NATIONAL ENERGY TECHNOLOGY LABORATORY

Fossil Energy and Carbon Capture: A Systems Perspective

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U.S. DOE/NETL

CAPD ESI Seminar Series
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Pittsburgh, PA

U.S. DEPARTMENT OF ENERGY

Outline

- **Overview of NETL**
- Definitions, Overview of Power Production
- Motivation – CO_2, Costs, Water Use
- Post-combustion carbon capture technology
- Process Synthesis, Design & Optimization
  - Overview
  - Results
- Conclusions

National Energy Technology Laboratory

- *Full-service DOE federal laboratory*
- *Dedicated to energy RD&D, domestic energy resources*
- *Fundamental science through technology demonstration*
- *Unique industry–academia–government collaborations*

Oregon

Pennsylvania

West Virginia

A Century of Energy Innovation

1943 – U.S. Rep. Jennings Randolph flies from Morgantown, WV, to Washington, DC, on coal-derived fuel

1910 Coal research begins in Pittsburgh, PA

1918 Petroleum research begins in Bartlesville, OK

1943 Materials research begins in Albany, OR

1946 Synthesis gas research begins in Morgantown, WV

1977 All four sites join new U.S. Department of Energy

1996 PA & WV sites form new Federal Energy Technology Center

1999 FETC becomes National Energy Technology Laboratory (NETL)

2000 National Petroleum Technology Office in OK joins NETL

2001 NETL opens Arctic Energy Office in Fairbanks, AK

2005 Albany Research Center joins NETL

2009 OK office moves to Sugar Land, TX

Electricity Delivery & Energy Reliability

Energy Efficiency & Renewable Energy

Systems & Policy Analysis

Climate & Energy

Collaborative R&D Management

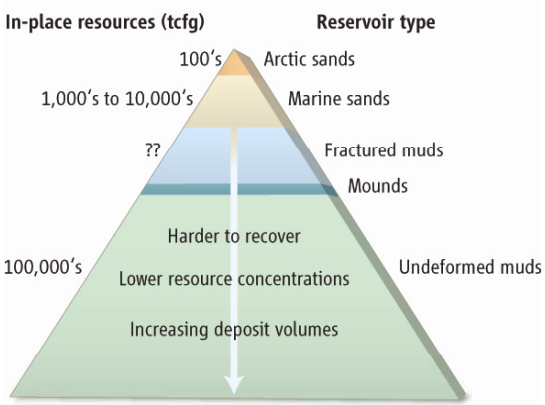
Alternative Fuels

Materials Science & Advanced Metallurgy

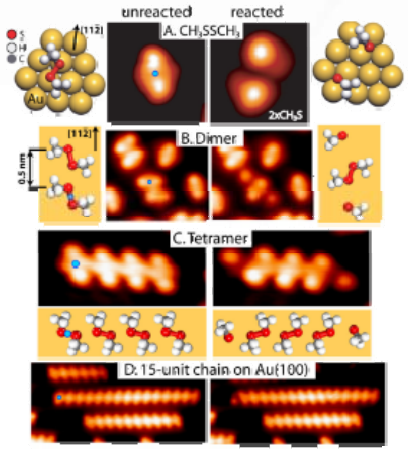
Enhanced Resource Recovery & Operational Safety

ORD Statistics

- **Employees:**
  - 205 Federal
  - 220 Contractor
- **University Collaboration:**
  - Regional University Alliance (CMU, Pitt, PSU, VT, WVU)
    - 91 Faculty Associates
    - 139 Graduate Students and Post-Docs
  - ORISE:
    - 63 Students and Post-Doctoral Students
- **Papers**
  - 140 papers in 2009
    - Up from 20 in 2000
    - Publications in high impact journals
  - 1900 citations to NETL papers
- **Recent Awards**
  - Nine R&D 100 Awards since 2007, including four in 2009
  - Five National FLC Excellence in Technology Transfer Awards; two in 2009
  - 70 Patent Applications in Process, 66 Total Issued Patents
  - 17 Active CRADAs
  - 11 Patent Licenses



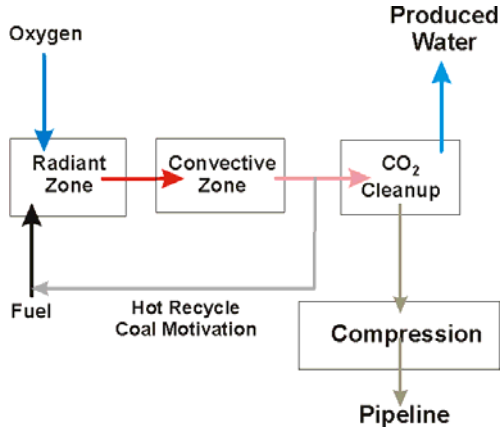
Science, vol. 325, 957-958 (2009).

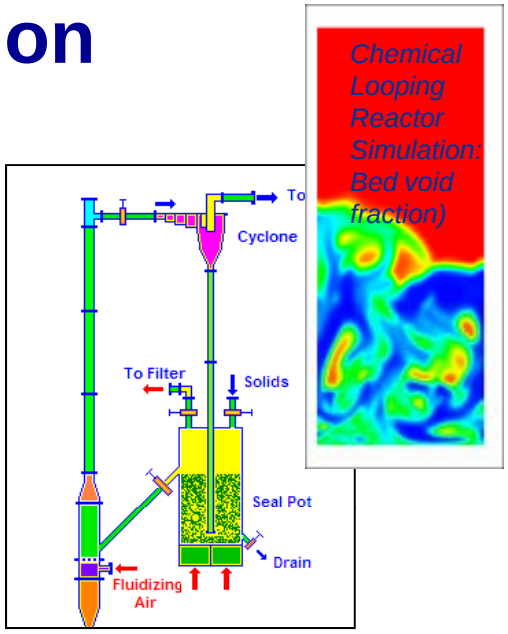


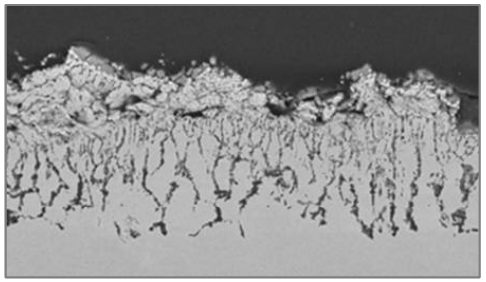
Science, vol. 322, 1664 (2008).

Reducing the Carbon Footprint in Fossil Energy Production

- Increased Efficiencies
  - Advanced Steam Cycles
  - Advanced Gasification
  - Next Generation Combustion Turbines
  - Fuel Cells
- Fuel Flexibility
- Carbon Capture
  - >90% CO_2 capture
  - Minimize increase in COE







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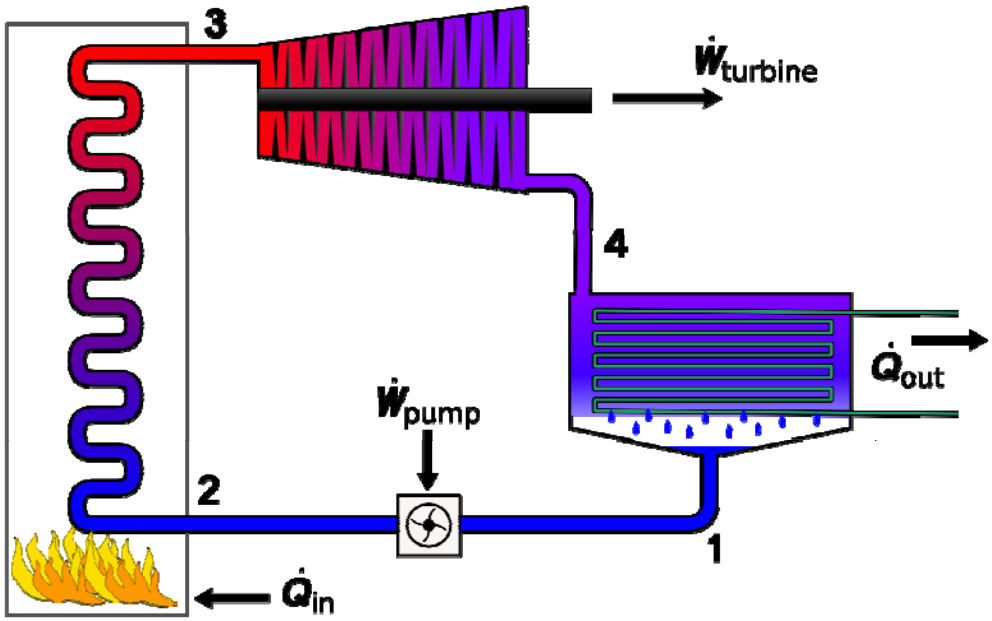
Definitions – Single Cycle

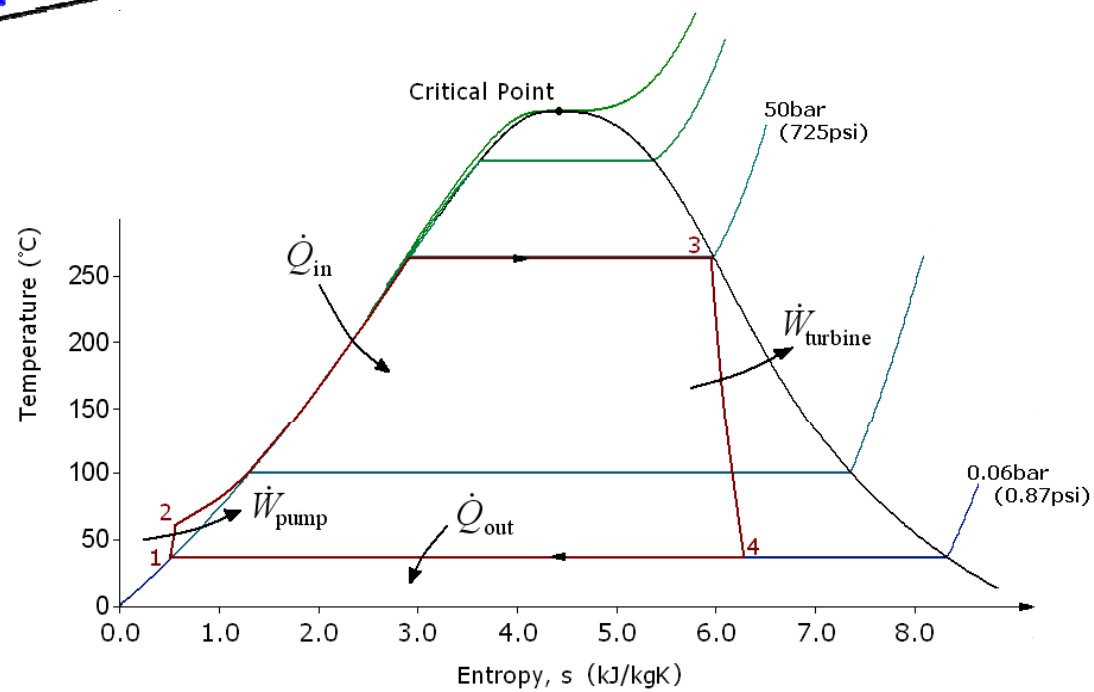
- Pulverized Coal (PC) Plant
  - Burns coal to generate steam to run turbines (Rankine Cycle)
  - Classifications
    - Subcritical (~2500 psia, 36-40% efficient)
    - Supercritical (~3500+ psia, 40-45% efficient)
    - Ultrasupercritical (~4400 psia, 48% efficiency)
  - Post-combustion capture
    - Aqueous amine (MEA)
- Gas Turbine – single Brayton cycle
  - Inexpensive capital cost
  - Higher operating cost
  - Used for peaking power

Definitions – Combined Cycle

- IGCC-Integrated Gasification Combined Cycle
  - Gasifies coal (CO, H_2, CO_2)
    - Electricity from Combined Cycle
      - burning syngas in gas turbine (Brayton cycle)
      - steam generated from cooling syngas, turbine exhaust (Rankine cycle)
  - Pre-combustion capture
    - Shift reactor (syngas to hydrogen & CO_2)
    - Physical solvent to remove CO_2
      - Selexol, Rectisol
- NGCC – Natural Gas Combined Cycle
  - Lower capital cost
  - Lower inherent CO_2 emissions
  - Requires post-combustion carbon capture

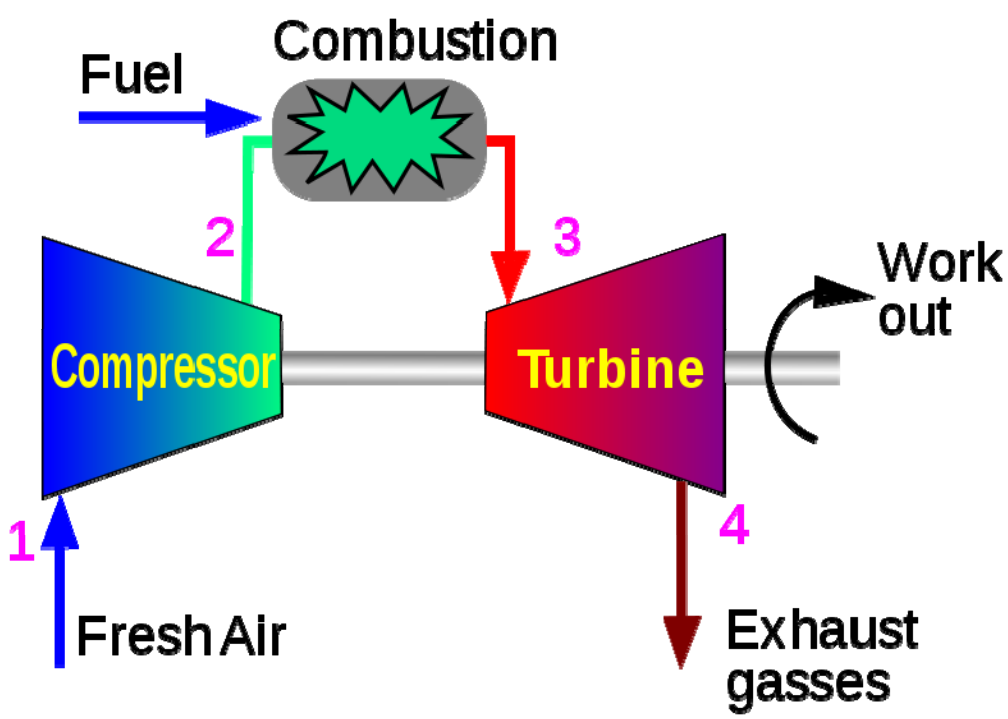
Rankine Cycle

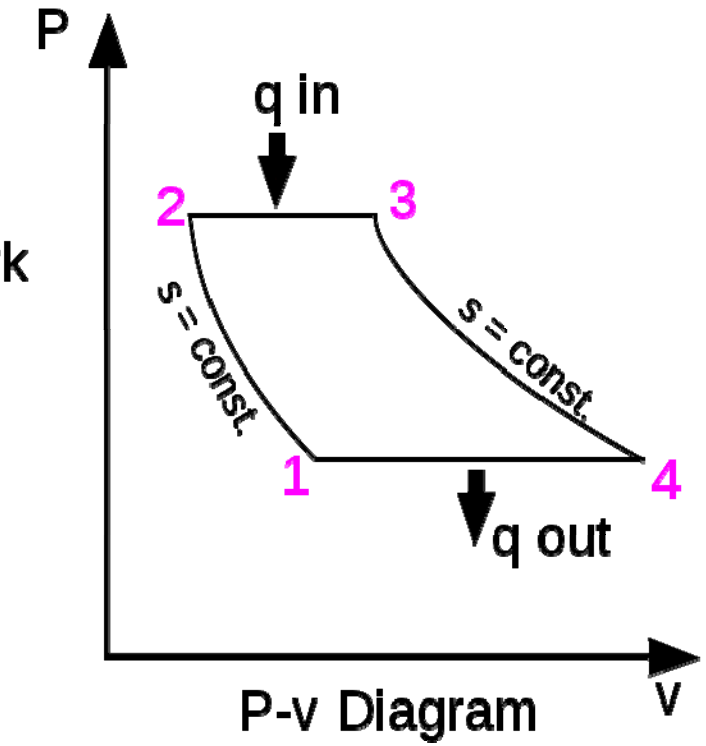




From http://en.wikipedia.org/wiki/Rankine_cycle

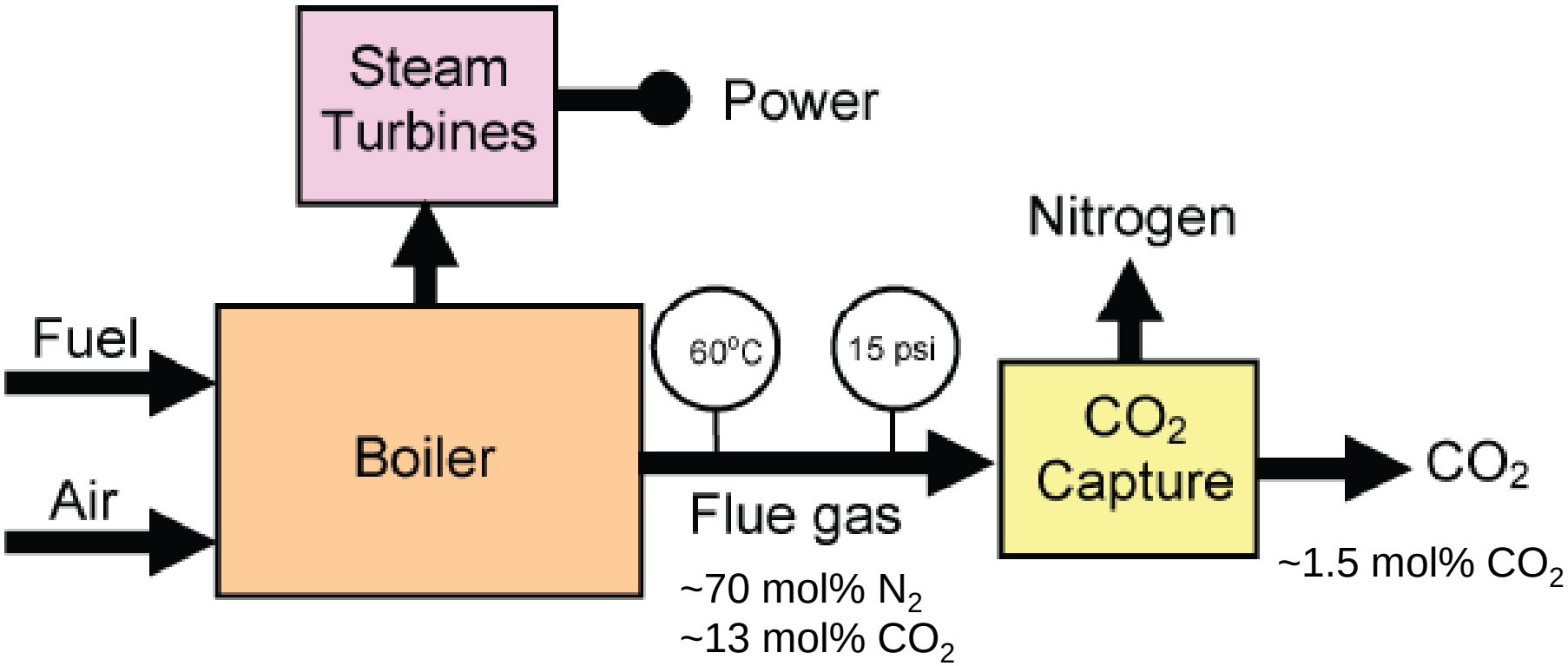
Brayton Cycle



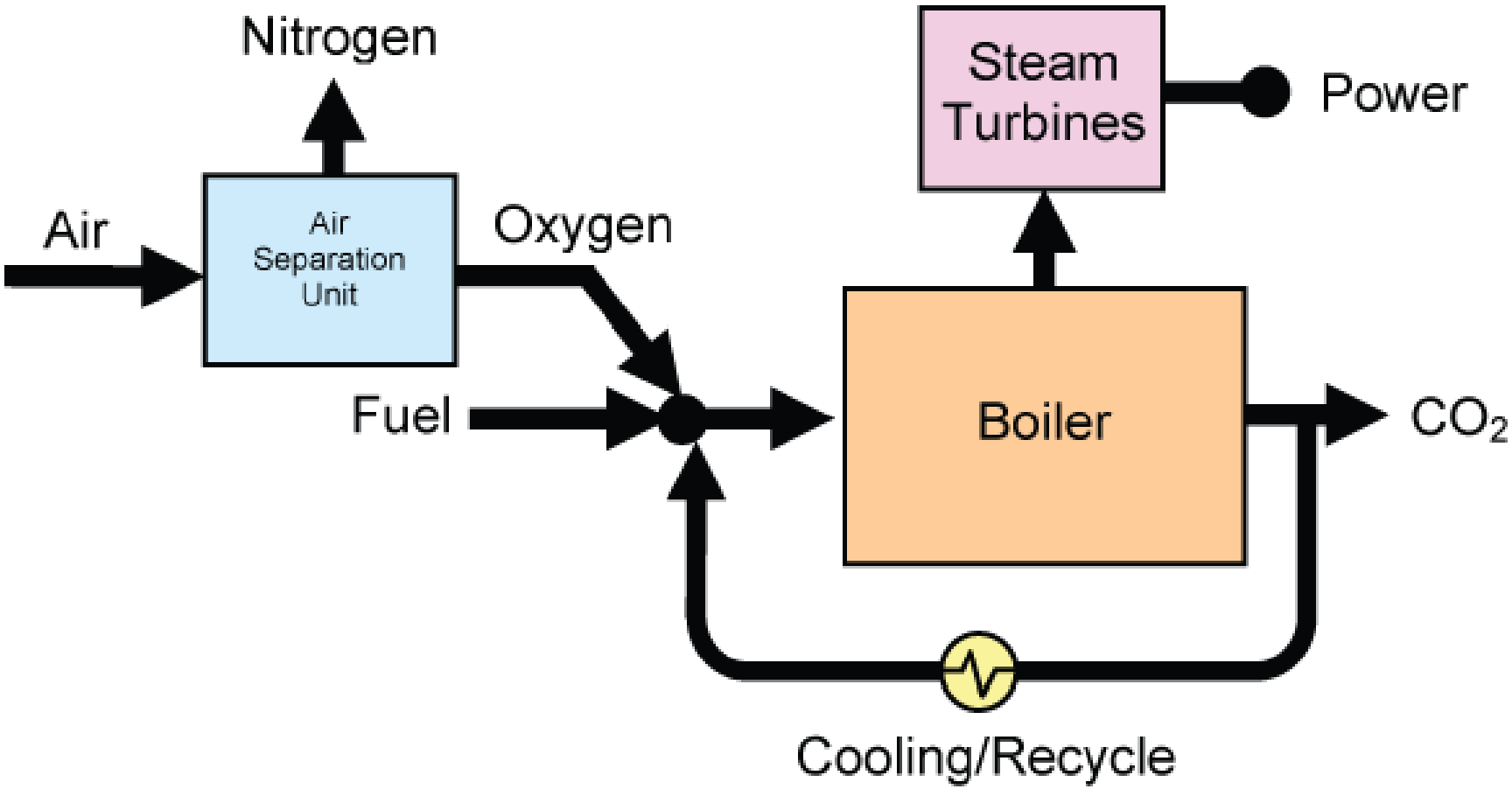


From http://en.wikipedia.org/wiki/Brayton_cycle

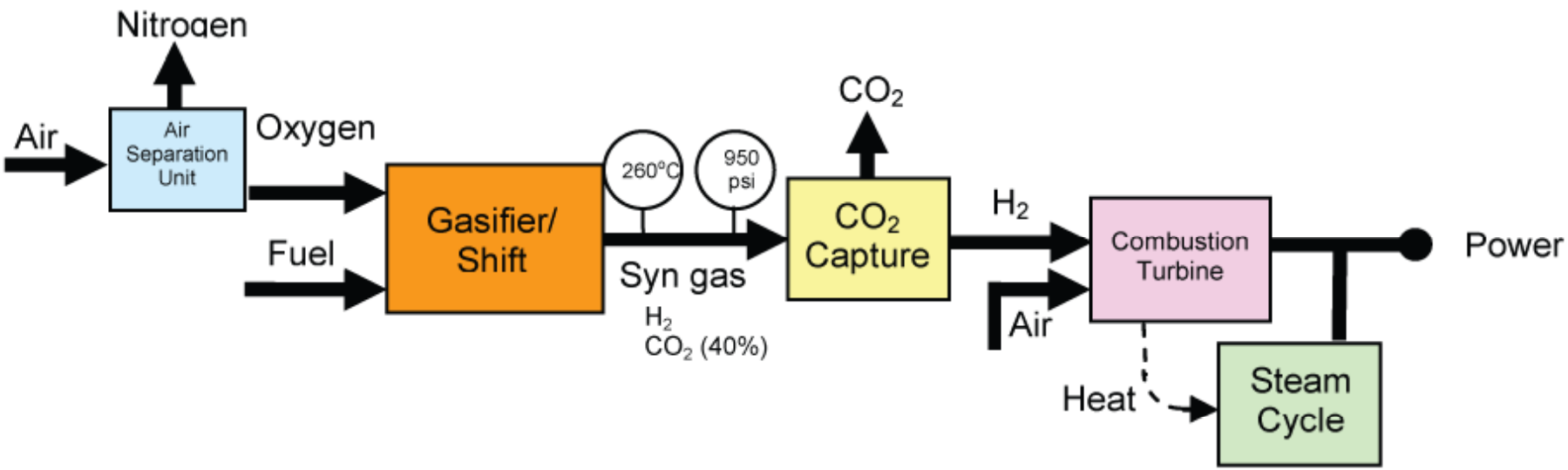
Post-combustion capture (PC)



Oxycombustion (PC)



Pre-combustion capture (IGCC)



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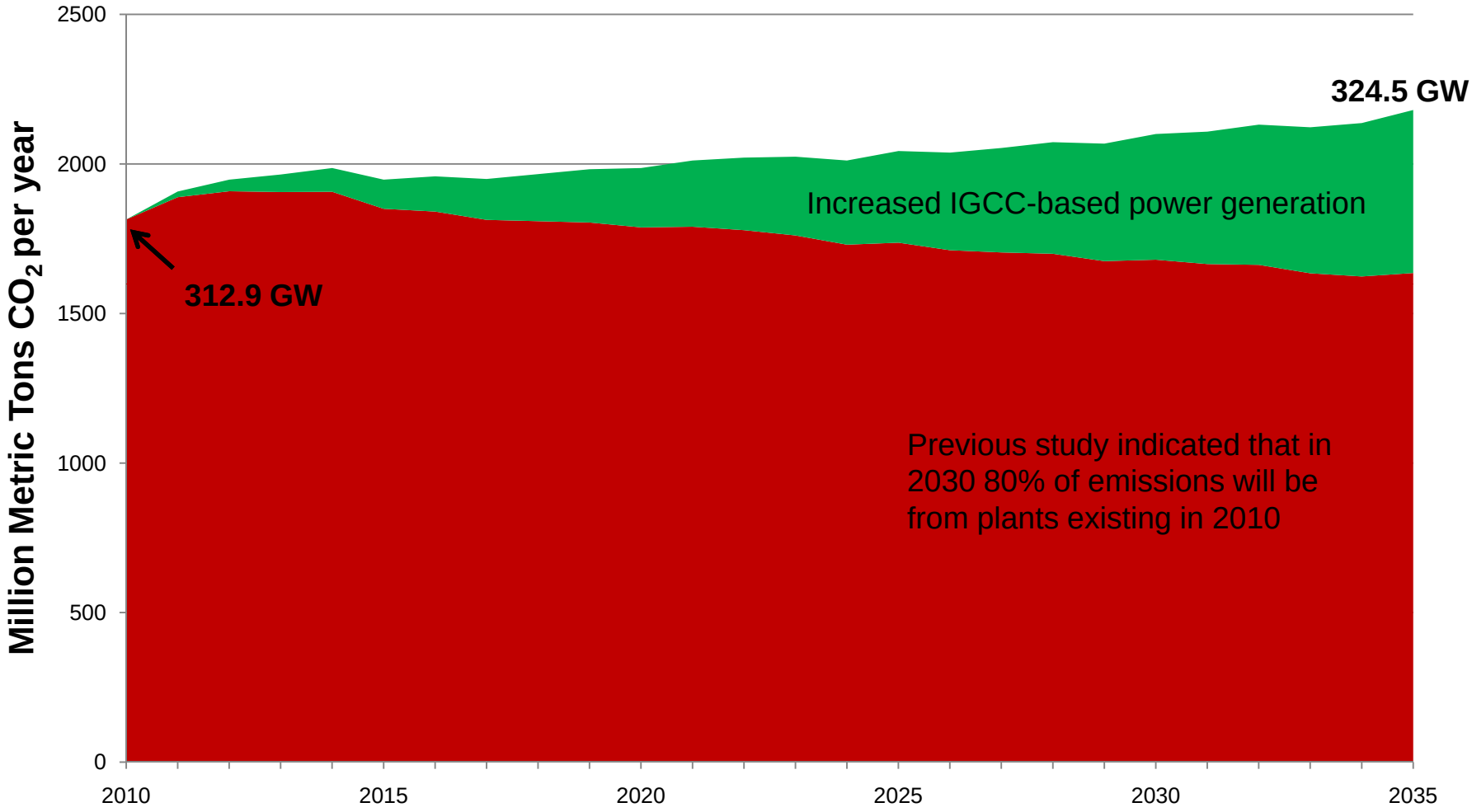
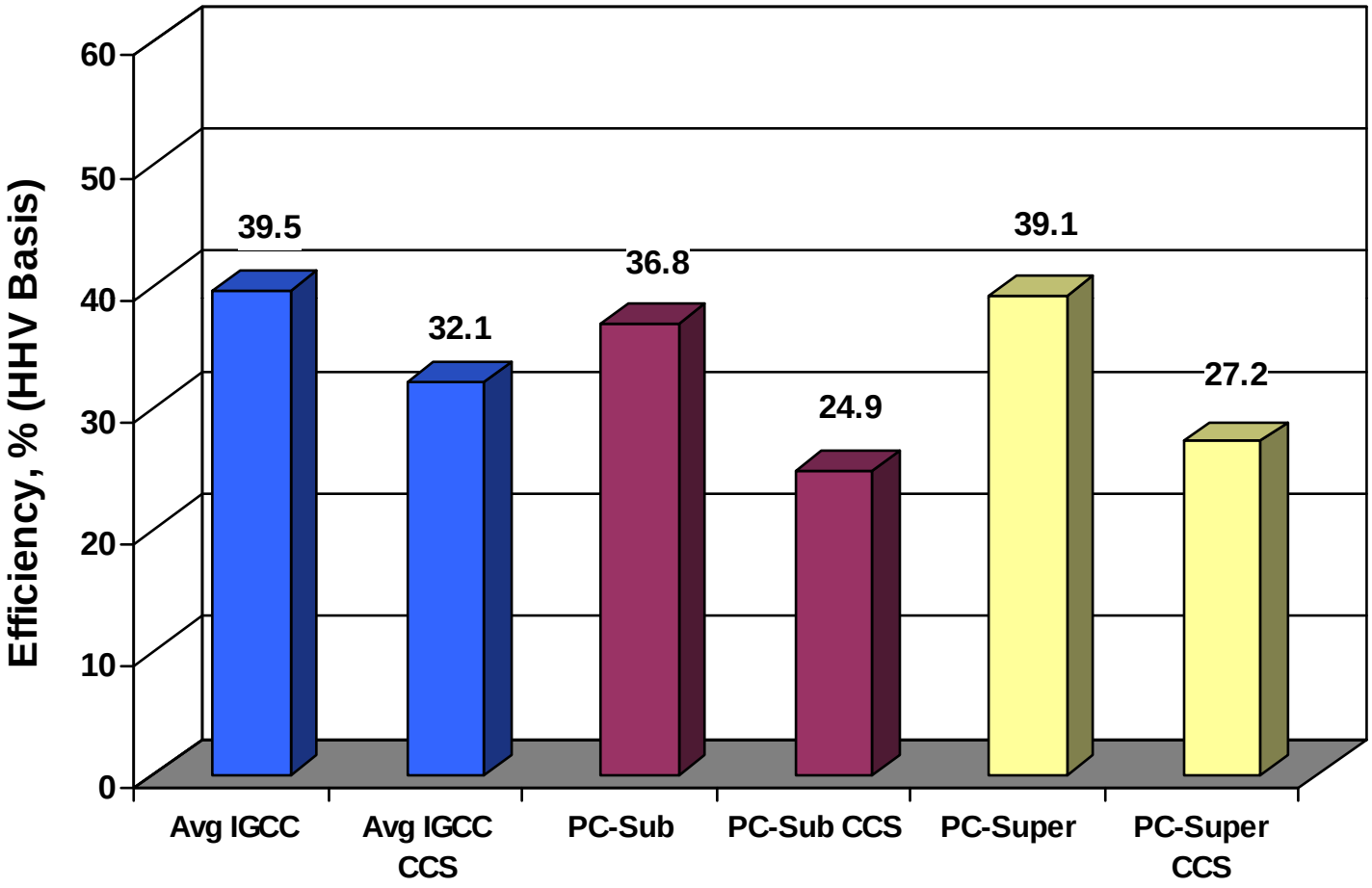
U.S. CO_2 Emissions from Coal Plants



Source: EIA, Annual Energy Outlook 2010 Early Release, Dec. 2009

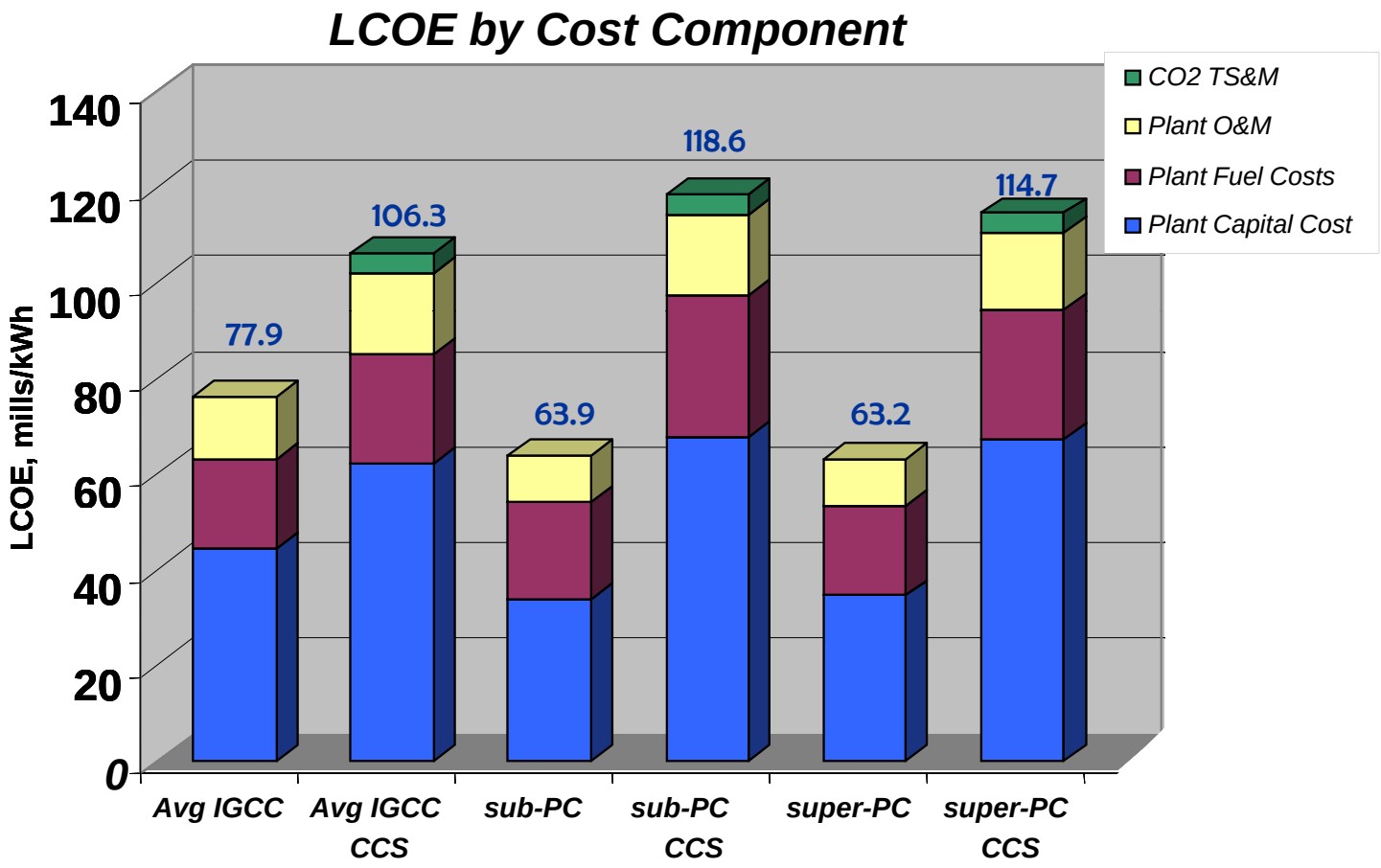
IGCC vs. PC with and without CCS

Net Plant Efficiency



"Cost and Performance Baseline for Fossil Energy Power Plants Study, Volume 1: Bituminous Coal and Natural Gas to Electricity," National Energy Technology Laboratory, www.netl.doe.gov, Aug. 2007.

IGCC vs. PC with and without CCS
Cost of Electricity

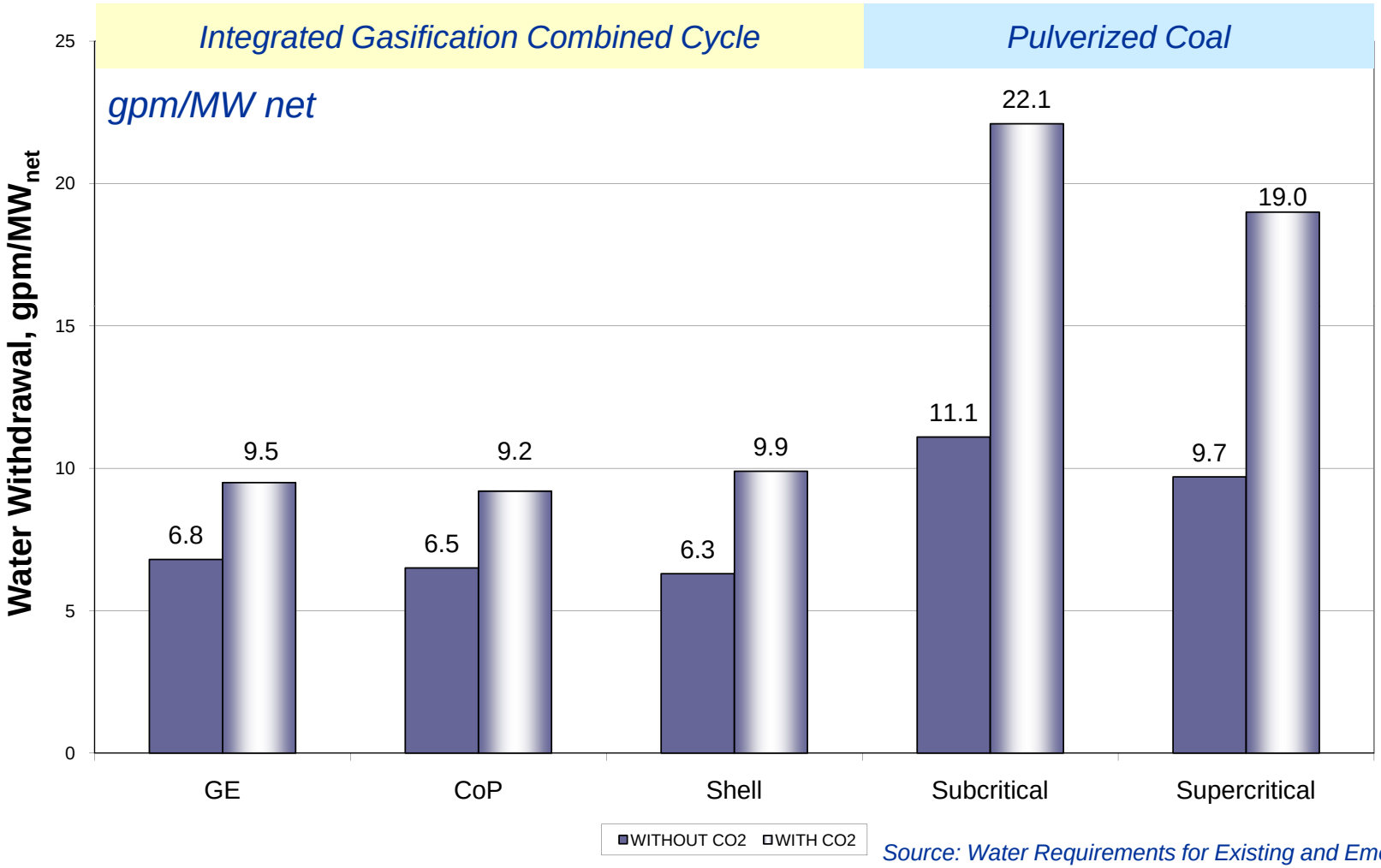


January 2007 Dollars, Coal cost $1.80/10^{6}Btu, Gas cost $6.75/10^{6}Btu CCS = Carbon capture and storage
TS&M = transport, storage, and monitoring

"Cost and Performance Baseline for Fossil Energy Power Plants Study, Volume 1: Bituminous Coal and Natural Gas to Electricity," National Energy Technology Laboratory, www.netl.doe.gov, May 2007.

Power Plant Water Withdrawal Requirements

with and without CO_2 capture



Source: Water Requirements for Existing and Emerging Thermoelectric Plant Technologies; NETL, August 2008

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

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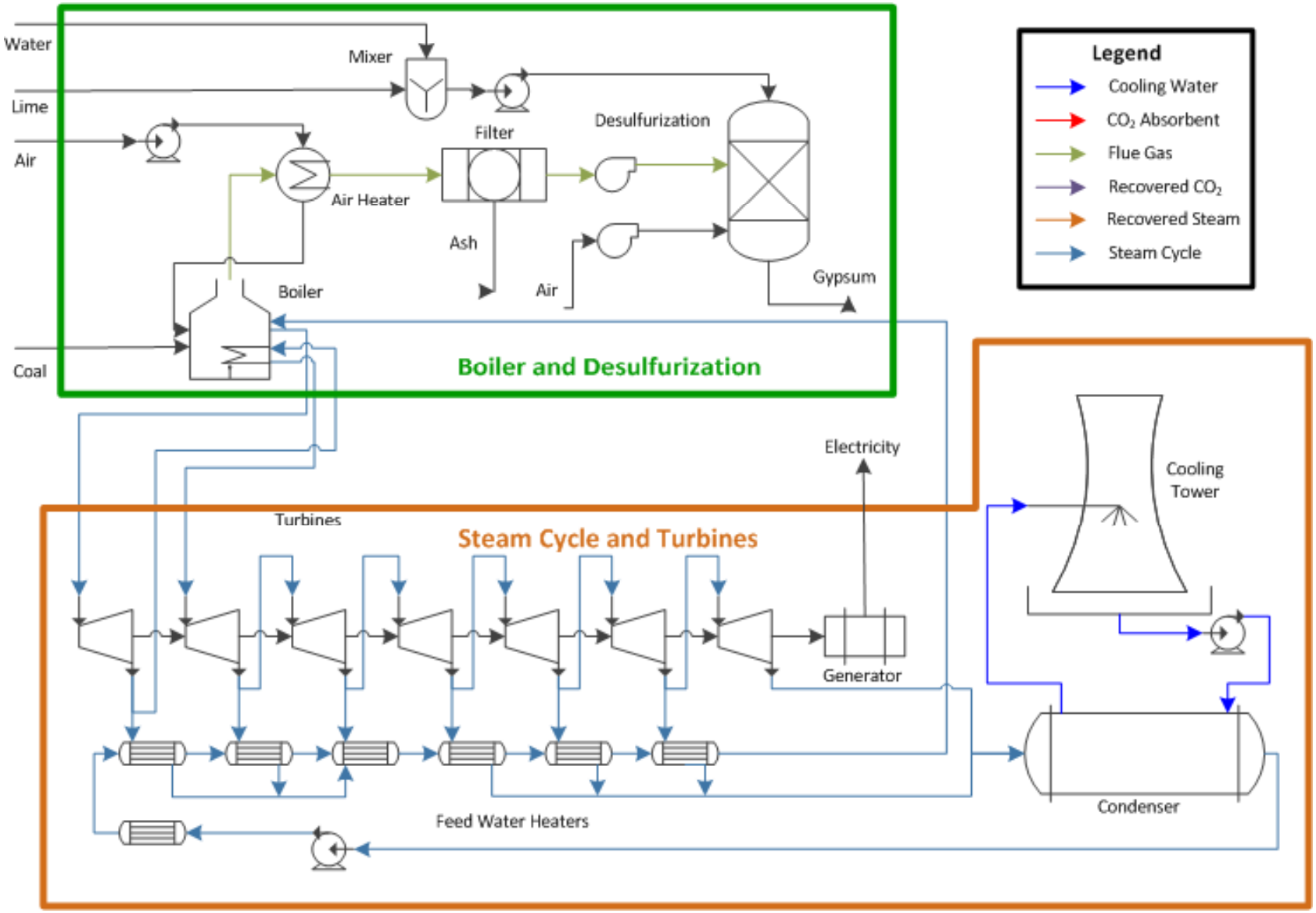
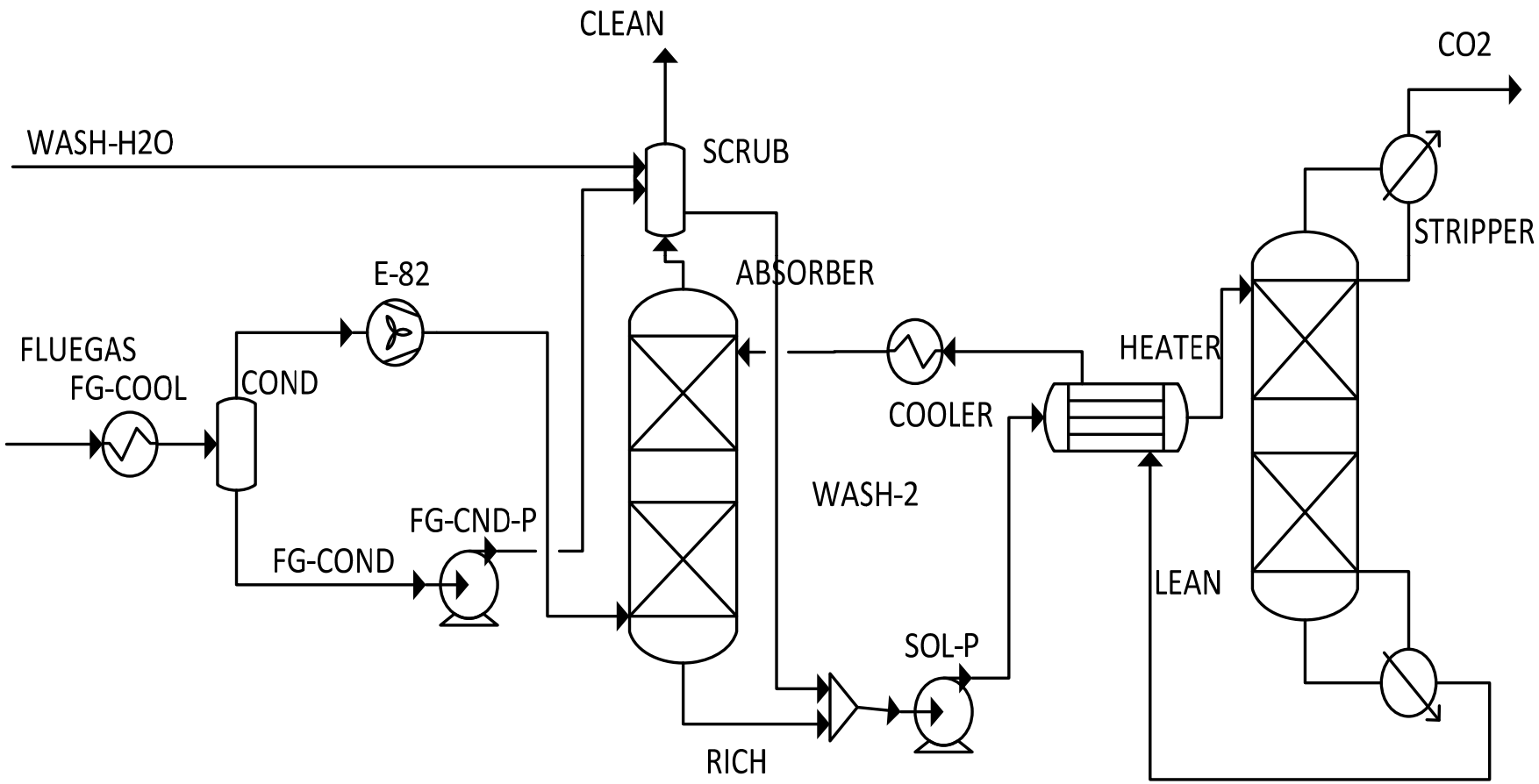
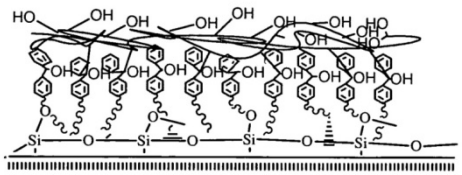
Subcritical PC Plant



Aqueous Amine Scrubbing



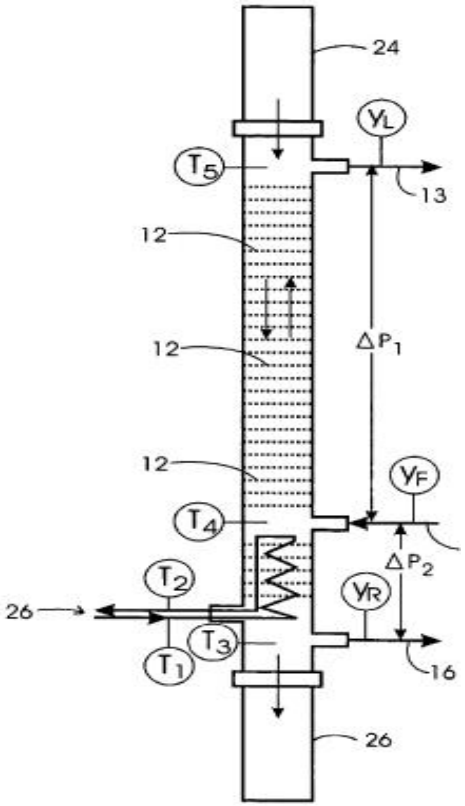
Solid Sorbents



Moving Bed

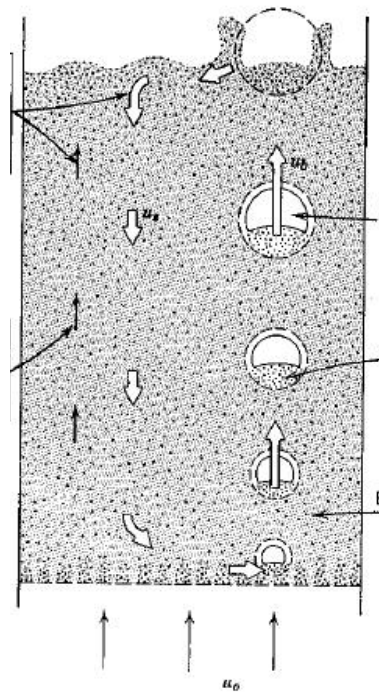
Steady-state

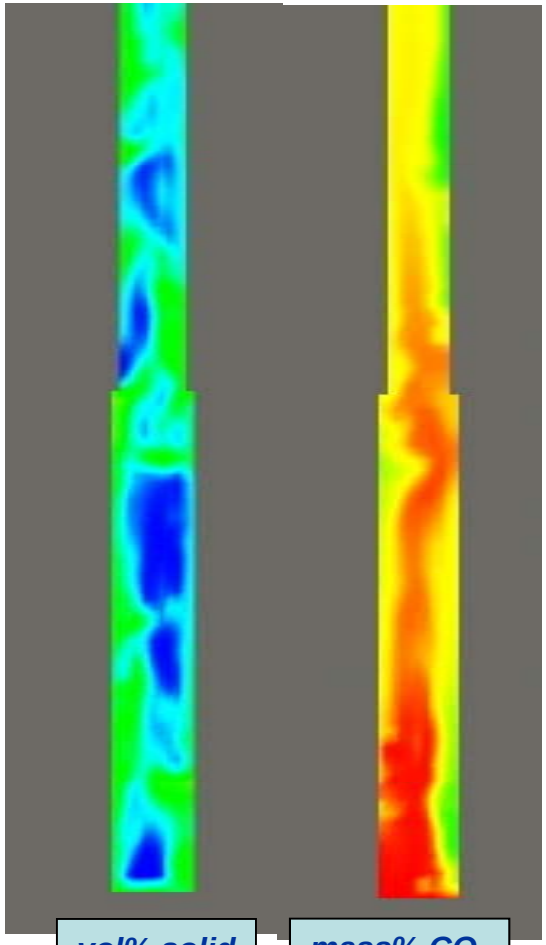
1 Dimensional PDE model



Fluidized Bed

Steady-state, three phase model (bubble, wake and emulsion) with interphase mass transfer

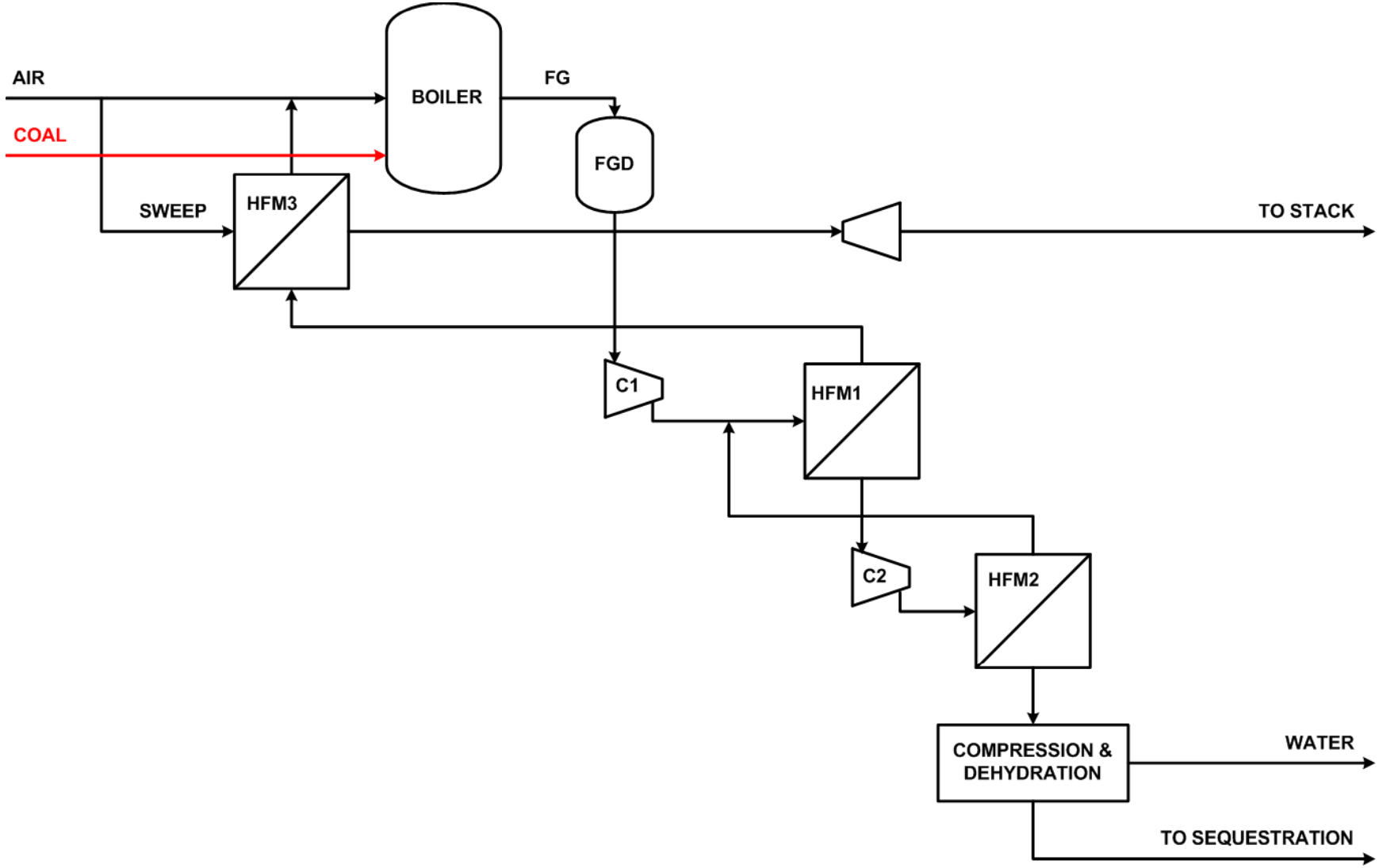




vol% solid
Green 50
Blue 0

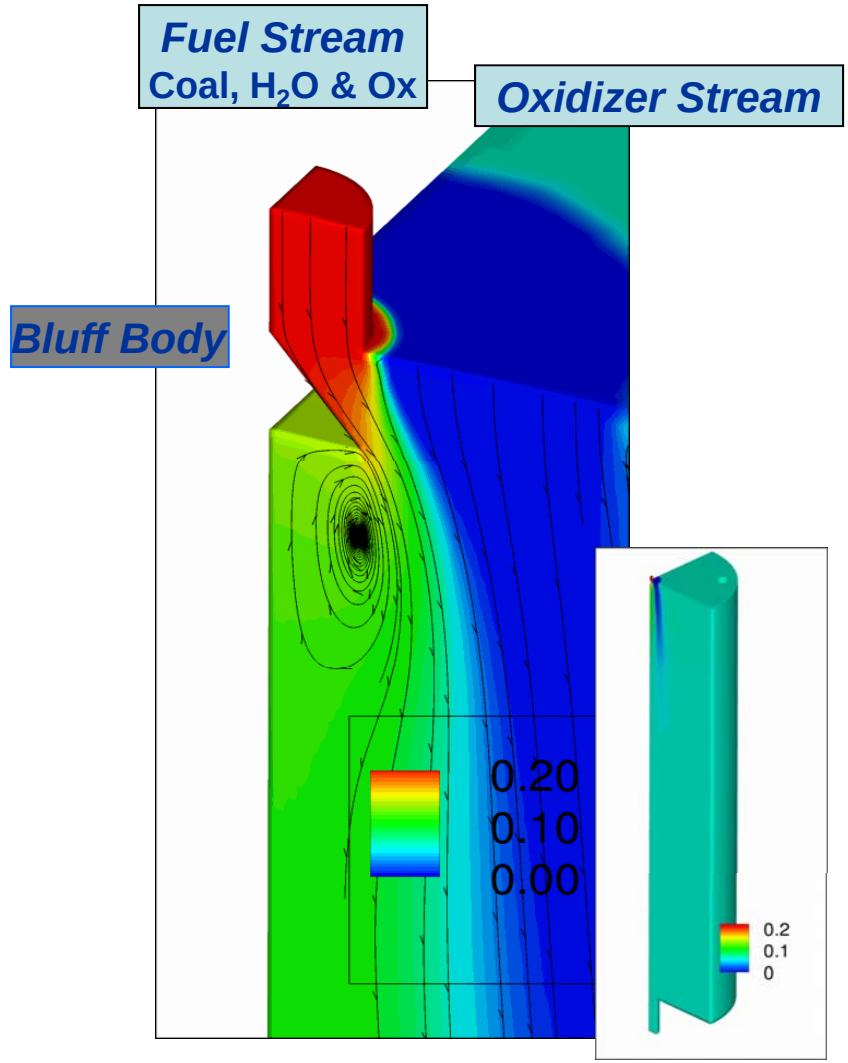
mass% CO_2
Red 10
Green 5

Membrane Systems



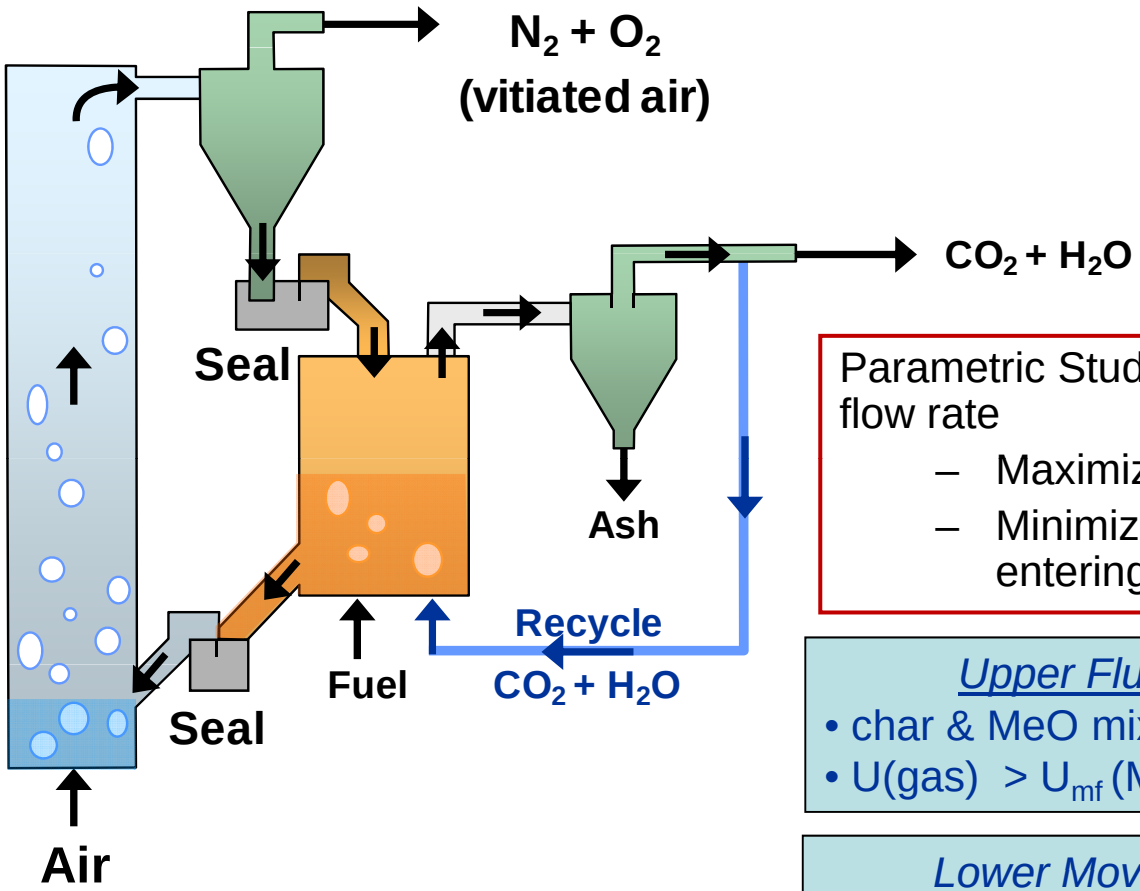
Oxy-fuel Combustion

- Oxygen + flue gas recycle = easy CO_2 capture.
- Innovative oxygen production technologies and <u>integration</u> with whole process needed.
- Validated simulation tools:
  - Enabling rapid & multiple retrofit and greenfield.
  - Requires establishing simulation appropriate to new combustion environment.



Chalmer's Furnace (Khare et. al, 2008)

Chemical Looping



Parametric Study of geometry and flow rate

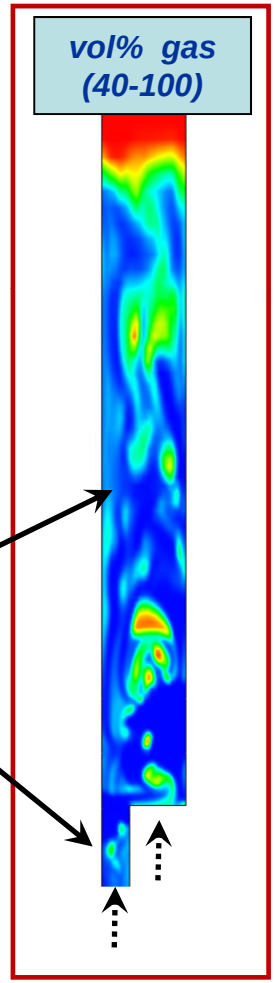
- Maximize Coal Utilization
- Minimize Char/Ash entering air reactor

Upper Fluid Bed Zone

- char & MeO mix and circulate
- $U(gas) > U_{mf}(MeO) > U_{mf}(char)$

Lower Moving Bed Zone

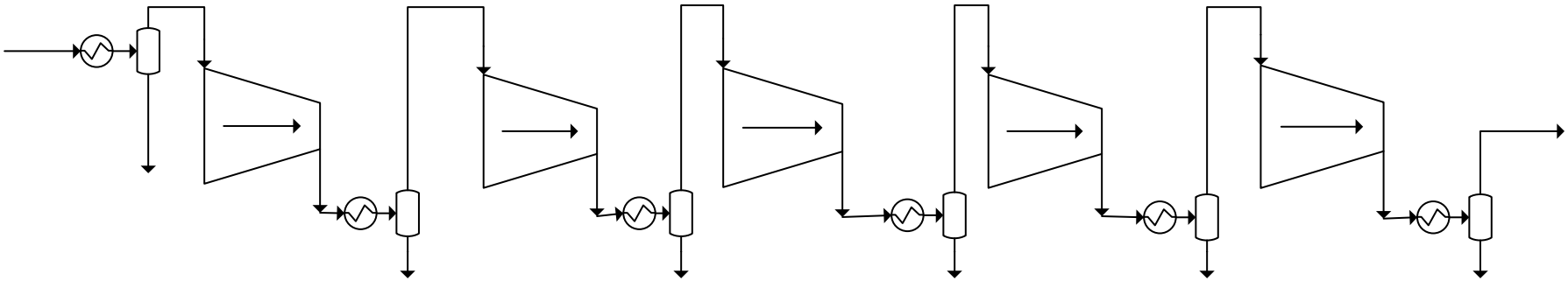
- char & MeO separate
- $U_{mf}(MeO) > U(gas) > U_{mf}(char)$



Carbon + metal oxide = CO_2 + metal

Metal + air (oxygen) = metal oxide

Compression



- 5 casing (10 stage) compression
- Intercoolers 265°F to variable T
- Water returned to process
- Final pressure 2200 psia

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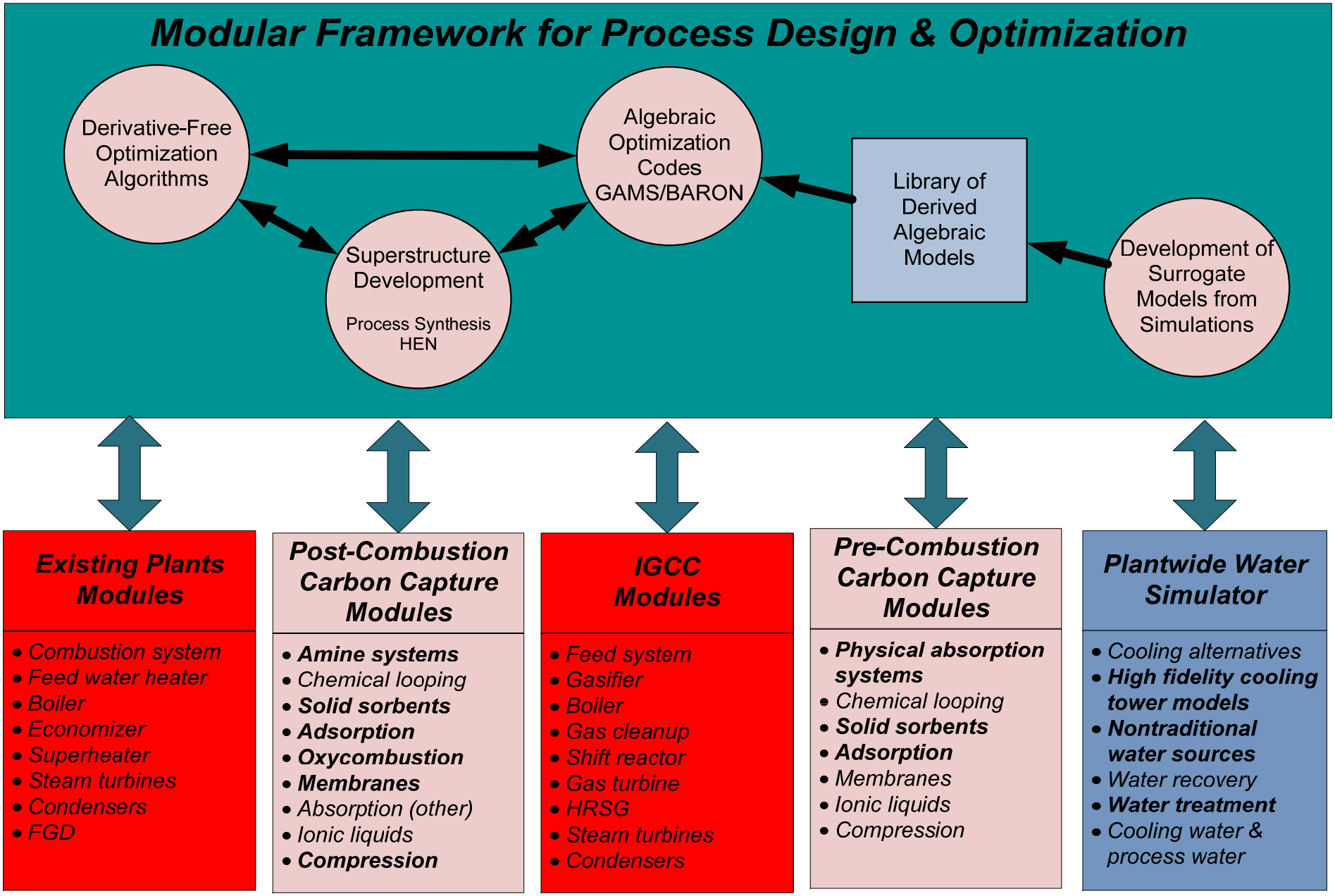
Challenges

- 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 <u>optimized</u> designs
- Difficulty re-using existing models/simulations
- Inconsistent assumptions & evaluation methods

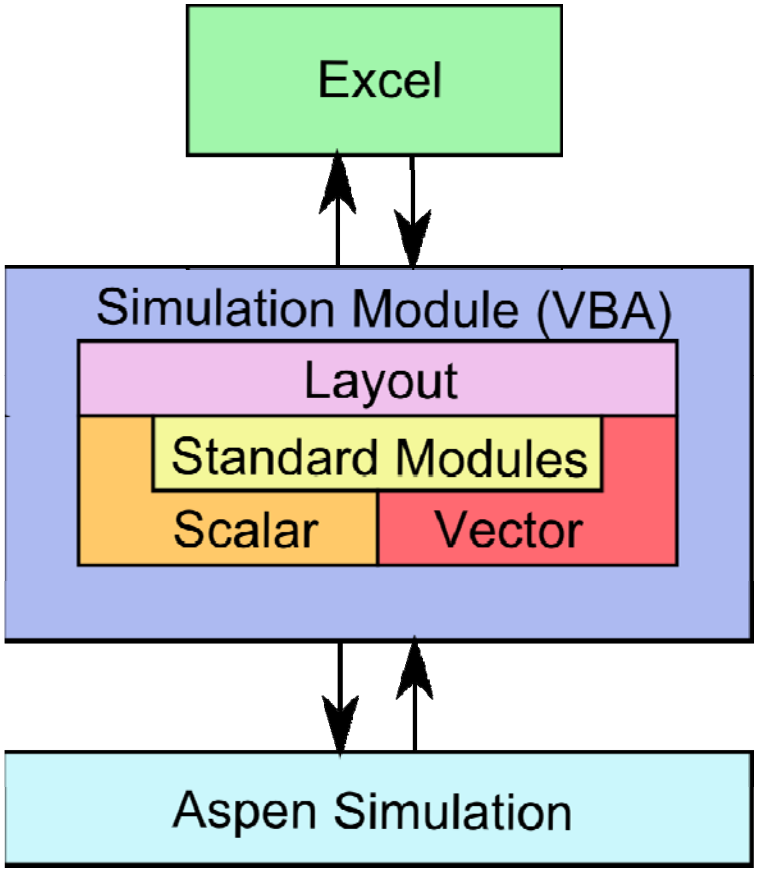
- Approach
  - Process synthesis, design & optimization
    - Process integration
    - Nonlinear interactions across units/subsystems
    - Simulation-based optimization
  - Multi-criteria decision-making tools
    - Include water resource considerations

Modular Framework for Process Design & Optimization

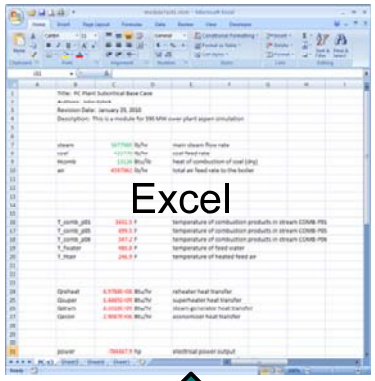


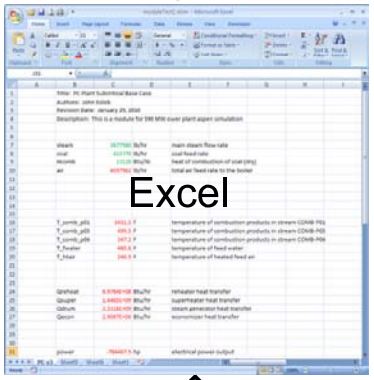
Simulation INTERface (SINTER)

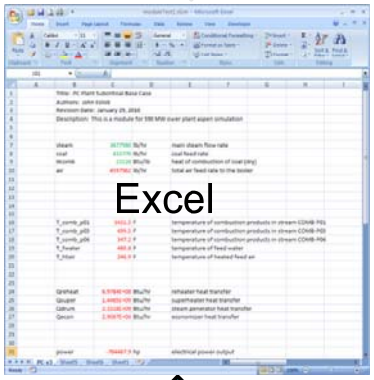
- Set simulation variables
- Supports structural changes
  - Feed stage
  - Number of stages
  - (not supported internally)
- Retrieves results
- Perform post-processing
  - Cost estimation
  - Objective function calculations



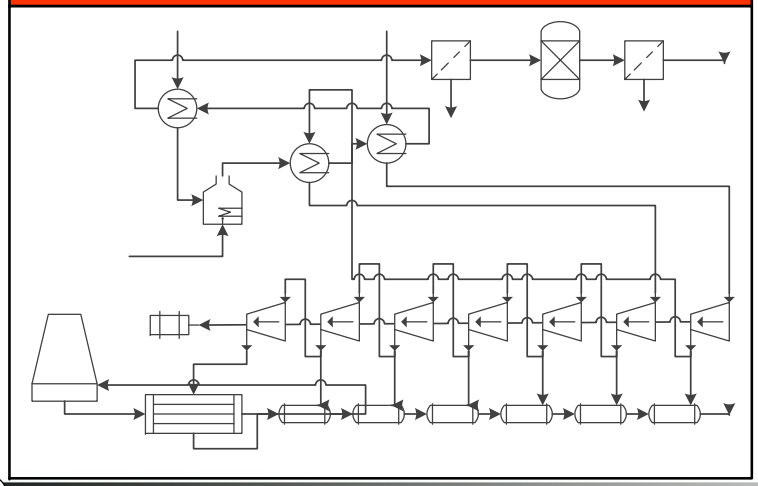
Modular Framework for Process Design and Optimization



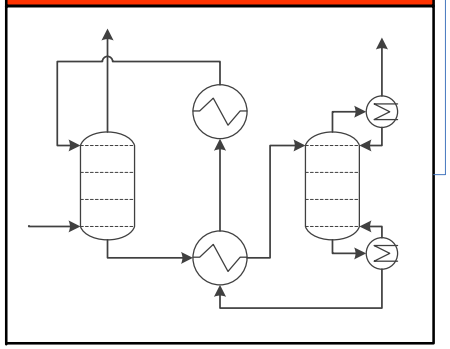




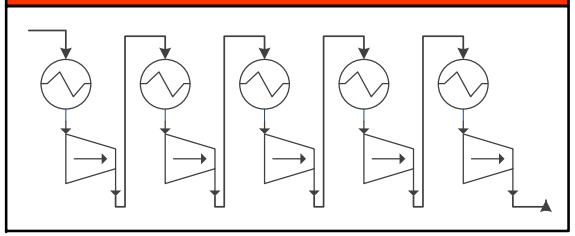
Power Plant Module



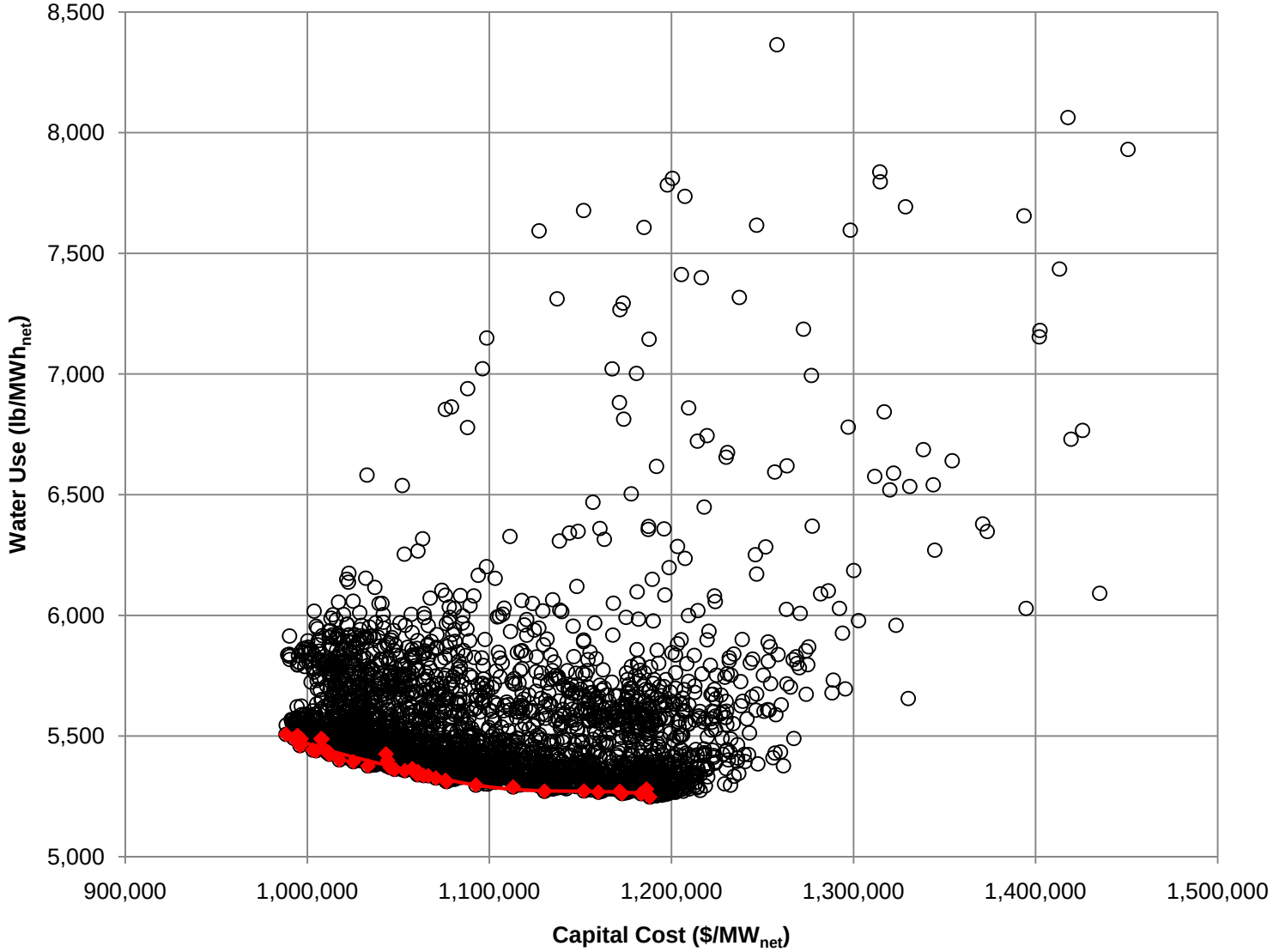
CO_2 Capture Module



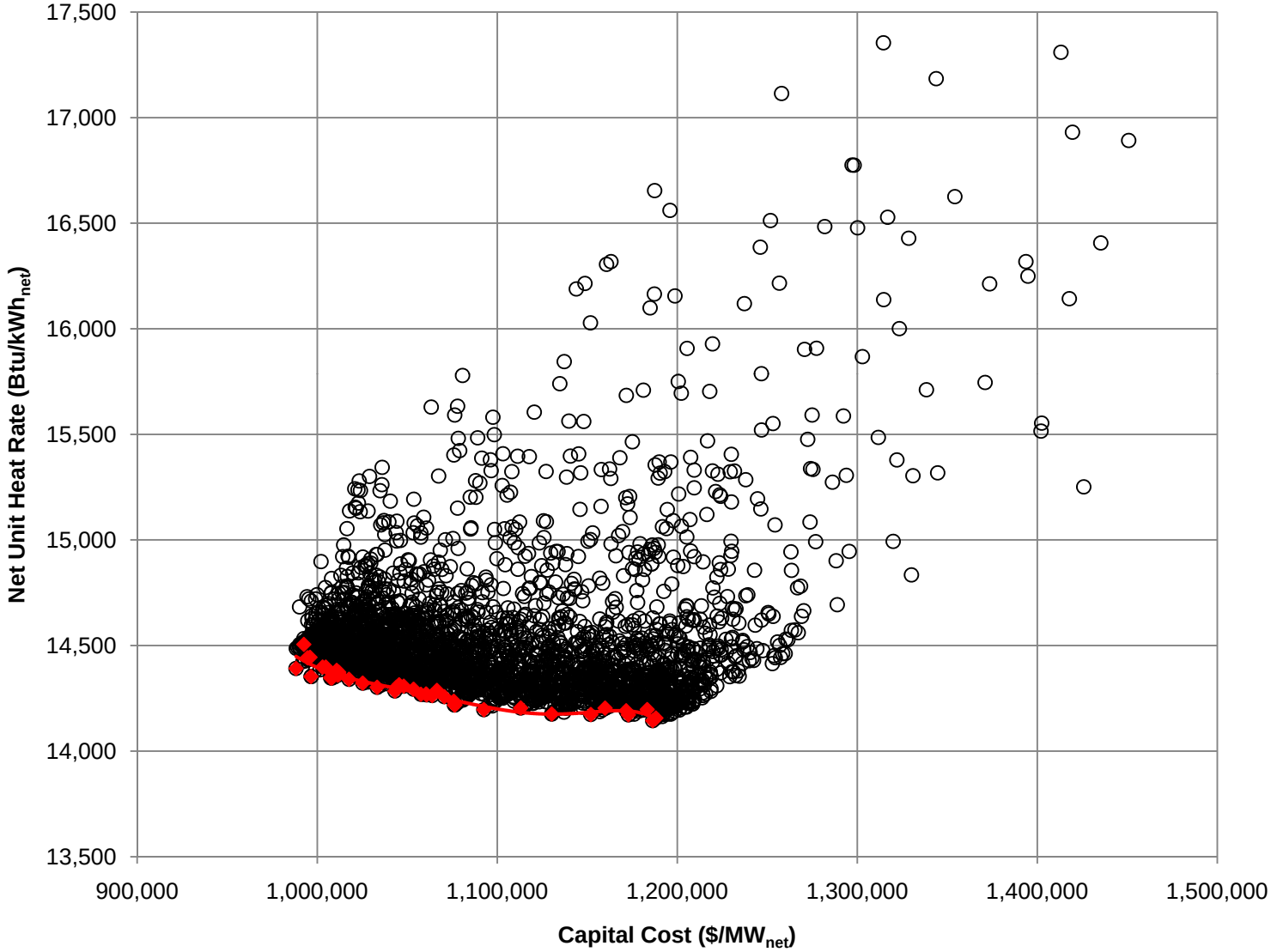
Compression Module



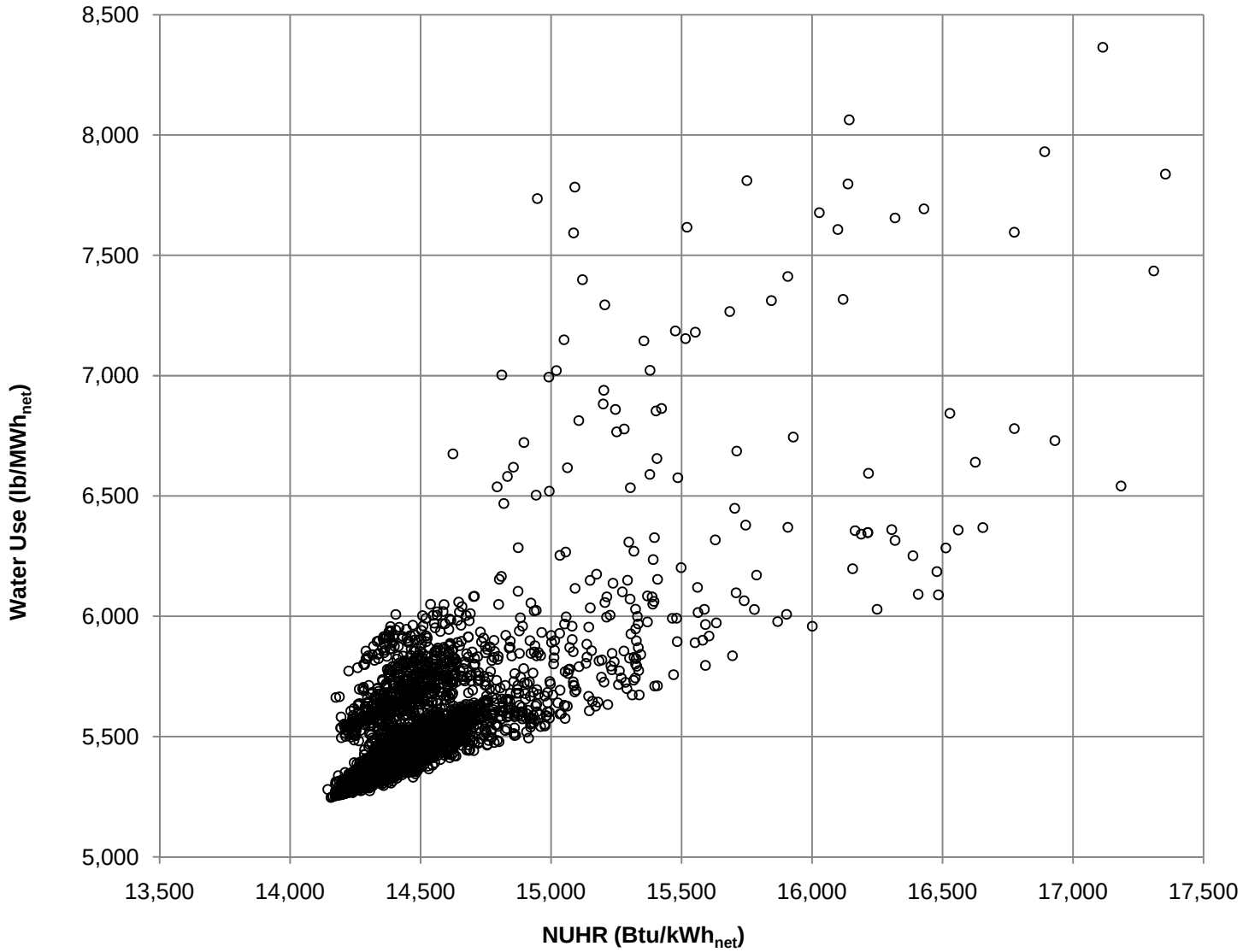
Capital Cost vs. Water Use



Capital Cost vs. NUHR



NUHR vs. Water Use

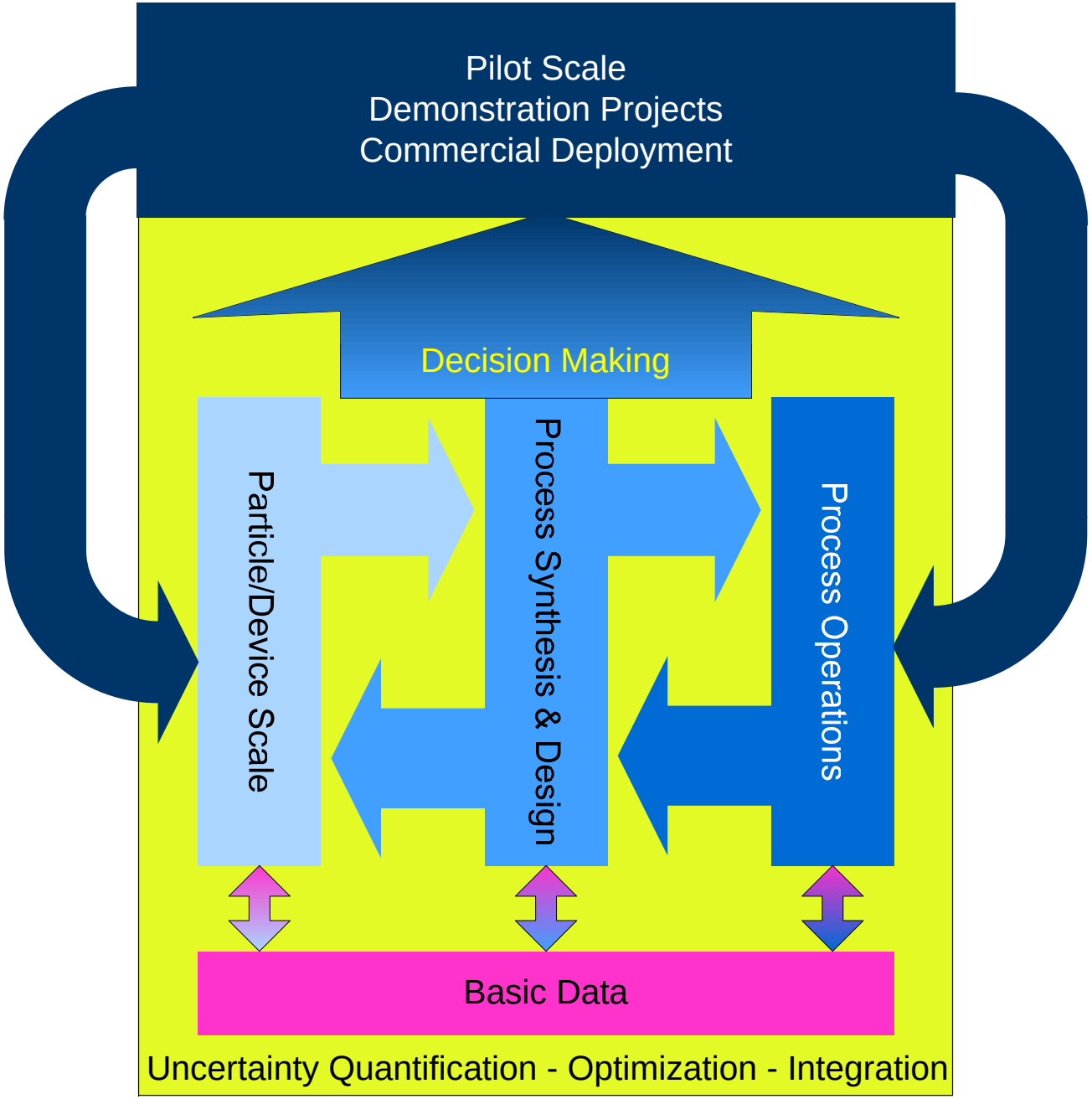


	Best Net Unit Heat Rate	Best Capital Cost	Best Water Use
NUHR (Btu/kWh)	14,145	14,392	14,157
Capital Cost ($/kW$_{net}$)	1,186	988	1,188
Overall Net Power Output (MW)	354.7	348.6	354.4
Total Capital Cost (Capture & Compression only)	$421 MM	$345 MM	$421 MM
Solvent Flow rate (gpm)	7,070	7,470	6,970
Lean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

Conclusions

- Demonstrated importance of optimizing systems
  - Large potential improvement over initial design
- Essential for comparing potential CC technology
  - Many non-intuitive interactions
  - Understand competing objectives
- Significant optimization/integration opportunities remain
  - Solid sorbents
  - Advanced solvents
  - Oxycombustion
  - IGCC
  - Compression

Tasks Required for Deployment



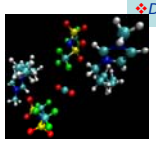
Carbon Capture Simulation Initiative

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

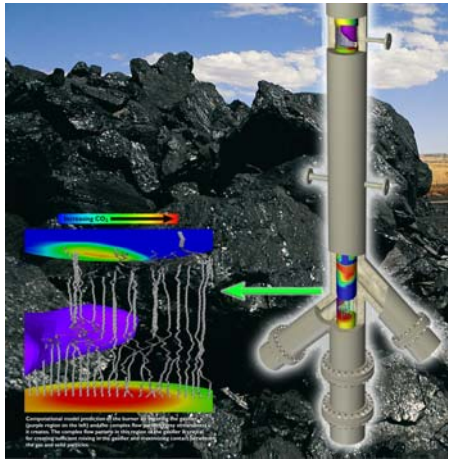
Monte Carlo
- *Thermo dynamic Properties*

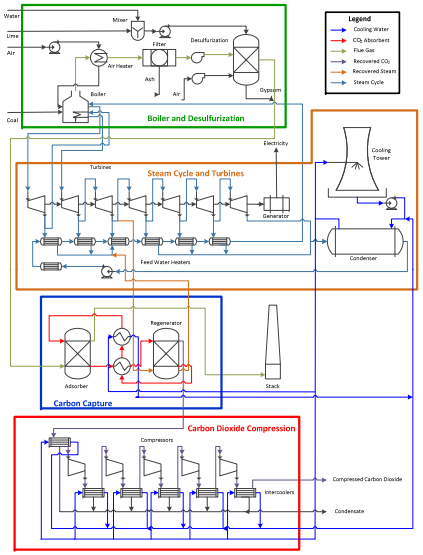
Molecular Dynamics
- *Transport Properties*

- *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

Acknowledgements: Research Team

- Optimization and computational infrastructure
  - ModeFrontier integration & multi-criteria, simulation-based optimization - NETL (Miller/Eslick)
  - Derivative-free surrogate model development – CMU (Sahinidis/Cozad/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)
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    - 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)