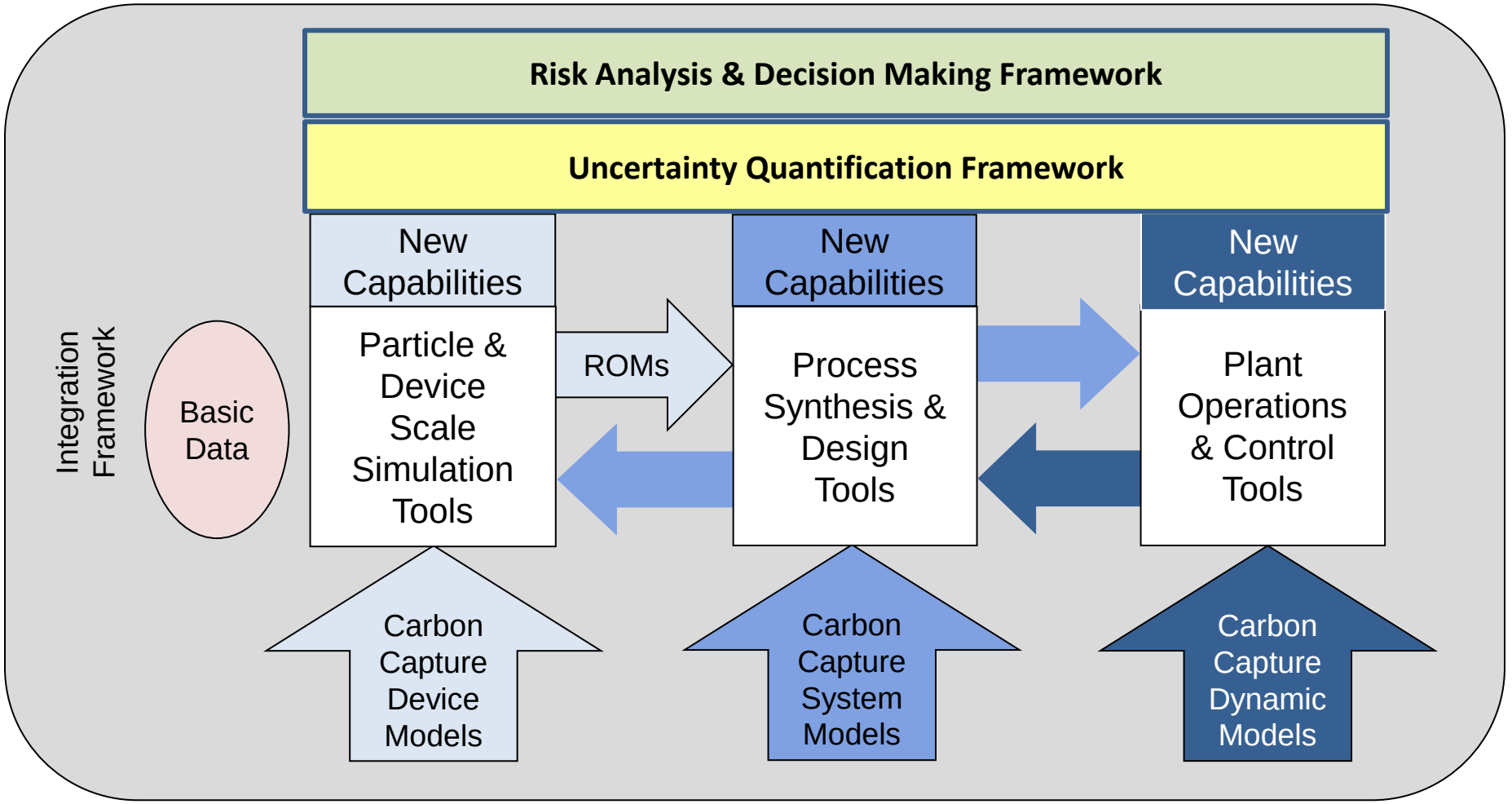
Industry

- Fluor
- ADA Environmental Solutions
- B&W
- GE
- EPRI Electric Power Research Institute
- Air Products
- Burns & McDonnell Since 1898
- Southern California Edison, An Edison International Company, San Onofre Nuclear Generating Station
- Alstom
- Southern Company
- Duke Energy
- URS
- Boeing
- DuPont
- ExxonMobil
- Chevron
- Phillips 66
- WorleyParsons resources & energy
- Eastman

CCSI™ Carbon Capture Simulation Initiative

NETL · Berkeley Lab · Lawrence Livermore National Laboratory · Los Alamos National Laboratory · Pacific Northwest National Laboratory · U.S. Department of Energy

Components of the CCSI Toolset



CCSI™ Carbon Capture Simulation Initiative

NETL

Berkeley Lab

Lawrence Livermore National Laboratory

Los Alamos National Laboratory

Pacific Northwest National Laboratory

U.S. DEPARTMENT OF ENERGY

CCSI Process Synthesis & Design

Facilitate the rapid screening of new concepts and technologies

Enable identification & development of optimized process designs

- Multiple potential technologies for carbon capture
  - Different reactors types
  - Different sorbent materials
  - Different regimes (high T, low T, PSA, TSA)
- Need systematic way to evaluate candidate processes, materials
  - Need to consider best process for different materials

- Identify configurations for more detailed simulation (i.e., CFD)
- Integrate and optimize the entire process system
  - PC plant, carbon capture process, and compression system

Basic Data

External Collaboration (Prof. Phil Smith, ICSE)

Flexible Modular Models

PC Plant Models
Thermoflex
(John Eslick)

Bubbling Fluidized Bed Reactor Model
ACM, gPROMS
(Juan Morinelly)

Moving Bed Carbon Capture Reactor Model
ACM, gPROMS
(Hosoo Kim)

Compression System Models
ACM, gPROMS
(John Eslick)

Membranes
ACM, gPROMS,
(Juan Morinelly)

Solvents
Aspen Plus
(John Eslick)

Oxy-combustion
GAMS
(Alex Dowling)

Algebraic Surrogate Models
(Alison Cozad)

Derivative Free Optimization

Industry Specific Collaboration

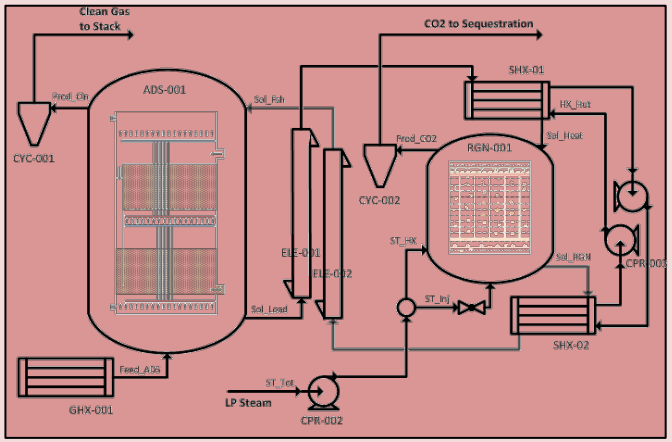
Process Synthesis

Superstructure for Optimal Process Configurations
(Zhihong Yuan)

Simultaneous Superstructure Approach
Power, Heat, Mass Targeting
(Linlin Yang)

Heterogeneous Simulation-Based Optimization Framework

PC Plant Model



Compression System Model

Heat/Power Integration

CCSI™ Carbon Capture Simulation Initiative

NETL

Berkeley Lab

Lawrence Livermore National Laboratory

Los Alamos National Laboratory

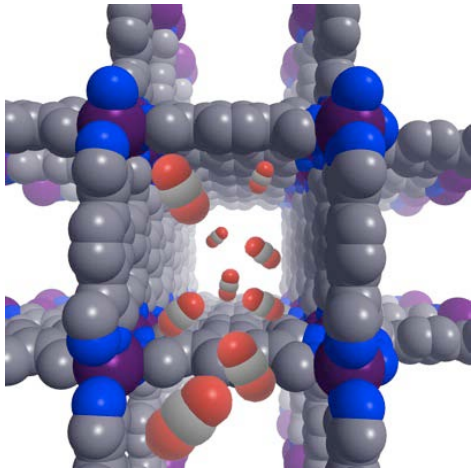
Pacific Northwest National Laboratory

U.S. DEPARTMENT OF ENERGY

Energy Frontier Research Center (EFRC)

Center for Gas Separations Relevant to Clean Energy Technologies

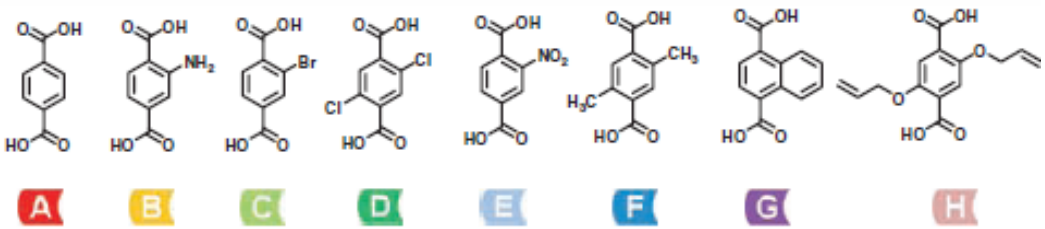
- Center for Gas Separations Relevant to Clean Energy Technologies
  - to develop new strategies and materials that allow for *energy efficient* selective *capture* or *separation* of CO_2 from gas mixtures based on molecule-specific chemical interactions.
- Plan and Direction
  - Capture of CO_2 from gas mixtures requires the molecular control offered by nanoscience to tailor-make those materials exhibiting exactly the right adsorption and diffusion selectivity to enable an economic separation process. Characterization methods and computational tools will be developed to guide and support this quest.



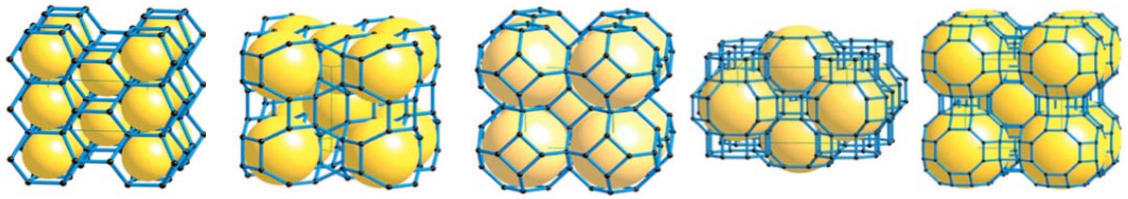
CCSI™ Carbon Capture Simulation Initiative · NETL · Berkeley Lab · Lawrence Livermore National Laboratory · Los Alamos National Laboratory · Pacific Northwest National Laboratory · U.S. Department of Energy

Millions of Potential Materials

- Metals: Fe, Mg, Ca, Zn, Cu, etc
- Linkers:



- Pore topologies:

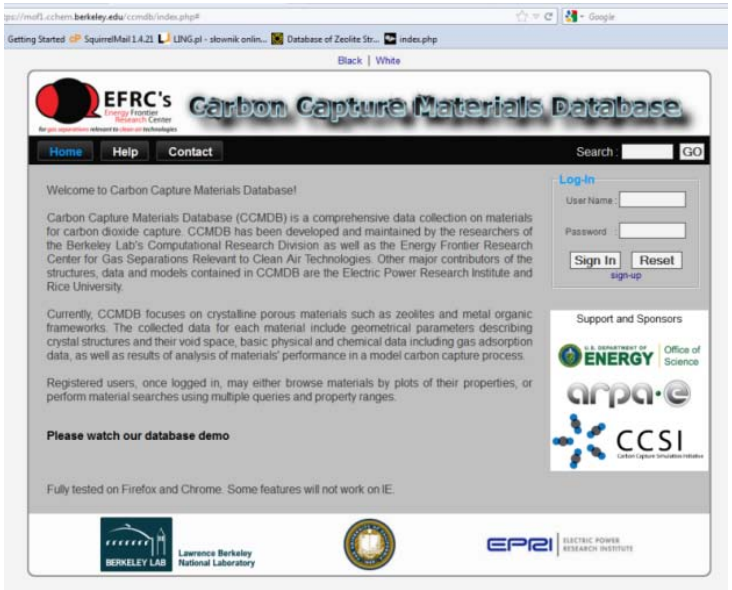


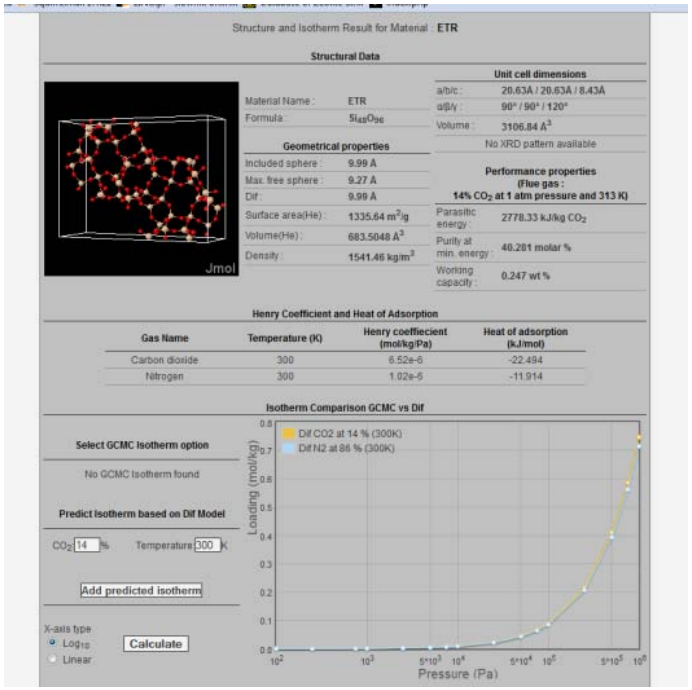
crb ***dft*** ***sod*** ***mer*** ***rho***

Any combination of the above !!

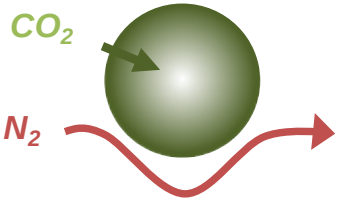
Carbon Capture Materials Database (CCMDB)

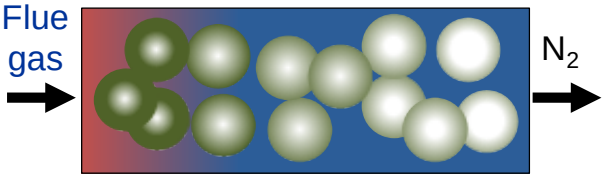
- EFRC's database is a large collection of basic physicochemical data on solid sorbents (Currently it contains data on ca. 200,000 crystalline porous materials such as zeolites, MOFs and ZIFs)
- The database incorporates LBNL and EFRC-developed algorithms and software tools for characterization of porous materials: HPVOID (GPU Molecular simulation code) and Zeo++ (high-throughput geometry-based analysis of porous structures)
- Users can access the data via a Web interface

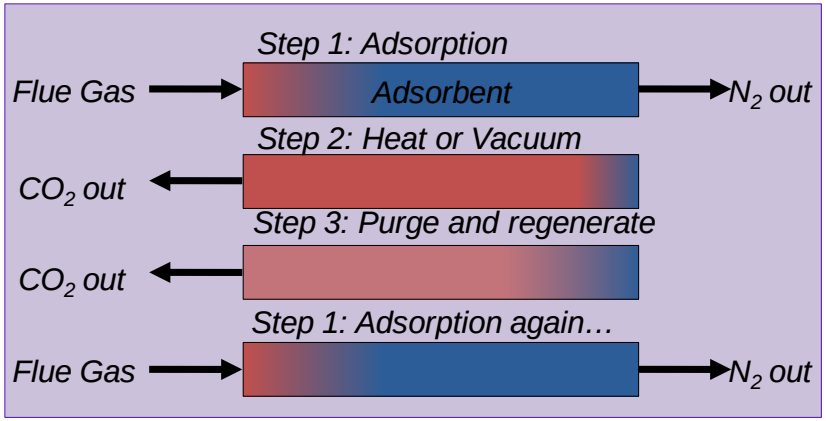




Material Screening using Fixed Bed Model





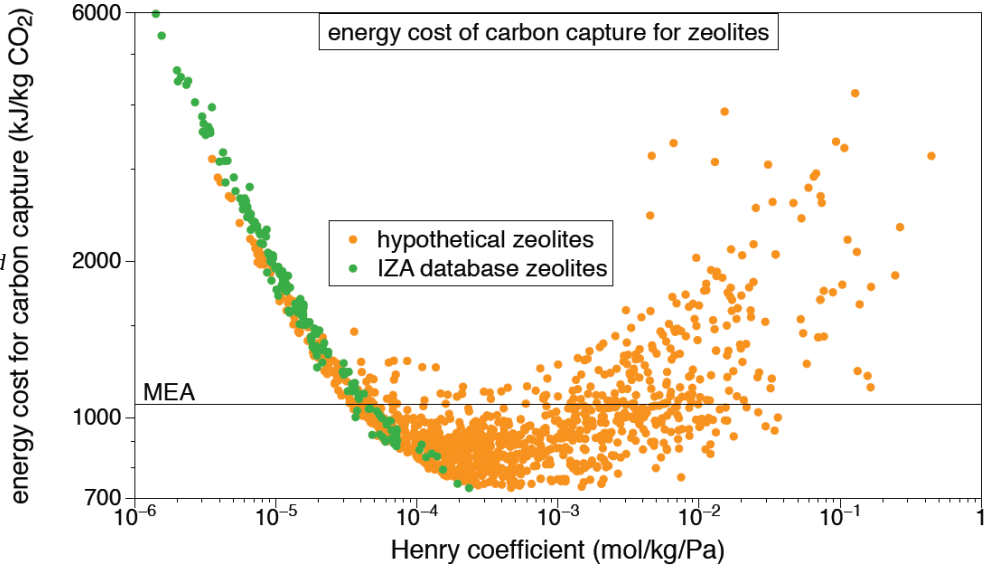


Calculation of energy penalty

$$Q = \left(C_p \rho_{sorbent} \Delta T + \Delta h_{CO2} \Delta q_{CO2} + \Delta h_{N2} \Delta q_{N2}\right) \Big/ CO_{2\,\mathrm{Produced}}$$

$$W_{eq} = \left(0.75Q \cdot \eta_{carnot} + W_{comp}\right)$$

- Fixed reactor configuration
- Equilibrium model
  - No heat or mass transfer

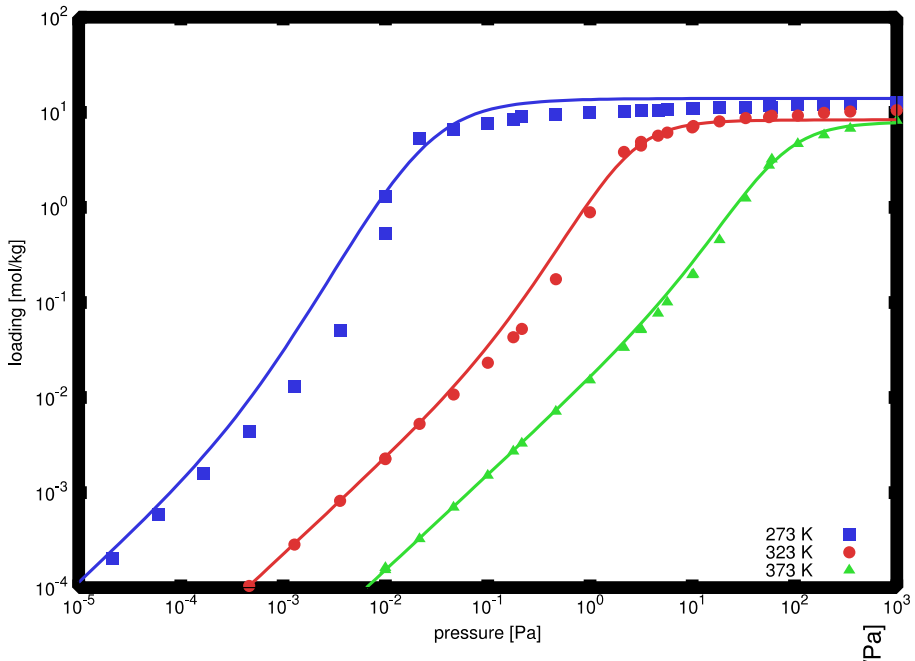


L.-C. Lin, A. H. Berger, R. L. Martin, J. Kim, J. A. Swisher, K. Jariwala, C. H. Rycroft, A. S. Bhown, M. W. Deem, M. Haranczyk, and B. Smit, In silico screening of carbon-capture materials, Nature Materials 11 (7), 633 (2012)

CCSI™ Carbon Capture Simulation Initiative · NETL · Berkeley Lab · Lawrence Livermore National Laboratory · Los Alamos National Laboratory · Pacific Northwest National Laboratory · U.S. Department of Energy

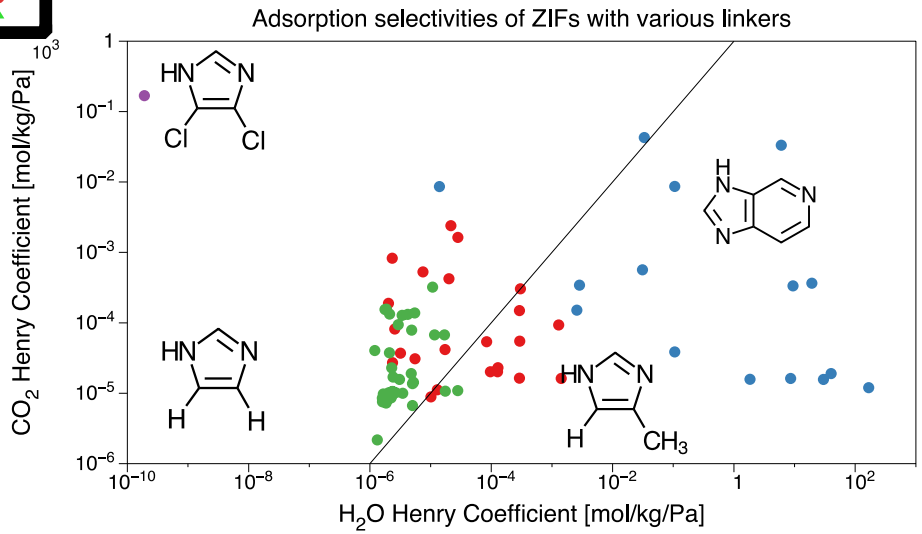
Estimating Potential Water Adsorption

simulated water adsorption in zeolite 13X (NaFAU, Si/Al ~ 1.24)



- Highly nonideal adsorption isotherm, with a convex isotherm – at low temperatures showing a discontinuity with an infinite slope.
- Once the water model is validated, it can be applied to various materials to predict adsorption selectivity for CO_2 over water.

- Zeolitic Imidizolite Frameworks (ZIFs)
- Water selective (bottom-right)
- CO_2 selective (top-left).



CCSI™ Carbon Capture Simulation Initiative

NETL

Berkeley Lab

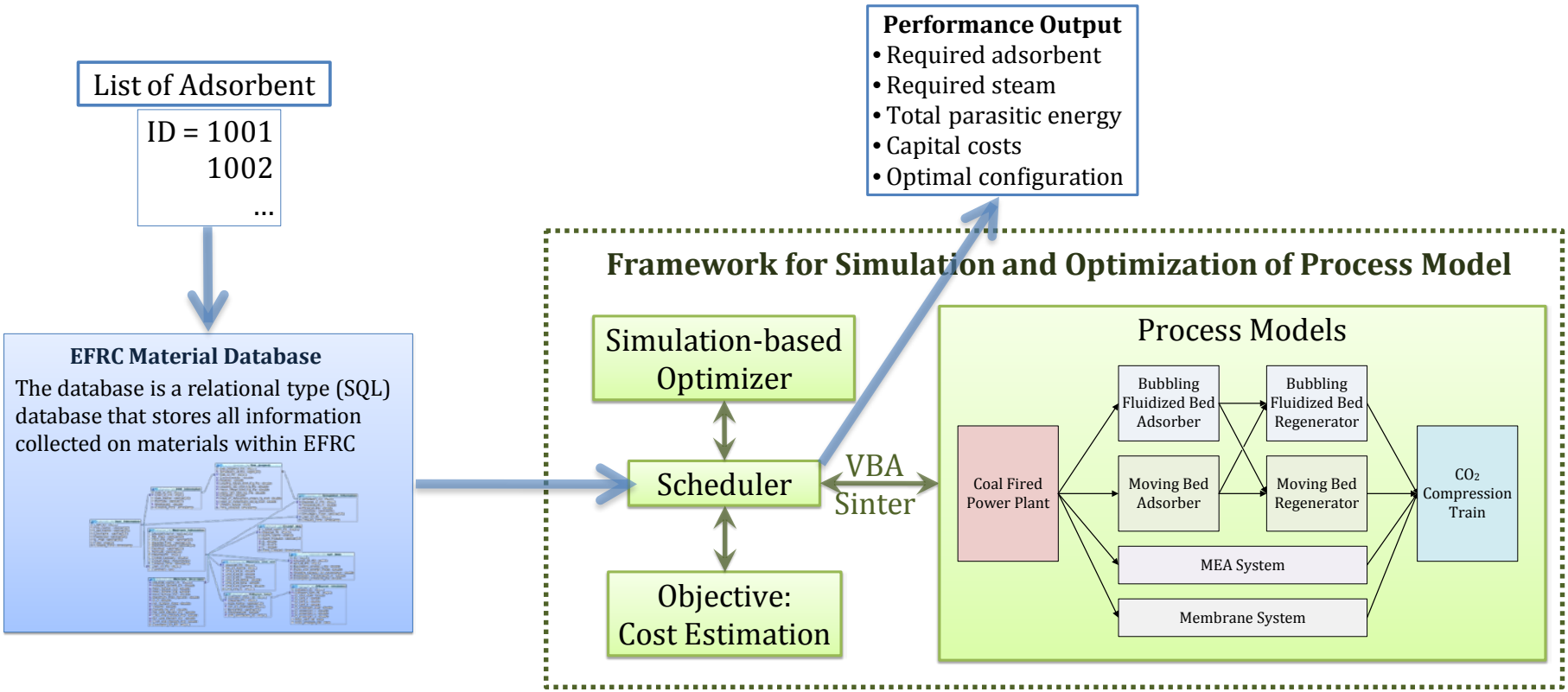
Lawrence Livermore National Laboratory

Los Alamos National Laboratory

Pacific Northwest National Laboratory

U.S. DEPARTMENT OF ENERGY

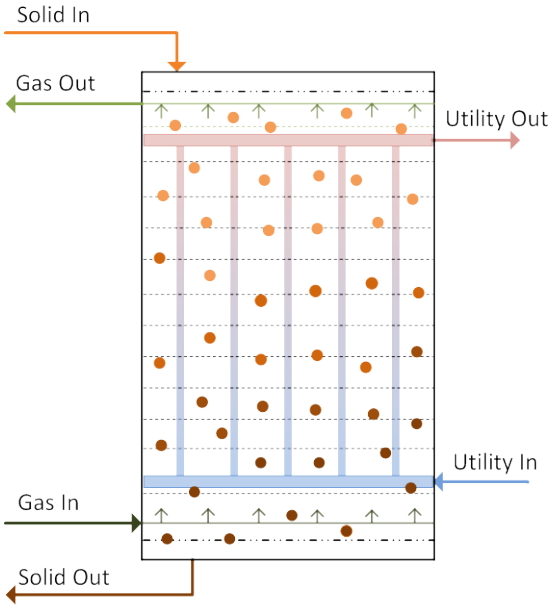
Linkage Scheme: EFRC's DB – CCSI Toolset

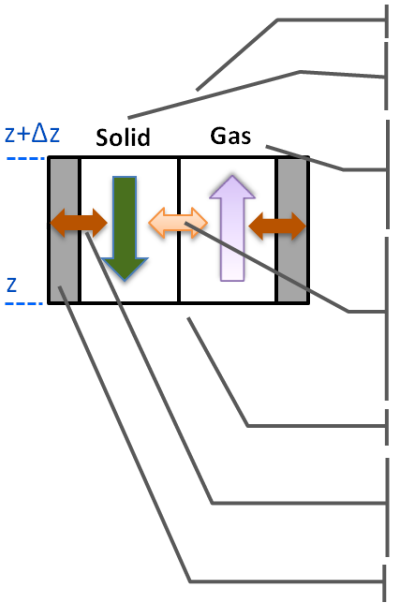


- CCSI designed and developed an Application Programming Interface (API) and corresponding data formats to provide CCSI access to the data in the EFRC's database.

Solid Sorbent Moving-Bed Reactor

Modeling Scheme





Shell (Gas, Solid) & Tube (Steam) Type
Uniform Flow for Solid Phase (Const. vel.)
Eff. Thermal Conductivity

Plug-Flow for Gas
Convection w/Axial Dispersion
Pressure Drop using Ergun Eqn

Mass Transfer
- External Film Resistance
- Intra-particle Diffusion

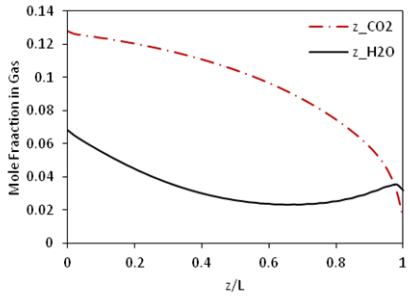
Heat Transfer
- Convective

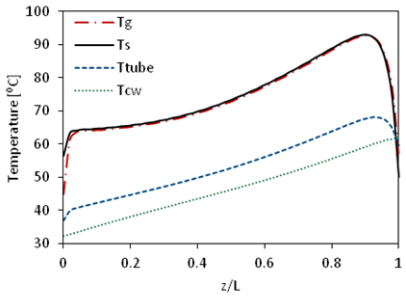
Adsorption & Desorption Kinetics

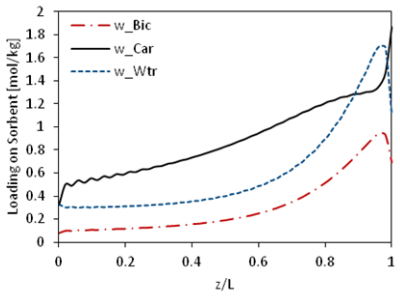
Heat Transfer
- Wall - Gas
- Wall - Solid

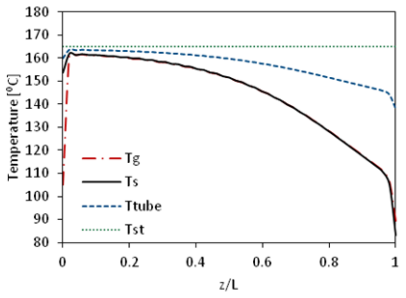
Heat Transfer Bet'n Wall & Steam

Simulation of Adsorber/Regenerator







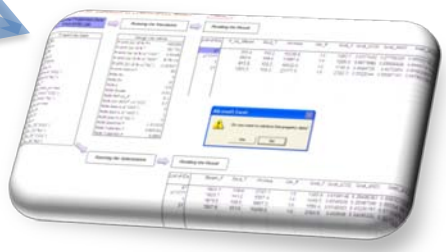


CCSI™ Carbon Capture Simulation Initiative | NETL | Berkeley Lab | Lawrence Livermore National Laboratory | Los Alamos National Laboratory | Pacific Northwest National Laboratory | U.S. Department of Energy

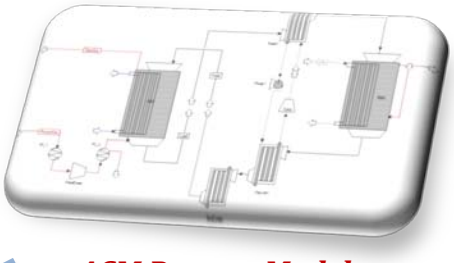
Estimating Material Performance using CCSI Moving Bed System

	Material ID	Material Name
1	87	JBW
2	471777	13X
3	1	ABW
4	21	ASV

CCMDB



Excel Interface



ACM Process Model

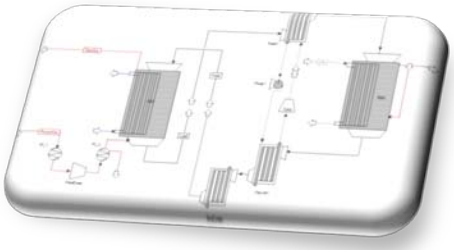
Performance Output

- *Adsorbent requirement*
- *Steam usage*
- Parasitic energy
- Capital costs
- Optimal configuration

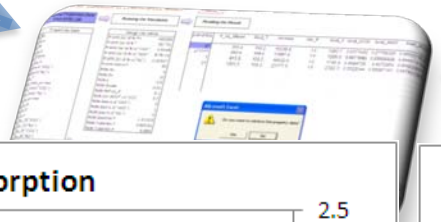
CCSI™ Carbon Capture Simulation Initiative | NETL | Berkeley Lab | Lawrence Livermore National Laboratory | Los Alamos National Laboratory | Pacific Northwest National Laboratory | U.S. Department of Energy

Example: Comparison of Material Performance using CCSI Moving bed System

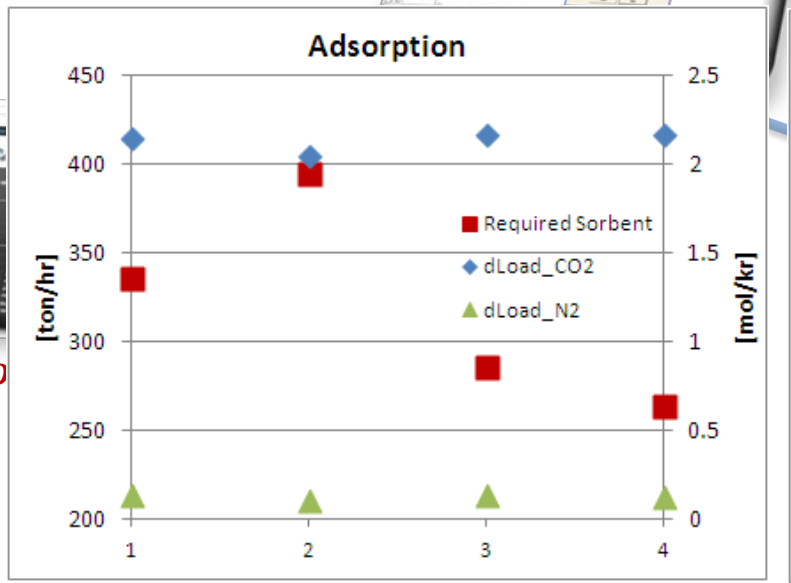
	Material ID	Material Name
1	87	JBW
2	471777	13X
3	1	ABW
4	21	ASV

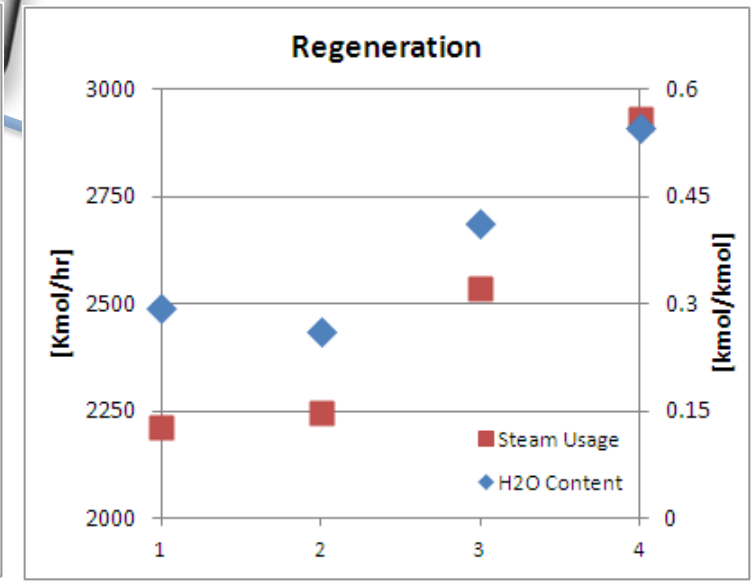


ACM Process Model



CCMD





CCSI™ Carbon Capture Simulation Initiative

NETL

Berkeley Lab

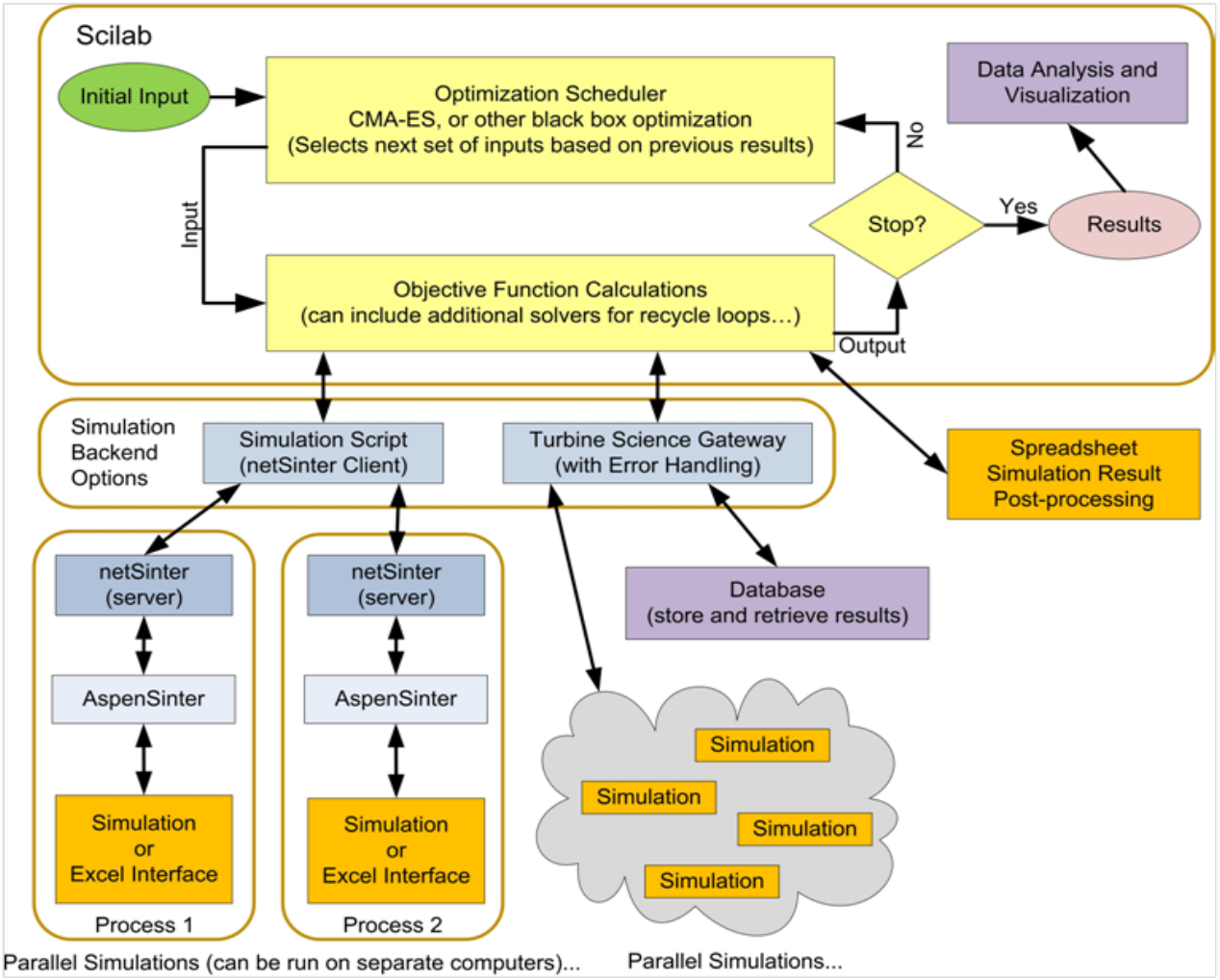
Lawrence Livermore National Laboratory

Los Alamos National Laboratory

Pacific Northwest National Laboratory

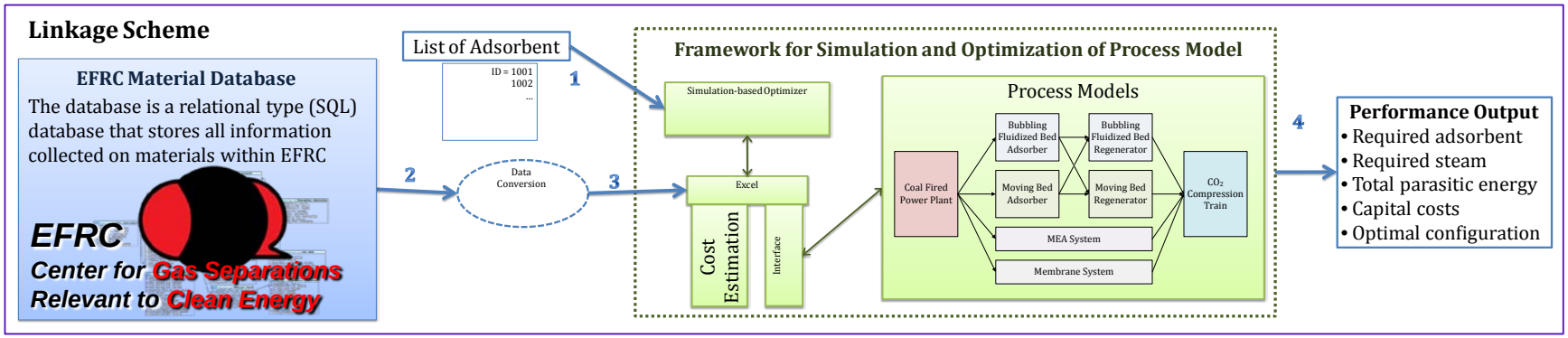
U.S. DEPARTMENT OF ENERGY

Potential Future Application – Automated System Optimization for Further Screening of Promising Database Sorbents



Conclusions: Identifying promising concepts

- **How?** Computationally screen sorbent materials, devices, and processes
- **CCSI Example**: Toolset was linked to database developed by UC Berkeley Energy Frontier Research Center (EFRC)
  - EFRC database contains over 100,000 zeolite and zeolitic imidazolate framework (ZIF) sorbent structures[1]
  - CCSI moving bed system used for comparing sorbent materials
- **Benefits**
  - By identifying promising concepts early, time and money are saved because the development efforts are only directed toward potentially successful systems



1. L.-C. Lin … B. Smit, In silico screening of carbon-capture materials, *Nat Mater* **11** (7), 633 (2012)

Questions?

Disclaimer