NATIONAL ENERGY TECHNOLOGY LABORATORY

# NETL Modular Framework for Design & Optimization of Carbon Capture Systems

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U.S. DEPARTMENT OF ENERGY

# Outline

- Motivation – $CO_2$ and Water
- Modular Framework – Design & Optimization
- Model details
  - PC Plant
  - MEA system
  - Compression system
- Results & Discussion
  - Power generation
  - Capital cost
  - Water use
- CCSI – Accelerating Process Scale Up

# DOE/NETL Goals: $CO_2$ Capture

| Minimum $CO_2$ Captured | Maximum Increase in COE |
| --- | --- |
| 90% | 30% for PC |
| | 10% for IGCC |

# DOE/NETL Goals: Freshwater Minimization

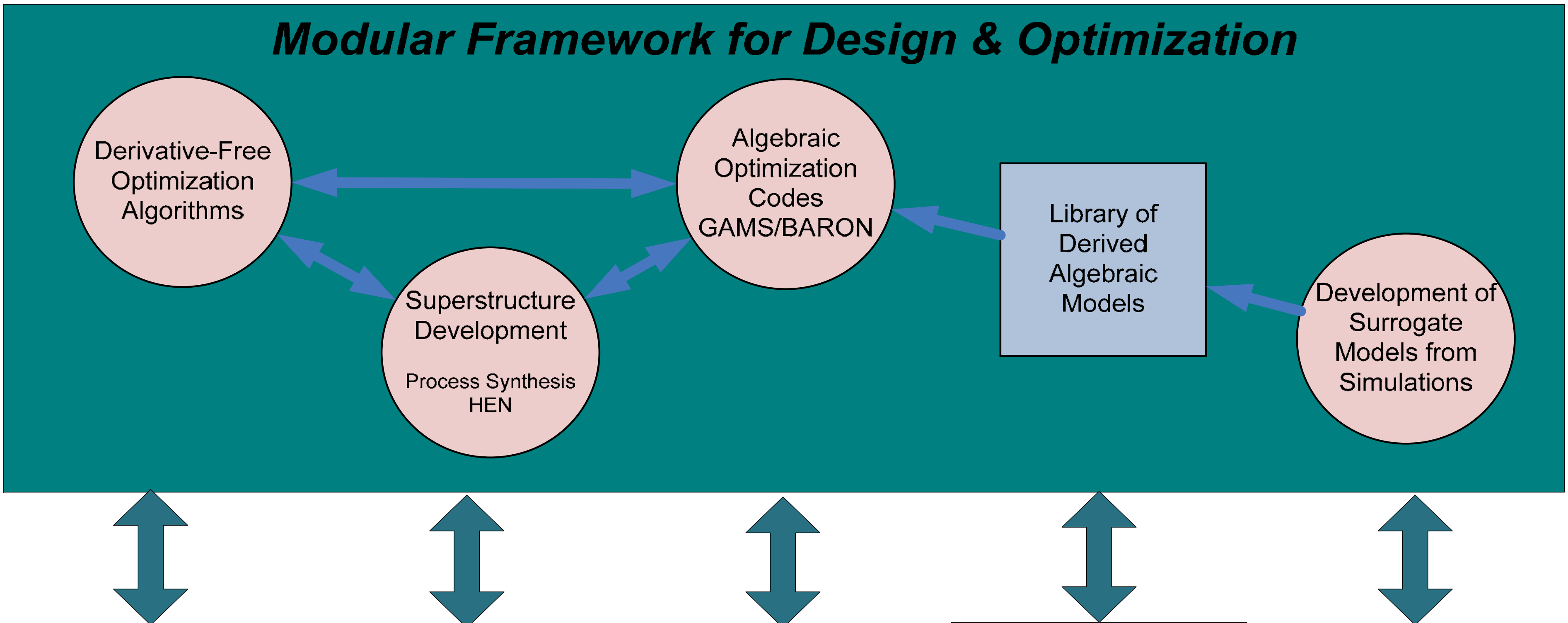
- **Short-term goals (ready for commercial demonstration by 2015)**
  - Reduce freshwater withdrawal and consumption by > 50% for thermoelectric power plants equipped with wet recirculating cooling technology
  - Levelized cost savings > 25% compared to state-of-the-art dry cooling
- **Long-term goals (ready for commercial demonstration by 2020)**
  - Reduce freshwater withdrawal and consumption by > 70% for thermoelectric power plants equipped with wet recirculating cooling technology
  - Levelized cost savings > 50% compared to state-of-the-art dry cooling

# Challenges

- Large-scale problem
  - 2 billion tons $CO_2$ from coal by 2020 in US
  - Flue gas: 5 million lb/hr for 550MW PC plant

- No existing economical solution
- No framework for developing & evaluating optimized designs
- Difficulty re-using existing models/simulations
- Inconsistent assumptions & evaluation methods

- Approach
  - Process synthesis, design & optimization
    - Process integration
    - Nonlinear interactions across units/subsystems
    - Simulation-based optimization
  - Multi-criteria decision-making tools
    - Include water resource considerations




### *Existing Plants Modules*

- *Combustion system*
- *Feed water heater*
- *Boiler*
- *Economizer*
- *Superheater*
- *Steam turbines*
- *Condensers*
- *FGD*

### *Post-Combustion Carbon Capture Modules*

- ***Amine systems***
- *Chemical looping*
- ***Solid sorbents***
- ***Adsorption***
- ***Oxycombustion***
- ***Membranes***
- *Absorption (other)*
- *Ionic liquids*
- ***Compression***

### *IGCC Modules*

- *Feed system*
- *Gasifier*
- *Boiler*
- *Gas cleanup*
- *Shift reactor*
- *Gas turbine*
- *HRSG*
- *Steam turbines*
- *Condensers*

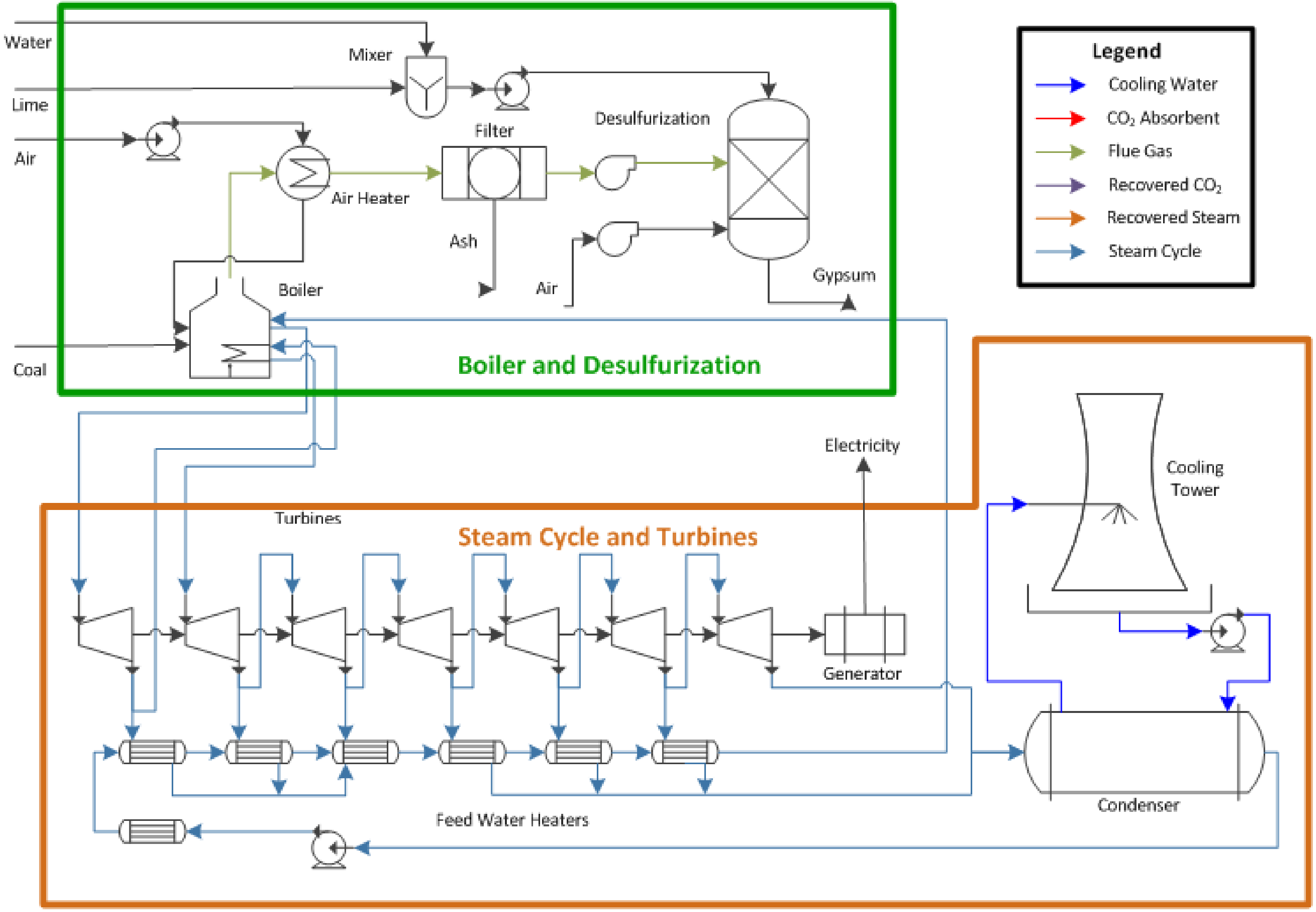
### *Pre-Combustion Carbon Capture Modules*

- ***Physical absorption systems***
- *Chemical looping*
- ***Solid sorbents***
- ***Adsorption***
- *Membranes*
- *Ionic liquids*
- *Compression*

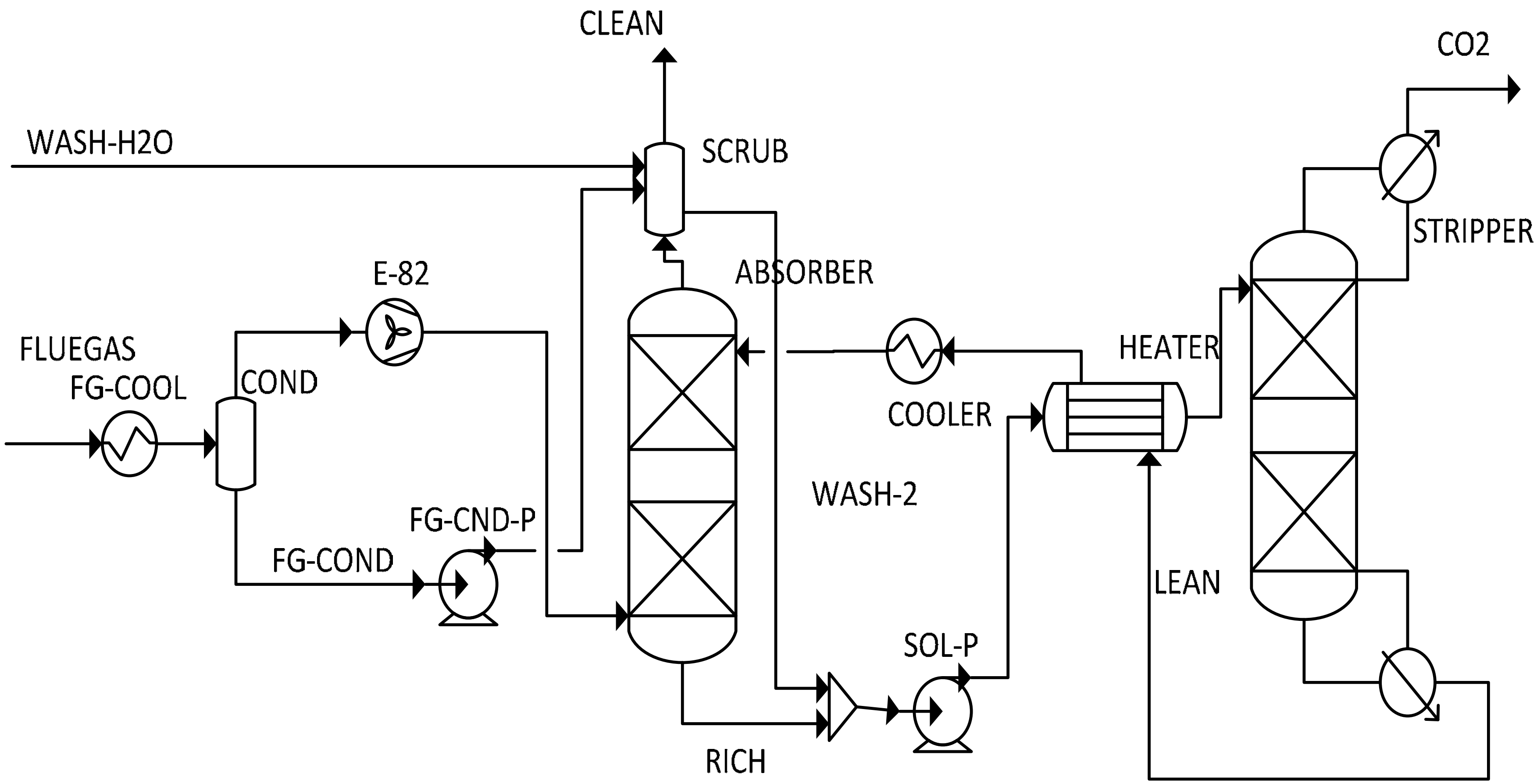
### *Plantwide Water Simulator*

- *Cooling alternatives*
- ***High fidelity cooling tower models***
- ***Nontraditional water sources***
- *Water recovery*
- ***Water treatment***
- *Cooling water & process water*

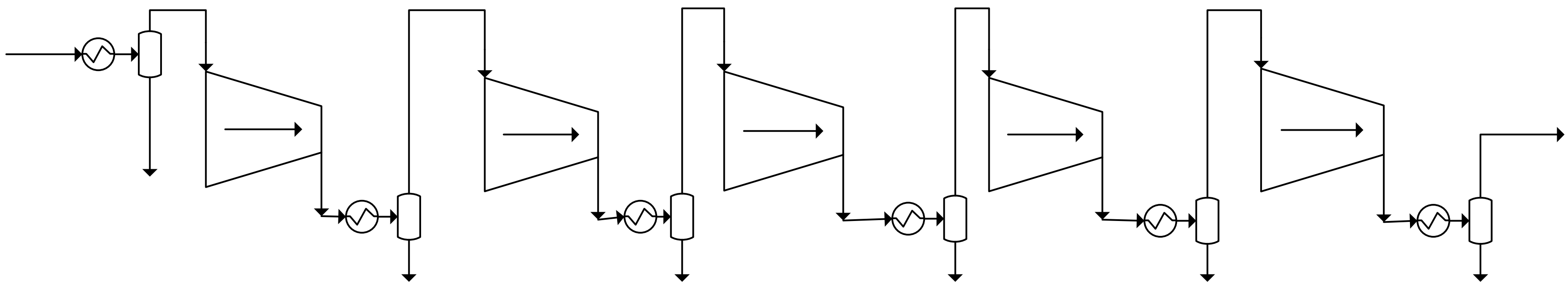
# Subcritical PC Plant



# MEA Module


CLEAN
CO2
WASH-H2O
SCRUB
STRIPPER
E-82
ABSORBER
FLUEGAS
FG-COOL
COND
HEATER
COOLER
WASH-2
FG-CND-P
FG-COND
LEAN
SOL-P
RICH

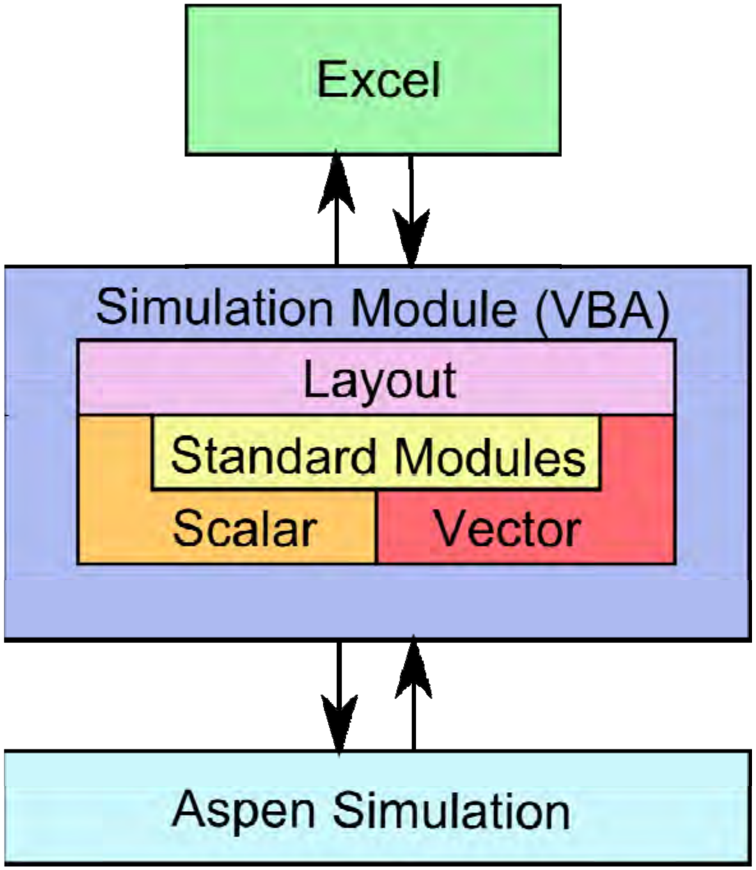
# Compression

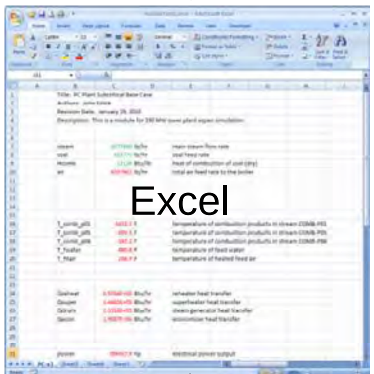


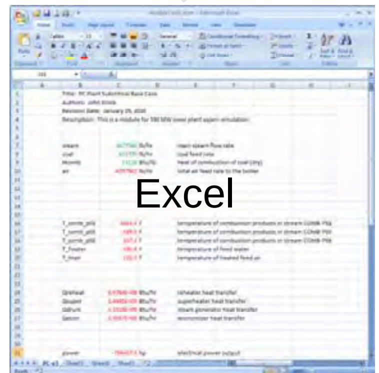
- 5 stage compression
- Intercoolers 265°F to variable T
- Water returned to process
- Final pressure 2200 psia

# Simulation Interface

- Set simulation variables
- Supports structural changes
  - Feed stage
  - Number of stages
  - (not supported internally)
- Retrieves results
- Perform post-processing
  - Cost estimation
  - Objective function calculations




Excel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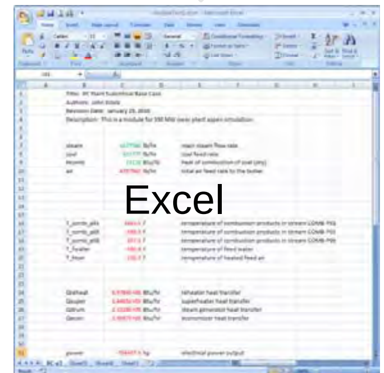
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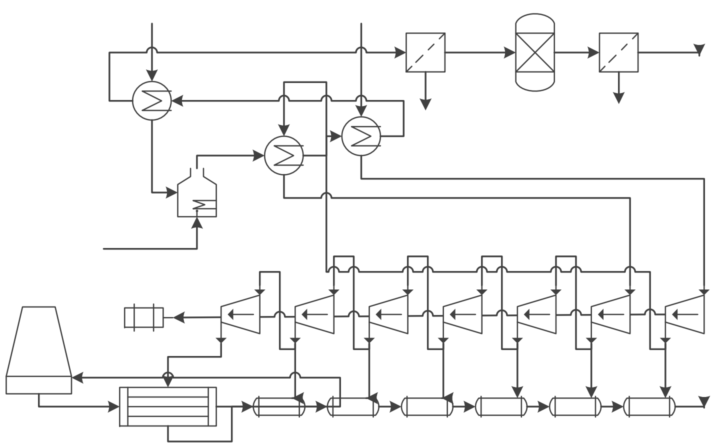
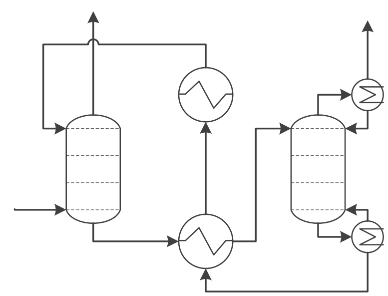
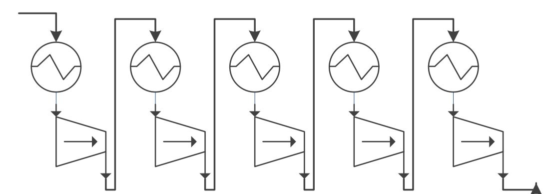
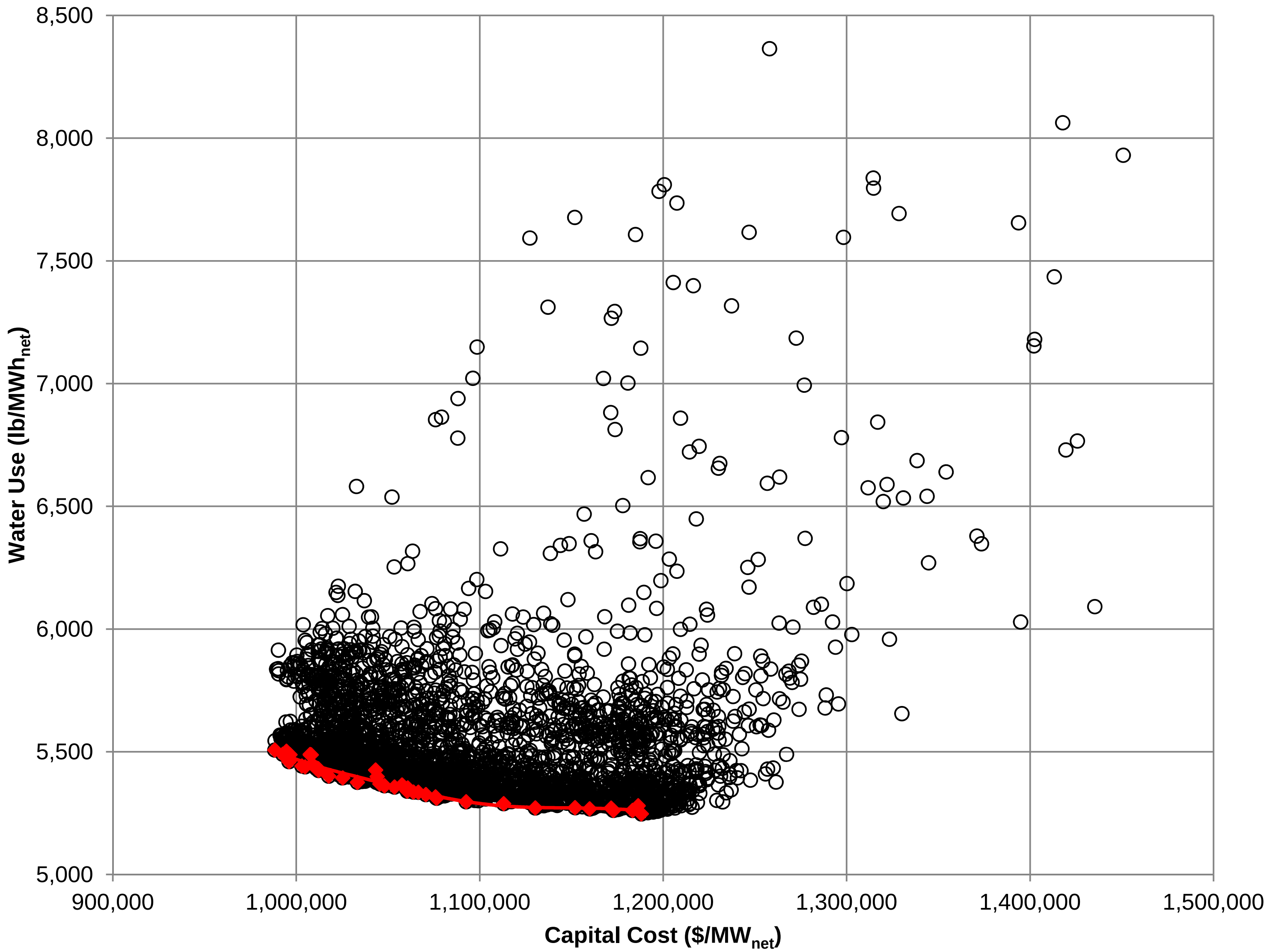


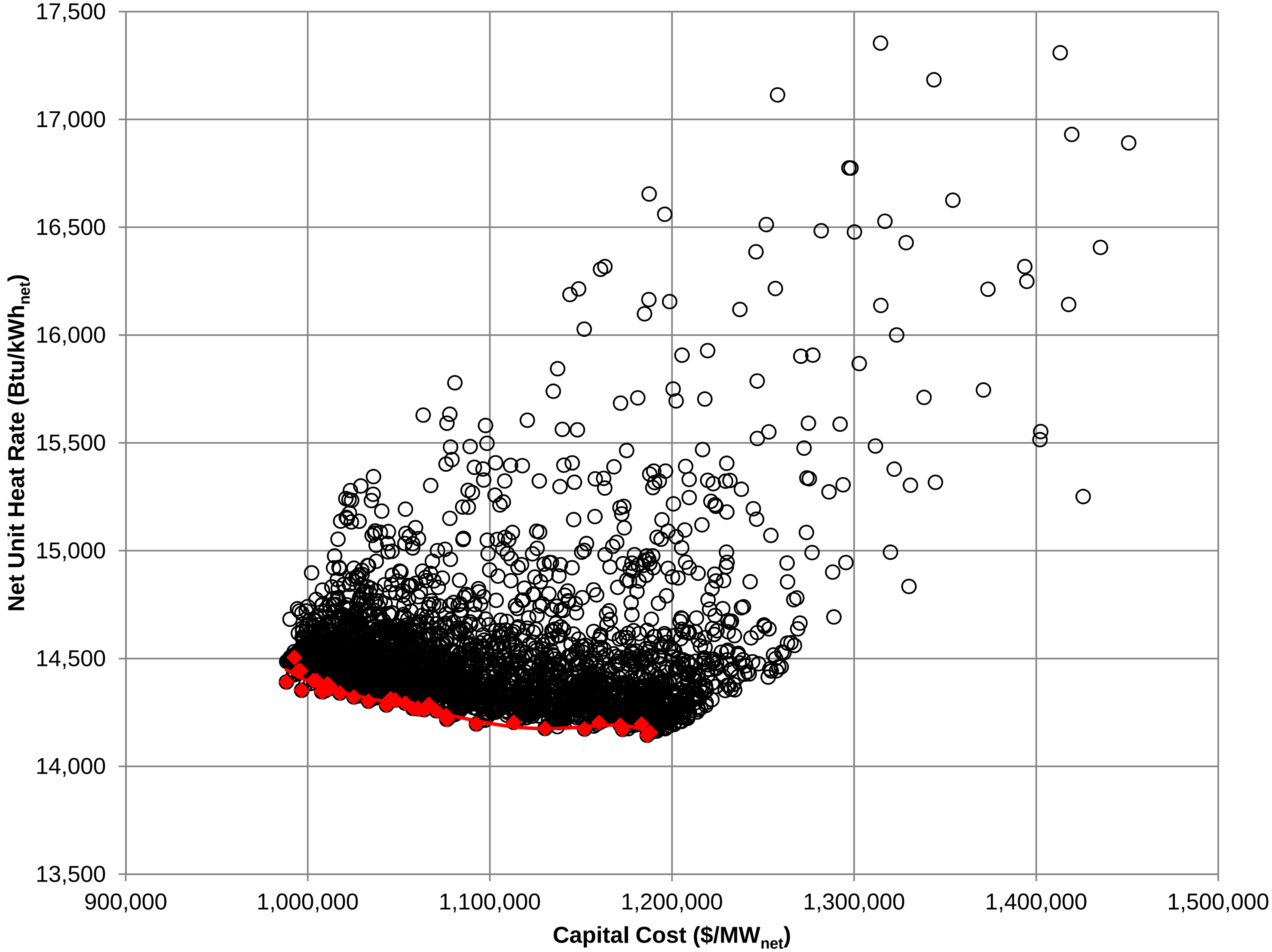




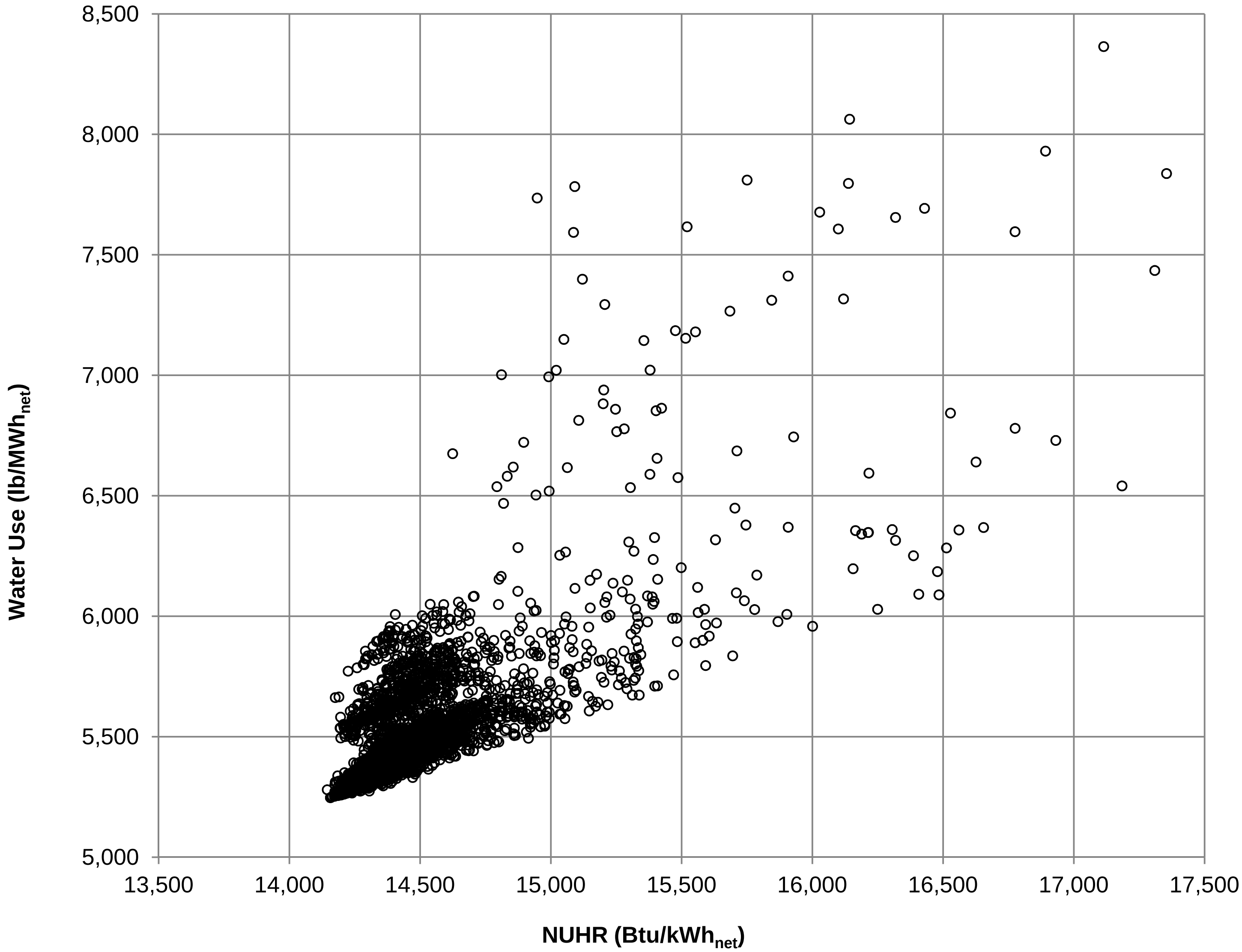
# Capital Cost vs. Water Use



# Capital Cost vs. NUHR



# NUHR vs. Water Use

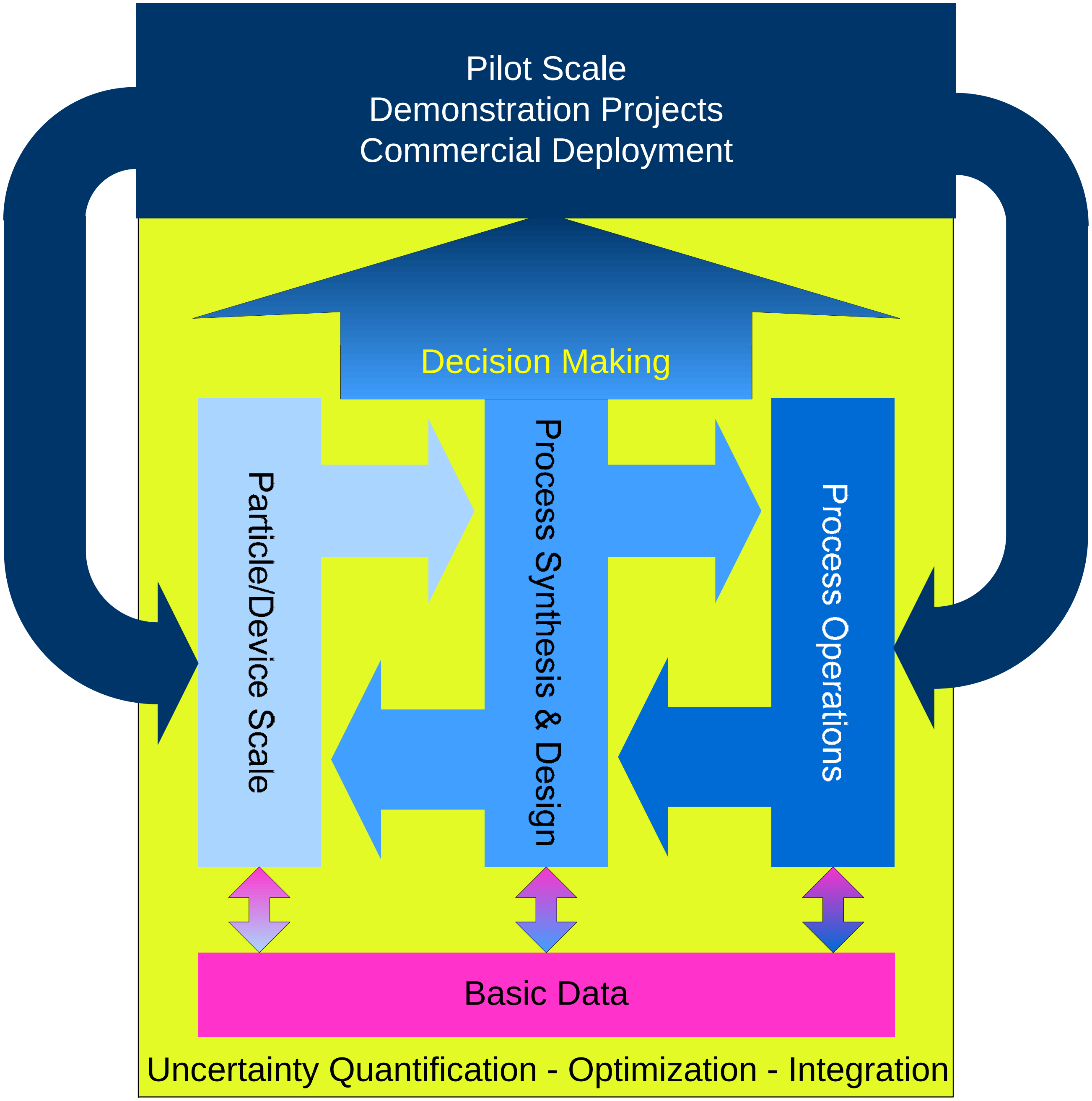


| | Best Net Unit Heat Rate | Best Capital Cost | Best Water Use |
|---|---|---|---|
| NUHR (Btu/kWh) | 14,145 | 14,392 | 14,157 |
| Capital Cost ($/kW$_{net}$) | 1,186 | 988 | 1,188 |
| Overall Net Power Output (MW) | 354.7 | 348.6 | 354.4 |
| Total Capital Cost (Capture & Compression only) | $421 MM | $345 MM | $421 MM |
| Solvent Flow rate (gpm) | 7,070 | 7,470 | 6,970 |
| Lean Solvent Loading (mol $CO_2$/mol amine) | 0.214 | 0.218 | 0.212 |
| Rich Solvent Loading (mol $CO_2$/mol amine) | 0.454 | 0.444 | 0.454 |
| No. Absorber Stages | 20 | 10 | 20 |
| No. Stripper Stages | 14 | 12 | 14 |
| Cooling Water Evaporation (lb/MWh$_{net}$) | 5,280 | 5,507 | 5,247 |

# Optimized Process Systems

- Large potential improvement over initial design
- Essential for comparing technology
- Many non-intuitive interactions
- Understand competing objectives

# Process Scale Up Tasks



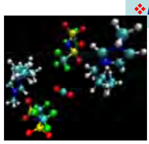
# Carbon Capture Simulation Initiative

*Ab initio QM*
- Energy, structure
- Charge, force field
- Interaction mechanisms

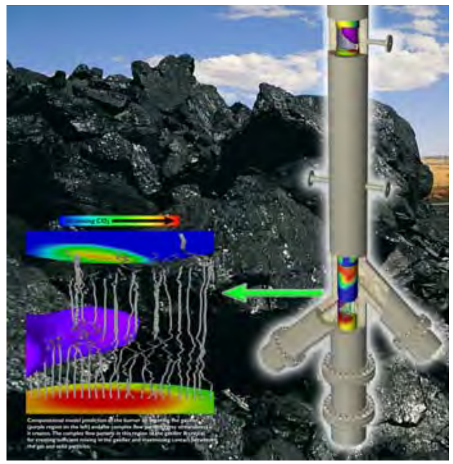
*Monte Carlo*
•Thermo dynamic Properties

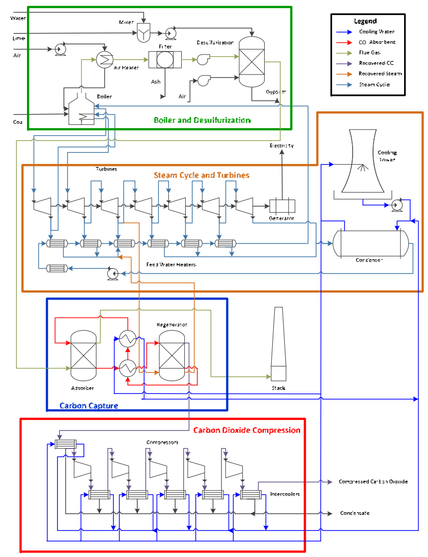
*Molecular Dynamics*
•Transport Properties

- ❖Search for better ILs
- ❖Modify IL functionality
- ❖Discover new IL



*A new ionic liquid that exhibits high $CO_2$ permeability and $CO_2/H_2$ selectivity was identified with this method.*






*Identify promising concepts and designs* → *Develop optimal designs* → *Quantify technical risk in scale up*

*Accelerate learning during development & deployment*

NETL · Berkeley Lab · Los Alamos National Laboratory EST. 1943 · Lawrence Livermore National Laboratory, Science in the National Interest · Pacific Northwest National Laboratory

# Modular Framework Research Team

- Optimization and computational infrastructure
  - ModeFrontier integration & multi-criteria, simulation-based optimization - NETL (Miller/Eslick)
  - Derivative-free "Blackbox" Optimization – CMU (Sahinidis/Cozad)
  - Surrogate model development – CMU (Sahinidis/Chang)
  - Simultaneous Superstructure-based Optimization – CMU (Grossmann/Yang)
  - Synthesis of Integrated IGCC Systems – CMU (Grossmann/Biegler/Kamath)
- Module development
  - Base plant modules
    - Predictive Plant Models (PC/IGCC) – NETL (Miller/Eslick)
    - Development of Predictive Turbine Models – NETL (Liese)
    - Oxycombustion Plant Model – NETL Albany (Summers/Oryshchyn/Harendra)
  - Carbon capture modules
    - Equilibrium & rate-based amine capture – NETL (Miller/Eslick)
    - Solid sorbent capture systems – NETL (Miller/Lee)
    - Membrane-based separation systems – NETL (Miller/Morinelly)
    - Compression system – NETL (Miller/Eslick)
    - Synthesis of Optimal PSA Cycles for CO2 Capture from Flue Gas – CMU (Biegler/Agarwal)
    - Synthesis of Optimal PSA Cycles for Hydrogen/CO2 Separation – CMU (Biegler/Vetukuri)
    - Cryogenic separation and hydrate-based separation – NETL (van Osdol)
  - Water-specific activities
    - Treated Municipal Wastewater for Power Plant Cooling – CMU (Dzombak/Hsieh)
    - Modeling Nontraditional Sources of Power Plant Water
      - IIT (Abbasian/Arastoopour/Walker/Safari/Strumendo)
    - Water from Oxycombustion – NETL Albany (Summers/Oryshchyn/Harendra)