



New Developments with IECM

Edward S. Rubin

Dept's of Engineering & Public
Policy, and Mechanical Eng'g.
Carnegie Mellon University
Pittsburgh, PA

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Outline of Talk

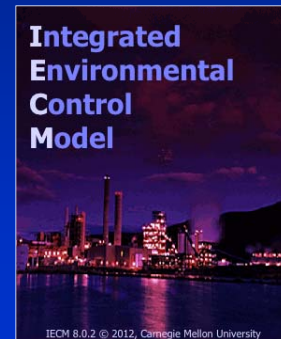
- Overview of the IECM
- Recent & planned work: Pre-combustion capture
- Recent & planned work: Post-combustion capture
- Recent & planned work: Oxy-combustion capture
- Recent & planned work: Other activities

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IECM Overview

IECM: A Tool for Analyzing Power Plant Design Options

- A desktop/laptop computer simulation model developed for DOE/NETL
- Provides systematic estimates of performance, emissions, costs and uncertainties for preliminary design of:
 - PC, IGCC and NGCC plants
 - All flue/fuel gas treatment systems
 - CO₂ capture and storage options (pre- and post-combustion, oxy-combustion; transport, storage)
- Free and publicly available at:
www.iecm-online.com



IECM 8.0.2 © 2012, Carnegie Mellon University

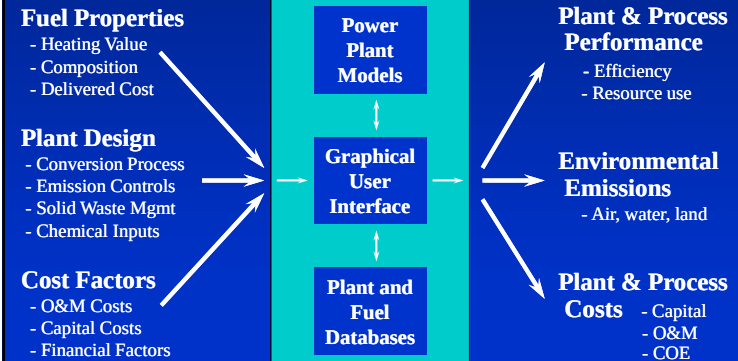
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IECM Modeling Approach

- Systems Analysis Approach
- Process Performance Models
- Engineering Economic Models
- Advanced Software Capabilities
 - User-friendly graphical interface
 - Probabilistic analysis capability
 - Versatile input/output features

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IECM Software Package



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IECM Technologies for PC Plants

(excluding CO₂ capture, transport and sequestration)

Boiler/Turbine Types

- Subcritical
- Supercritical
- Ultra-supercritical

Furnace Firing Types

- Tangential
- Wall
- Cyclone

Furnace NO_x Controls

- LNB
- SNCR
- SNCR + LNB
- Gas reburn

Flue Gas NO_x Removal

- Hot-side SCR

Mercury Removal

- Carbon/sorbent injection

Particulate Removal

- Cold-side ESP
- Fabric filter
 - Reverse Air, Pulse Jet

SO₂ Removal

- Wet limestone
 - Conventional, Forced oxidation
 - Additives
- Wet lime
- Lime spray dryer

Solids Management

- Ash pond, Landfill, Co-mixing
- Byproducts (for export)

Cooling and Wastewater Systems

- Once-through cooling
- Wet cooling tower
- Dry cooling tower
- Chemical treatment
- Mechanical treatment

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Technologies for IGCC and NGCC Plants

(excluding CO₂ capture, transport and sequestration)

Air Separation Unit

- Cryogenic

Slurry Preparation

Coal Pretreatment

Gasification

- Slurry-feed gasifier (GE-Q)
- Dry-feed gasifier (Shell)

Syngas Cooling and

Particulate Removal System

Mercury Removal

- Activated carbon

H₂S Removal System

- Selexol
- Sulfinol

Sulfur Recovery System

- Claus Plant
- Beavon-Stretford Unit

FOR BOTH IGCC and NGCC:

Gas Turbine

- GE 7FA
- GE 7FB

Heat Recovery Steam Generator

Steam Turbine

Boiler Feedwater System

Process Condensate Treatment

Auxiliary Equipment

Cooling Water System

- Once-through
- Wet cooling tower
- Air cooled condenser

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IECM Technologies for CCS

(version 8.0.2)

- CO₂ Capture Options
 - *Pre-Combustion (IGCC):*
 - Water gas shift + Selexol
 - Chemical looping
 - *Oxy-Combustion (PC)*
 - *Post-Combustion (PC, NGCC):*
 - Amine systems (MEA, FG+)
 - Chilled ammonia
 - Membrane systems
 - Auxiliary NG boiler or power plant (optional)
- CO₂ Transport Options
 - Pipelines (six U.S. regions)
- CO₂ Sequestration Options
 - Geologic: Deep Saline or Other Formations
 - Geologic: Enhanced Oil Recovery (EOR)

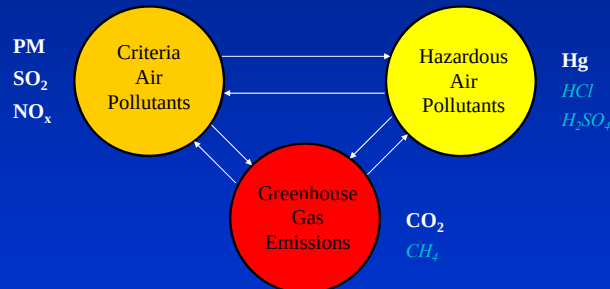
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Process Performance Models

- Detailed mass and energy balances for each major component and overall plant
- For components with complex chemistry and/or heat integration schemes, multi-variate regression or other reduced-order models are derived from experimental data and detailed process models
- Approximately 10-20 performance parameters for each component technology

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Performance Models Account for Multi-Pollutant Interactions



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Technology Cost Models

- Direct cost models for each major process area (typically 5-10 areas per technology) based on detailed engineering design studies
- Explicit links to process performance models via key parameters (e.g., flow rate, temp., pressure, etc.)
- Calculate total capital cost, variable O&M costs, fixed O&M costs and annualized cost of electricity
- Approximately 20-30 cost elements per technology

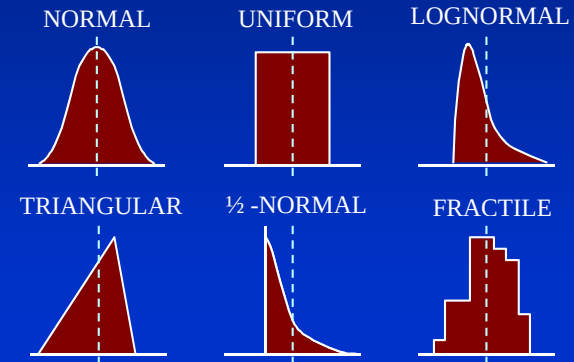
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Probabilistic Capability

- Allows users to explicitly model and quantify the effects of uncertainty and/or variability on component and system performance, emissions and cost
- Values for user-selected parameters are specified as a probability distribution function, which is sampled using a selected method and sample size (default = median latin hypercube sampling, LHS)
- Results are displayed as a cumulative distribution function, yielding confidence intervals and probability of different outcomes for selected parameters

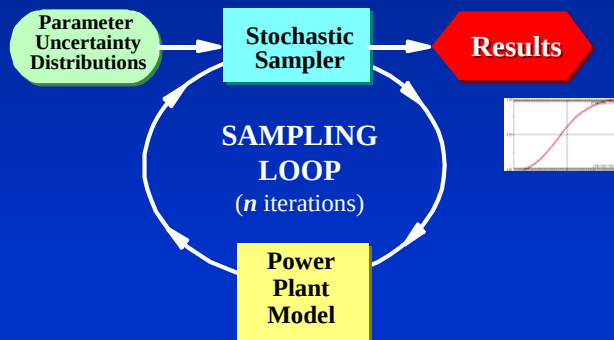
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Examples of IECM Parameter Uncertainty Distributions



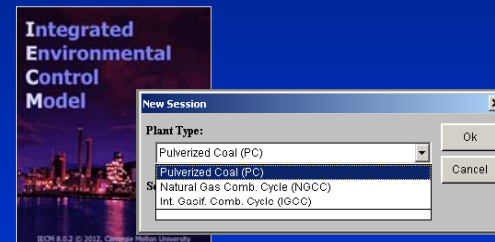
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Stochastic Simulation



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Graphical User Interface



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Configure Plant Screens

The image displays two screenshots of the 'Configure Plant' software interface, which is used for configuring industrial processes like IGCC (Integrated Process for Gasification and Chemicals).

Left Screenshot: 'Configure Plant' - IGCC Base Configuration

- Configuration:** Base Unit - Simul
- Configuration Options:**
 - Gas Cleanup: Catalytic Oxidation
 - CO2 Control: Pre-combustion
- Combustion Controls:**
 - NOx Control: None
- Sulfide Management:**
 - Nag: Lanth
 - Sulfur: Sulfur Recovery

The process flow diagram shows Air entering a compressor, then a burner, followed by a series of heat exchangers and a CO2 separator.

Right Screenshot: 'Configure Plant' - Pre-combustion Configuration

- Configuration:** Pre-combustion
- Combustion Controls:**
 - Fuel Type: Coal
 - NOx Control: None
- Post-Combustion Controls:**
 - NOx Control: Hot Side SCR
 - Particulate: Cold Side ESP
 - H2S FGD: None
 - Mercury: None
 - CO2 Capture: Amine Systems
- Water and Waste Management:**
 - Cooling Water: Hot Cooling Tower
 - Wastewater: No Wastewater System
 - Flyash Disposal: Mixed w/ Bottom Ash

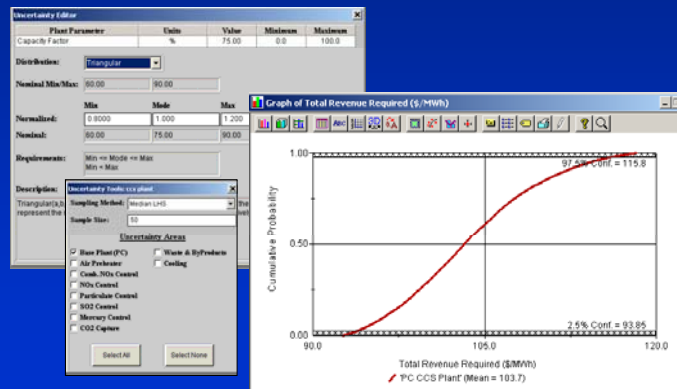
The process flow diagram shows Air entering a compressor, then a burner, followed by a series of heat exchangers and a CO2 separator, with additional components for SO2, H2S, and Flyash disposal.

Set Parameters Screens: Plant Components

Get Results Screens: Overall Plant

Get Results Screens: Components

Probabilistic Results: *Uncertainty in COE*



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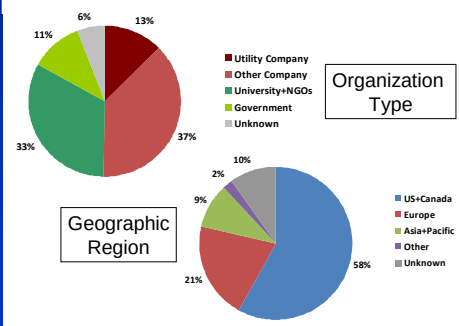
Some Questions of Interest

- What technologies are available to control emissions from a given power plant system? What levels of pollution reduction are possible?
- What are the associated impacts and uncertainties on:
 - resource requirements
 - efficiency
 - cost?
- How *likely* is it that a given advanced technology can:
 - Achieve lower cost and/or better performance than current systems?
 - Meet DOE goals for “high risk, high payoff” technology?

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IECM Users and Uses

n >2200 Users >800 Organizations > 50 Countries



IECM IS USED FOR:

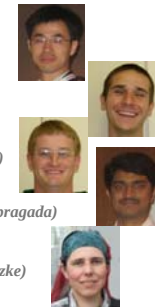
- Process design
- Technology evaluation
- Cost estimation
- R&D management
- Risk analysis
- Environmental compliance
- Marketing studies
- Strategic planning
- Teaching/Education

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The IECM Project Team

Performance and Cost Models of Advanced CO₂ Capture Systems

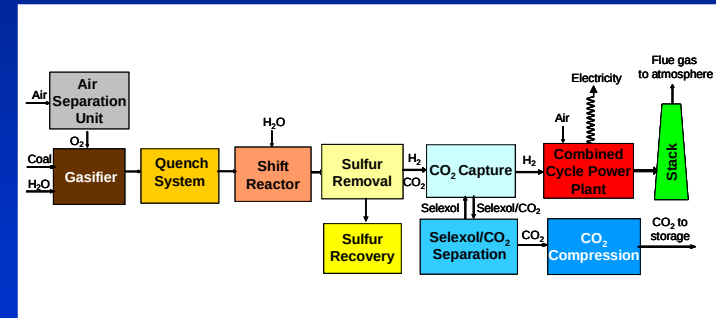
- Membrane capture systems (Haibo Zhai)
- Solid sorbent systems (Justin Glier)
- Advanced oxy-combustion (Kyle Borgert)
- Chemical looping combustion (Hari Mantripragada)
- Software Development & Dist. (Karen Kietzke)



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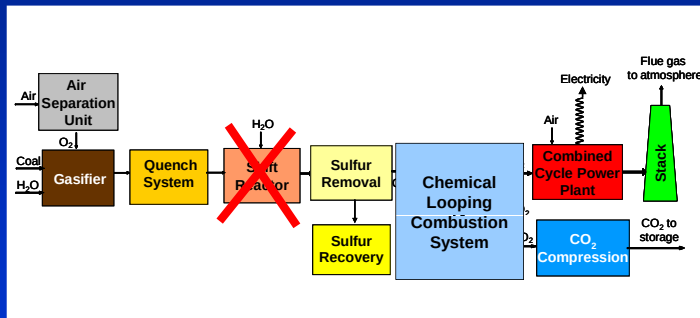
*Recent and planned activities:
Pre-combustion capture*

Current IGCC Power Plant with Pre-Combustion CO₂ Capture



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Chemical Looping Combustion System for CO₂ Capture

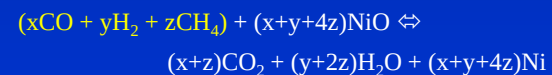


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CLC System Reactions

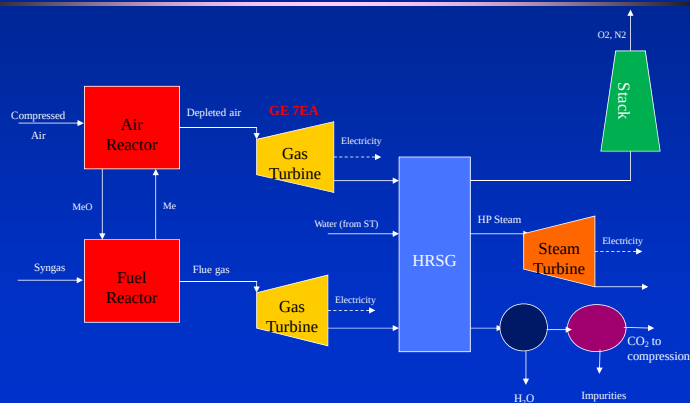
- $\text{CH}_4 + 4\text{NiO} \rightleftharpoons \text{CO}_2 + 2\text{H}_2\text{O} + 4\text{Ni} \quad (\Delta H = 134 \text{ kJ/mol})$
- $\text{CH}_4 + 3\text{NiO} \rightleftharpoons \text{CO} + 2\text{H}_2\text{O} + 3\text{Ni}$
- $\text{CO} + \text{NiO} \rightleftharpoons \text{CO}_2 + \text{Ni} \quad (\Delta H = -43.3 \text{ kJ/mol})$
- $\text{H}_2 + \text{NiO} \rightleftharpoons \text{H}_2\text{O} + \text{Ni} \quad (\Delta H = -2.1 \text{ kJ/mol})$
- $\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + \text{H}_2$

Overall Reaction:



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Schematic of CLC Combined Cycle Power Plant



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CLC Model in IECM (v 8.0.2)

Configure Plant		Set Parameters		Get Results																																																																																																																																																									
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18 CLC Power Requirement	% MWg		9.731	☒	0.0	100.0	calc																																																																																																																																																						

| Process Type: 1. Chemical Looping | | | | | |

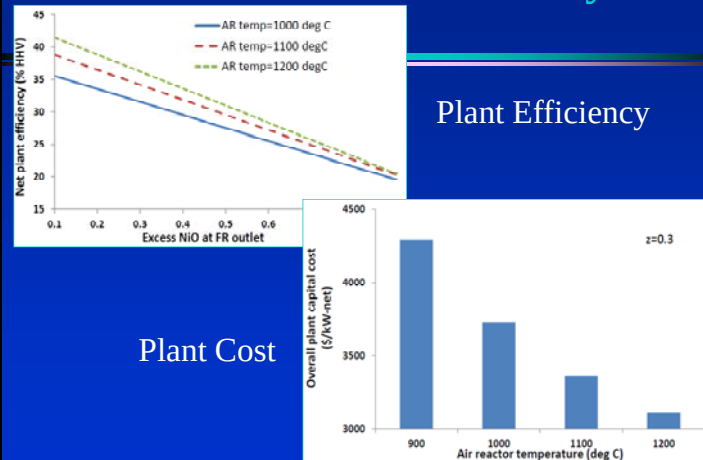
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CLC Model in IECM (v 8.0.2)

Configure Plant		Set Parameters		Get Results																																					
Overall Plant	Fuel	Air Separation	Gasifier Area	Sulfur Removal	CO2 Capture																																				
<table border="1"> <tr> <td>Air Out (tonne/hr)</td> <td>2153</td> <td>Flue Gas Out (tonne/hr)</td> <td>329.5</td> </tr> <tr> <td>Air Temp. Out (deg. C)</td> <td>1100</td> <td>Gas Temp. Out (deg. C)</td> <td>1045</td> </tr> <tr> <td colspan="4">Oxygen Carrier (OC)</td> </tr> <tr> <td>Oxidized OC (tonne/hr)</td> <td>2106</td> <td>OC Temp. (deg. C)</td> <td>1100</td> </tr> <tr> <td>OC Makeup (kg/hr)</td> <td>18.38</td> <td>OC Makeup (kg/hr)</td> <td>18.38</td> </tr> <tr> <td>Reduced OC (tonne/hr)</td> <td>1979</td> <td>OC Temp. (deg. C)</td> <td>1045</td> </tr> <tr> <td>OC Degradation (kg/hr)</td> <td>18.38</td> <td>OC Degradation (kg/hr)</td> <td>18.38</td> </tr> <tr> <td>Air In (tonne/hr)</td> <td>2279</td> <td>Syngas In (tonne/hr)</td> <td>204.3</td> </tr> <tr> <td>Air Temp. In (deg. C)</td> <td>379.2</td> <td>Syngas Temp. In (deg. C)</td> <td>29.44</td> </tr> </table>						Air Out (tonne/hr)	2153	Flue Gas Out (tonne/hr)	329.5	Air Temp. Out (deg. C)	1100	Gas Temp. Out (deg. C)	1045	Oxygen Carrier (OC)				Oxidized OC (tonne/hr)	2106	OC Temp. (deg. C)	1100	OC Makeup (kg/hr)	18.38	OC Makeup (kg/hr)	18.38	Reduced OC (tonne/hr)	1979	OC Temp. (deg. C)	1045	OC Degradation (kg/hr)	18.38	OC Degradation (kg/hr)	18.38	Air In (tonne/hr)	2279	Syngas In (tonne/hr)	204.3	Air Temp. In (deg. C)	379.2	Syngas Temp. In (deg. C)	29.44
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Illustrative Results for CLC System



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IECM Work Plan for FY2014

- New pre-combustion system and capture technologies
 - Chemical looping systems using low-cost metal oxygen carriers
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- Develop and test a new IECM release (v9.0) with the added technologies and capabilities above

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New Pre-Combustion Tasks (1)

- Building on the current CLC model we will:
 - Model two new low-cost oxygen carriers, copper and iron
 - Develop performance models for air and fuel reactors
 - Develop new performance model for GE 7EA gas turbine
 - Develop performance model for CO_2 purification system
 - Develop cost models for all the above
 - Implement and test in the IECM
 - Prepare technical documentation for all the above

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New Pre-Combustion Tasks (2)

- Implement model of a GE-Radiant gasification system (based on NETL Baseline studies)
 - Develop performance model for gasifier
 - Modified IGCC power block model
 - Develop cost models for the above
 - Implement and test in the IECM
 - Prepare technical documentation for all the above

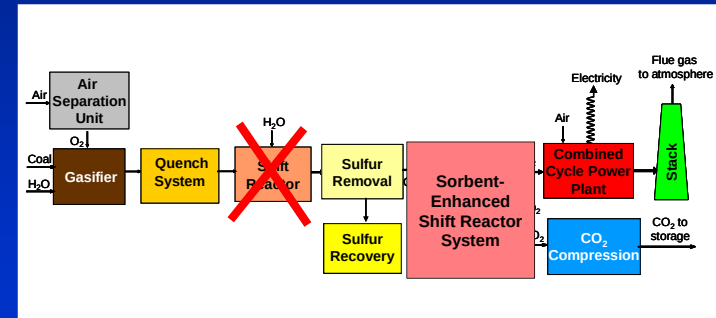
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New Pre-Combustion Tasks (3)

- Develop and implement new model of a sorbent-enhanced WGS reactor system:
 - Performance models
 - Cost models
 - Implement and test in the IECM
 - Prepare technical documentation

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Sorbent Enhanced Shift Reactor System for CO₂ Capture



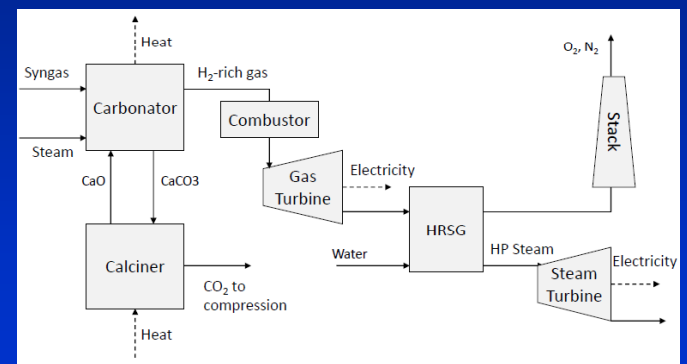
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Performance Characteristics for Sorbent-Enhanced WGS

- Chemical Reactions
 - Shift reaction: $\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$
 - Carbonation: $\text{CaO} + \text{CO}_2 \rightarrow \text{CaCO}_3$
 - Overall reaction: $\text{CaO} + \text{CO} + \text{H}_2\text{O} \rightarrow \text{CaCO}_3 + \text{H}_2$
 - Calcination: $\text{CaCO}_3 \rightarrow \text{CaO} + \text{CO}_2$ (to storage)
- Carbonator temperature: 650°C
- Calciner temperature: 950°C
- Variable H₂O/CO ratio

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Schematic of Sorbent-Enhanced Shift Reactor System



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Recent and planned work:

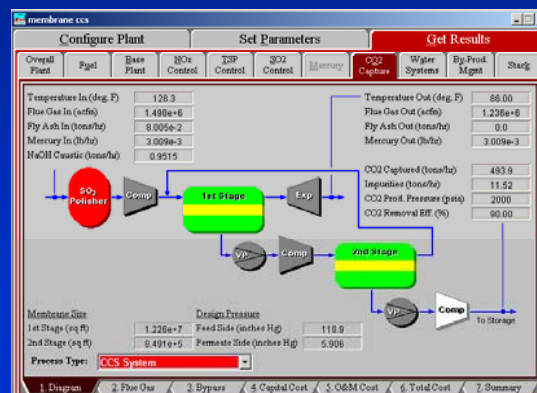
Post-combustion capture

IECM Work Plan for FY2014

- New pre-combustion system and capture technologies
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2-Stage Membrane System Model in IECM (v. 8.0.2)



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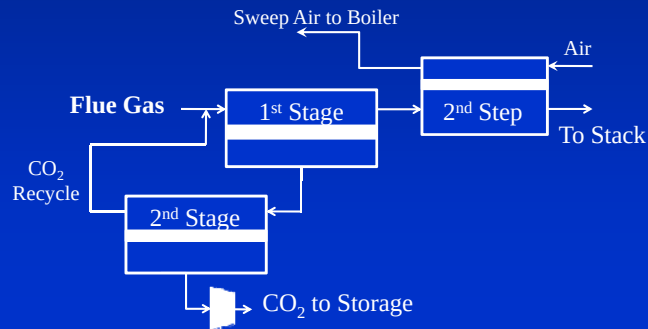
Performance Parameters for the Membrane Capture System Model

Configure Plant			Set Parameters			Get Results		
Overall Plant	Fuel	Base Plant	NOx Control	CO ₂ Control	CO ₂ Capture	Water Systems	By-Prod. Mgmt	
Performance Parameters								
Title	Units	Use	Value	Calc	Min	Max	Default	
1 Membrane Operating Temp	deg F		86.00		50.00	150.0	86.00	
2 Ideal CO ₂ Permeance (G.T.F.)	gms	Y	1000		500.0	5000	1000	
3 Ideal CO ₂ /N ₂ Selectivity (G.T.F.)	ratio		50.00		40.00	75.00	50.00	
4 Percent of Ideal CO ₂ Permeance	%		100.0		1.000	100.0	100.0	
5 Percent of Ideal CO ₂ /N ₂ Selectivity	%		100.0		1.000	100.0	100.0	
6								
7 Permeate-side Pressure	inches Hg		5.906		2.953	29.53	5.906	
8 Pressure Ratio at Stage 1 and 2	ratio		20.13		0.0	200.0	calc	
9 Feed-Side Pressure	inches Hg		118.9		39.53	147.7	calc	
10 Stage Out at 1st Stage	barrels		9.2967		0.0	1.000	calc	
11 Stage Out at 2nd Stage	barrels		8.4979		0.0	1.000	calc	
12								
13								
14								
15 Feed-side Compressor Efficiency	%		85.00		50.00	100.0	85.00	
16 Vacuum Pump Efficiency	%		85.00		50.00	100.0	85.00	
17 Expander Efficiency	%		85.00		50.00	100.0	85.00	
18 Capture System Cooling Duty	MBtu CO ₂		39.84		0.0	200.0	calc	
Process Type: CCS System								
1 Config / 2 Performance / 3 Capture / 4 T&E Config / 5 Revenue Cost / 6 Capital Cost / 7 O&M Cost								

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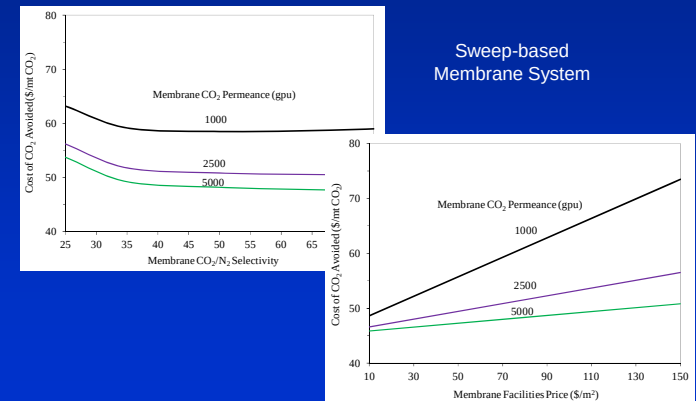
Sweep-based 2-Stage, 2-Step Membrane System Model

(Model developed but not yet implemented in IECM)



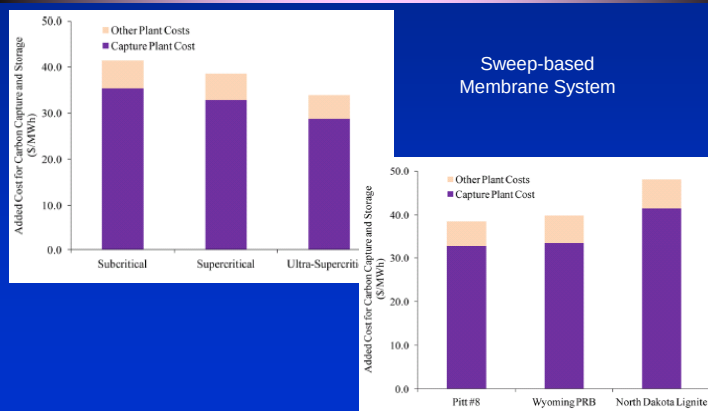
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Effects of Membrane Properties and Price on Cost of CO₂ Avoided



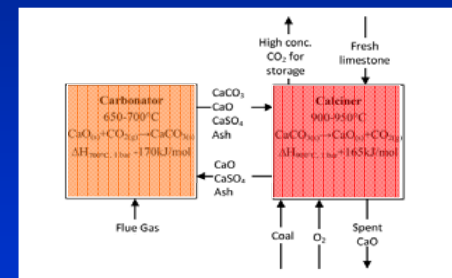
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Effects of Power Plant and Coal Type on Membrane System Cost



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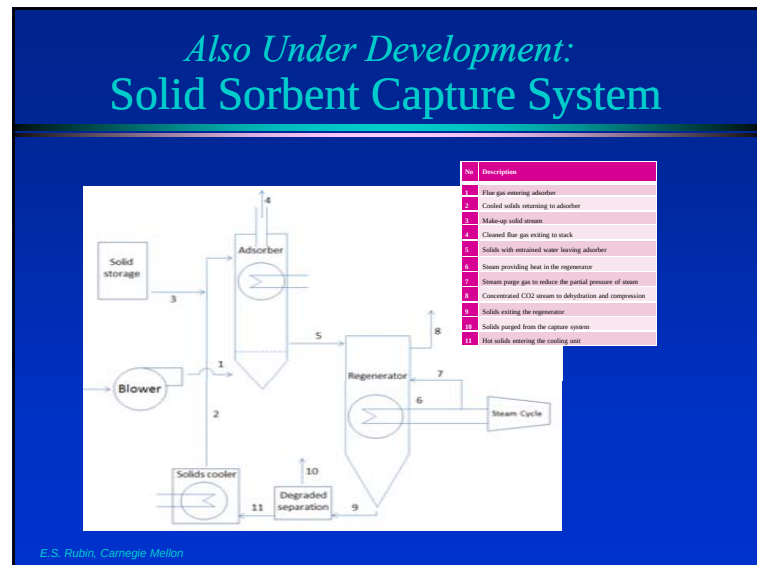
Under Development: Post-Combustion Chemical Looping



Source: Dean, et al., 2011

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New Calcium-based Chemical Looping Module (in IECM v9.0 dev)



Recent and planned work:

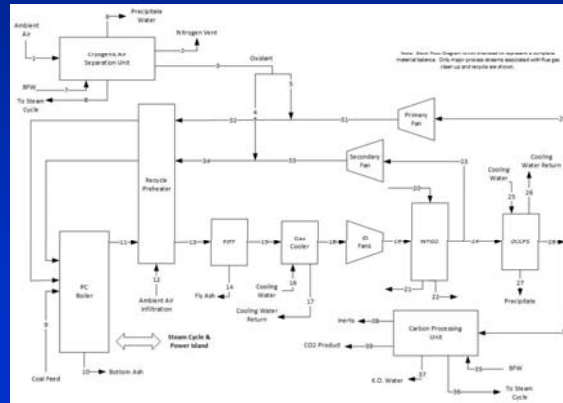
Oxy-combustion capture

IECM Work Plan for FY2014

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PC Oxyfuel Combustion Model



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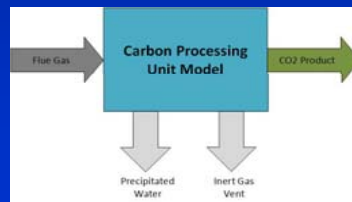
Air Separation Unit

- Updated performance and cost models:
 - Are functions of oxidant flow rate, purity, and delivery pressure
 - Include cooling water consumption for main air compressor
 - Include main air compressor water generation from ambient humidity removal prior to cold box

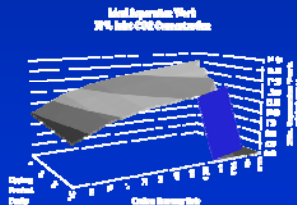
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Carbon Processing Unit

- New generalized model to handle a wide variety of inlet flue gas compositions
- Second law calculations used to determine the minimum separation energy as performance baseline



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Recent and planned work:

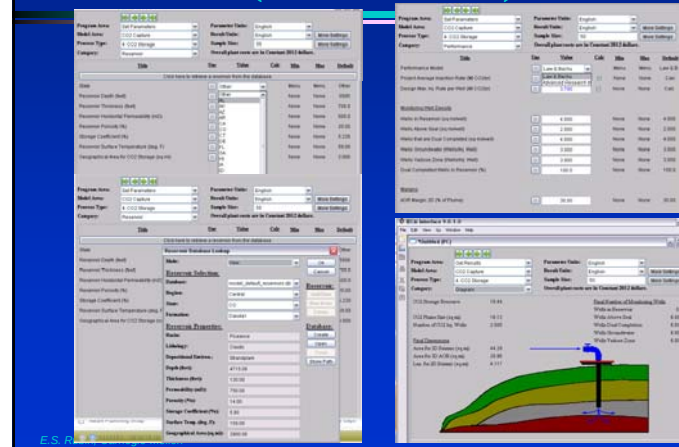
Other activities

IECM Work Plan for FY2014

- New pre-combustion system and capture technologies
 - The GE-radiant gasification system
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 - Sorbent-enhanced water gas shift reactor system
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 - Air-sweep membrane system
 - Calcium looping system
 - Solid sorbent system
 - Ionic liquid-based system
- New oxy-combustion system and capture technologies
 - ASU, DCC, CPU and other new or enhanced components
- Develop and test a new IECM release (v9.0) with the added technologies above plus other new capabilities

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New CO₂ Storage Cost Module (IECM v.9.0 dev)



2013 IECM-Related Publications

- Borgert, K.J., & Rubin, E. S. (2013). Oxyfuel combustion: technical and economic considerations for the development of carbon capture from pulverized coal power plants. *Energy Procedia*, 37:1291–1300.
- Glier, J.C. & Rubin, E. S. (2013). Assessment of solid sorbents as a competitive post-combustion CO₂ capture technology. *Energy Procedia*, 37:65–72.
- Mantripragada, H.C. & Rubin, E. S. (2013). Chemical Looping for Pre-combustion CO₂ Capture - Performance and Cost Analysis. *Energy Procedia*, 37:618–625.
- Versteeg, P., Oates, D.L., Hittinger, E. & Rubin, E.S. (2013). Cycling coal and natural gas-fired power plants with CCS. *Energy Procedia*, 37:618–625.
- Versteeg, P., Zhai, H. and Rubin, E.S., Comparative Assessments of Advanced Amine and Ammonia Systems for Post-combustion CO₂ Capture. *2013 Carbon Capture Utilization & Sequestration*, May, 2013, Pittsburgh, PA.
- Zhai, H., & Rubin, E. S. (2013). The Effects of Membrane-based CO₂ Capture System on Pulverized Coal Power Plant Performance and Cost. *Energy Procedia*, 37:1117–1124.
- Zhai, H., & Rubin, E. S. (2013). Techno-Economic Assessment of Polymer Membrane Systems for Postcombustion Carbon Capture at Coal-Fired Power Plants. *Environmental Science & Technology*, 47(6), 3006-3014.
- Zhai, H., & Rubin, E. S. (2013). Comparative Performance and Cost Assessments of Coal- and Natural-Gas-Fired Power Plants under a CO₂ Emission Performance Standard Regulation. *Energy & Fuels*, 27(8):4290-4301.

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Thank You

rubin@cmu.edu