Center for Advanced Process Decision-making

Energy Systems Initiative Kickoff Meeting

March 7, 2010
Department of Chemical Engineering
Carnegie Mellon University
Pittsburgh, PA 15213

http://capd.cheme.cmu.edu

Collaboration with NETL

2004 - Formation of RDS – Parsons, SAIC, CMU, Pitt, WVU

2007 - Establish Institute for Advanced Energy Solutions (IAES)

2009 - Rebid of Operating Contract – URS, CMU, Pitt, PSU, VPI&SU, WVU

IAES Research Thrusts

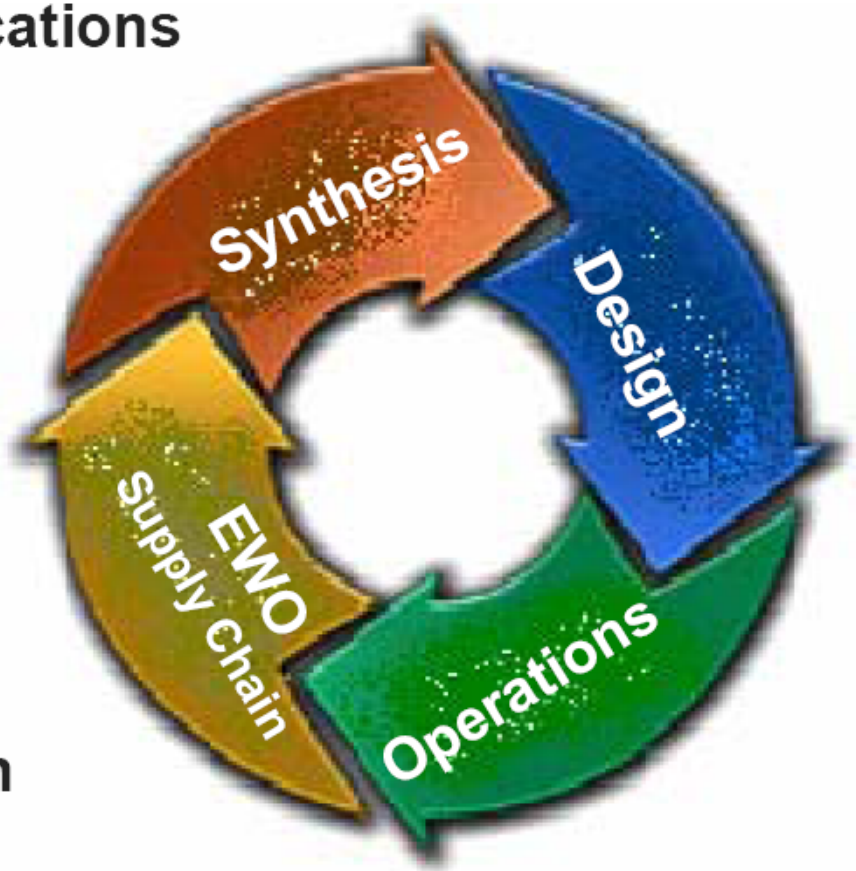
1 - Materials for Energy Technologies
2 - **Process and Dynamic Systems Modeling**
3 - Catalyst and Reactor Development
4 - Carbon Management
5 - Sensors Systems and Diagnostics
6 - Energy Conversion Devices
7 – Gas Hydrates

24 Resident Institute Fellows, ~80 students & postdocs.

Topics in IAES/NETL Thrust 2

Optimization of Fossil Energy Systems

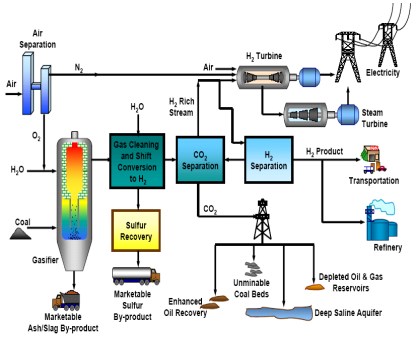
- **FE Systems Engineering Applications across the Plant Lifecycle**
  - **Process Synthesis**
  - **Process Design**
    - Steady-State
    - High-Fidelity
    - Stochastic
  - **Process Operations**
    - Dynamics
    - Control
  - **Enterprise-Wide Optimization**
    - Planning/Scheduling
    - Supply Chain



Fossil Energy Plant Lifecycle

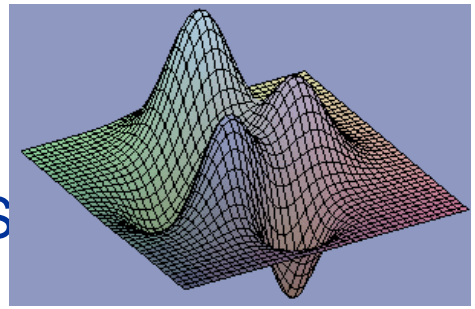
Collaboratory for Process & Dynamic Systems Research

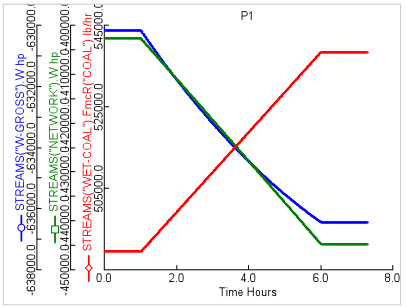
Goals and Objectives



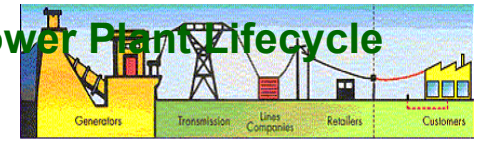
Accelerate R&D on advanced models, methods, and tools for process systems engineering

Apply to existing and emerging fossil energy systems, such as gasification-based plants with carbon capture & storage (CCS





Address technical barriers across power plant lifecycle– process innovation, design, operations, and management



Synergies with Other IAES Thrust Areas

Thrust 4: Carbon Management

- Develop aggregate CO_2 capture models for use in optimal synthesis of fossil energy power plants
- Develop rate-based separation models for the design of CO_2 capture processes
- Extend APECS technology to include CO_2 pipeline/ transport, and storage simulations
- Make use of IECM cost models for CO_2 compression, transport, and storage in APECS
- Develop and apply dynamic simulations to evaluate the performance, economics, and environmental impacts of advanced fossil energy systems with CCS under uncertain conditions

Synergies with Other IAES Thrust Areas

Thrust 3: Catalyst and Reactor Development

- Development and validation of high-fidelity reactor models for use in APECS co-simulations
- Modeling and simulation of fuel and air reactors for chemical looping processes

Thrust 6: Energy Conversion Devices

- Development of high-fidelity, CFD device/equipment models for use in APECS co-simulations of advanced energy systems
  - Gasifiers, Combustors
  - Syngas coolers, HRSGs
  - Turbines, Fuel cells

ESI Kickoff Meeting Agenda

Sunday, March 7

CAPD CONFERENCE ROOM, Doherty Hall 4201

Noon	**(Lunch) Overview and Introduction**	Larry Biegler
12:15	*Computer-Aided Process Decision-making R&D for Advanced Energy Systems*	Steve Zitney (NETL)
12:30	*Energy Process Synthesis and Integration*	Ignacio Grossmann
12:35	*Synthesis of Integrated IGCC Systems*	Ravi Kamath
12:50	*Water and Energy Optimization of Biofuel*	Mariano Martin
1:05	*Reduced Order Modeling for CFD Units*	Larry Biegler (Yi-dong Lang)
1:20	*PSA Opt. for CO2 Capture from Flue Gas*	Anshul Agarwal
1:35	*PSA Synthesis for H2/CO2 Separation*	Sreeram Vetukuri
1:50	*Dynamic Optimization for Air Separation Units*	Rui Huang

ESI Kickoff Meeting Agenda (cont'd)

2:05	**Break**	
2:25	*Advanced Optimization for Energy Processes*	Nick Sahinidis
2:30	*Design of High Performance Drilling Fluids*	Apurva Samudra
2:45	*Risk assessment for CO2 sequestration*	Yan Zhang
3:00	*Advances in Solar Processes*	Erik Ydstie
3:15	*NETL Modular Framework*	David Miller (NETL)
3:30	*Energy Systems Research at ExxonMobil*	Greg Martin (ExxonMobil)
3:45	*Reducing Carbon Footprint of Processes*	Jeff Siirola (Eastman)
4:00	*Energy Systems Research at ECOPETROL*	Ariel Uribe (Ecopetrol)
4:15	*Open Discussion and Next Steps*	

Institute for Complex Engineered Systems

ENGINEERING PITA Project

Special industrial interest group:
"Enterprise-wide Optimization for Process Industries"

Multidisciplinary team:

Chemical engineers, Operations Research, Industrial Engineering

Researchers:

Carnegie Mellon:	**Ignacio Grossmann (ChE)**
	Larry Biegler (ChE)
	Nicola Secomandi (OR)
Lehigh University:	**Larry Snyder (Ind. Eng)**
Univ. Pittsburgh:	**Andrew Schaeffer (Ind. Eng.)**

Carnegie Mellon

LEHIGH UNIVERSITY

University of Pittsburgh

Overall Goal:

- *Novel planning and scheduling models, including consideration of uncertainty*
- *Effective integration of Production Planning, Scheduling and Real–time Optimization*
- *Optimization of Entire Supply Chains*

ABB, Air Products, bp, Dow, ExxonMobil, ecopetrol, NOVA Chemicals, Praxair, Total, Unilever

Special industrial interest group:
"Enterprise-wide Optimization for Process Industries"

Case studies with partner companies

ABB: Batch Scheduling with Electric Power Constraints
Contact: Iiro Harjunkoski — Ignacio Grossmann, Pedro Castro

Air Products: Design of Resilient Supply Chain Networks for Chemicals and Gases
Contact: James Hutton — Larry Snyder, Peng Peng

BP: Refinery Planning with Process Models
Contact: Ignasi Palou-Rivera — Ignacio Grossmann, Abdul Alattas

Dow: Design of Reliable Integrated Sites
Contact: John Wassick — Ignacio Grossmann, Sebastian Terrazas

ExxonMobil: Global optimization of Bilinear GDP Models
Contact: Kevin Furman/Nick Sawaya — Ignacio Grossmann, Juan Ruiz

NOVA Chemicals: Polymerization optimization
Contact: Hany Farag — Larry Biegler, Weijie Lin

PPG: Planning and Scheduling for Glass Production
Contact: Jiao Yu — Ignacio Grossmann, Ricardo Lima

Praxair: Merchant Liquid Supply Chain Design and Management
Contact: Jose Pinto — Ignacio Grossmann, Fengqi You

TOTAL: Scheduling of crude oil operations
Contact: Pierre Pestiaux — Ignacio Grossmann, Sylvain Mouret

Industrial funding:
(@$12,500/yr for CAPD Members or major project)

Discussion Points
Research Topics

Advanced Fossil Fuel Power Plants

- process synthesis and design
- modeling and simulation
- operation and control

Biofuels

Alternative Fuels and Power Sources

Expand industrial involvement and application areas

Discussion Points
Mechanism for Project Support

- Unrestricted grants from industry
  - full application of NDAs and confidentiality of sensitive data
  - requires publication of research results
  - flexible for short-term projects
  - minimal bureaucracy, no overhead costs
- Strong leveraging for CAPD members from federal/state sources (~$2M/yr from NSF, DOE, PITA…)
- Applications, interactions and involvement from industry
- Suggest to Emulate EWO Model

Resources

NETL and associated DOE and academic partners

CAPD/largest concentration of PSE research in US

Recent Developments

Establishment of Energy Systems Initiative (ESI)

Motivation:

-Need for development of energy-efficient and sustainable processes

-Activities in CAPD group *(NETL, NSF funding):*

refinery operations, deep-water oilfield development

IGCC, CO_2 sequestration, water management

biofuels, fuel cells, solar cells

Leader: Larry Biegler

ESI modeled after successful EWO

Companies join by supplying case studies

Kick-off meeting: March 7

Industrial funding:

(@$12,500/yr for CAPD Members or major project)

Enterprise-wide Optimization (EWO)

EWO involves optimizing the operations of R&D, material supply, manufacturing, distribution and financial activities of a company to reduce costs and inventories, and to maximize profits, asset utilization, responsiveness and customer satisfaction.

Major operational items include planning, scheduling, real-time optimization and inventory control.

Key features:
- Integration of the information, modeling and solution methods
- Integrate strategic, tactical and operational decision-making