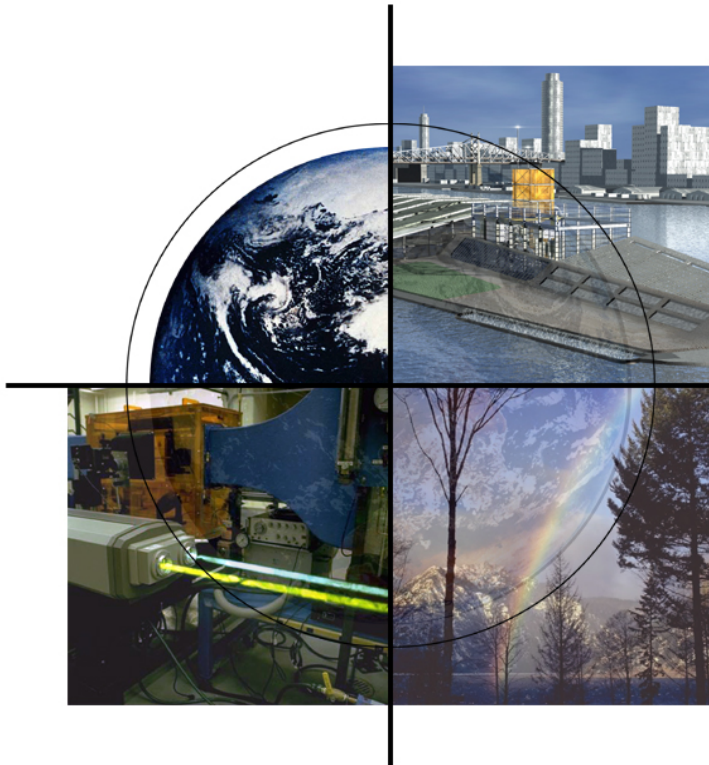# Process Systems Engineering R&D for Advanced Fossil Energy Systems

Stephen E. Zitney

Director, Collaboratory for Process & Dynamic Systems Research

stephen.zitney@netl.doe.gov

MIT Energy Initiative

Massachusetts Institute of Technology
Cambridge, MA
September 11, 2007

National Energy Technology Laboratory
Morgantown, WV
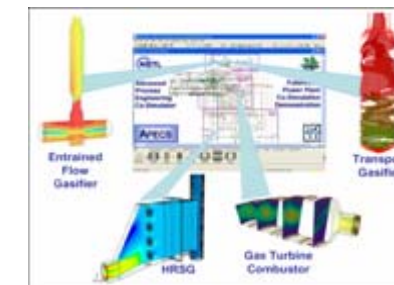
Outline of Presentation

- **Introduction**

- **US Fossil Energy Outlook**

- **NETL's Fossil Energy Mission**
  - Energy Policy Support
    - Clean Coal Power Initiative
    - *FutureGen*
  - Extramural RD&D
  - Onsite Research and Analysis

- **Process Systems Engineering**
  - Industry R&D Challenges
  - NETL R&D Activities

- **Concluding Remarks**

FutureGen **Plant**

NETL Onsite R&D

APECS Co-Simulation

National Energy Technology Laboratory

- **Only DOE national lab dedicated to fossil energy**
- **One lab, five locations, one management structure**
- **1,200 Federal and support-contractor employees**
- **NETL History**
  - 1910: Coal Research Center in Pittsburgh
  - 1954: Morgantown site with coal/syngas research
  - 1975: Energy Technology Centers (PETC, METC)
  - 1976-1981: ASPEN Project at MIT with DOE (METC)
  - 1996: Federal Energy Technology Center (PETC/METC)
  - 1999: FETC becomes DOE national laboratory (NETL)

Pittsburgh, PA (1910)

Morgantown, WV (1954)

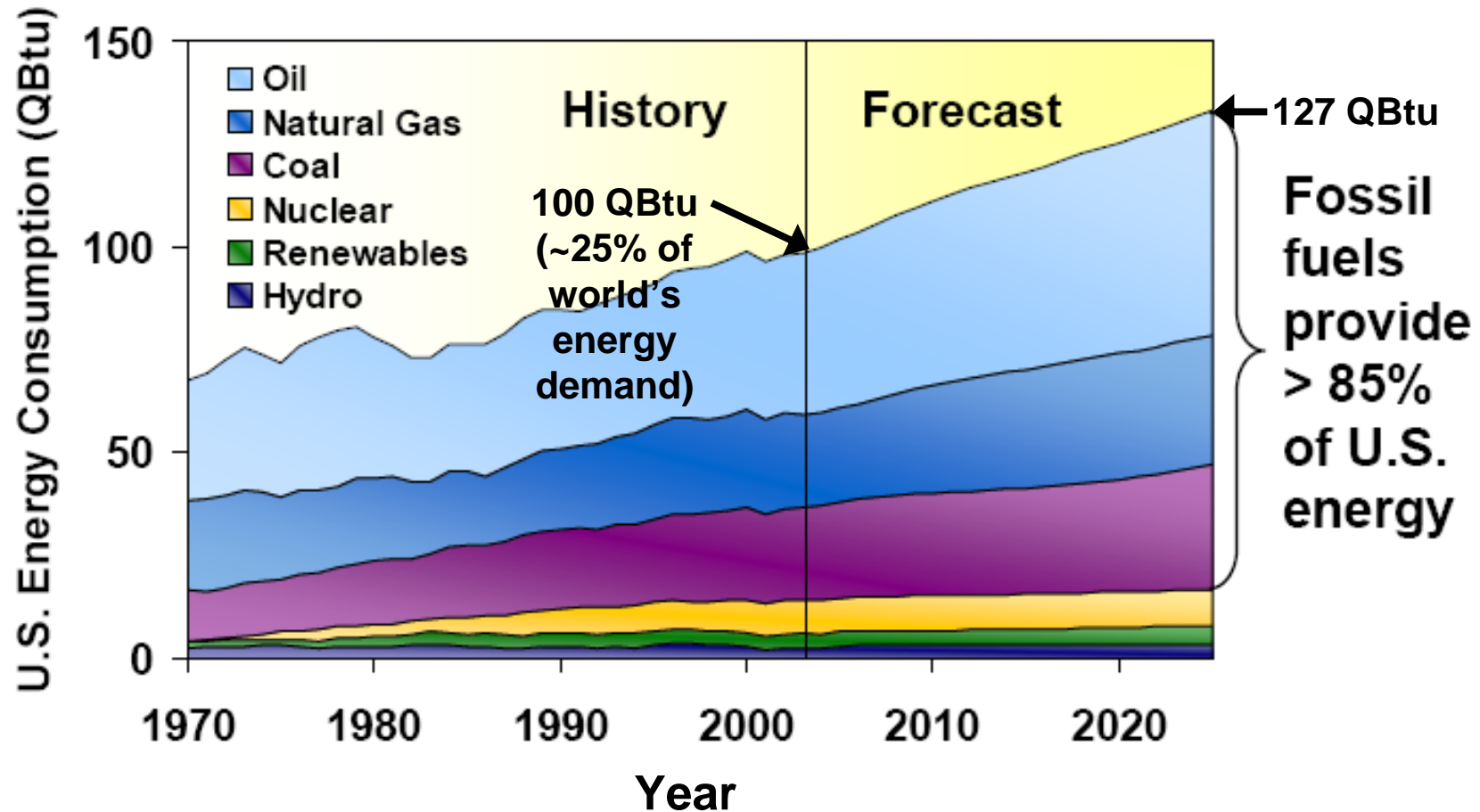**Tulsa, Oklahoma (2000)**

Fairbanks, Alaska (2001)

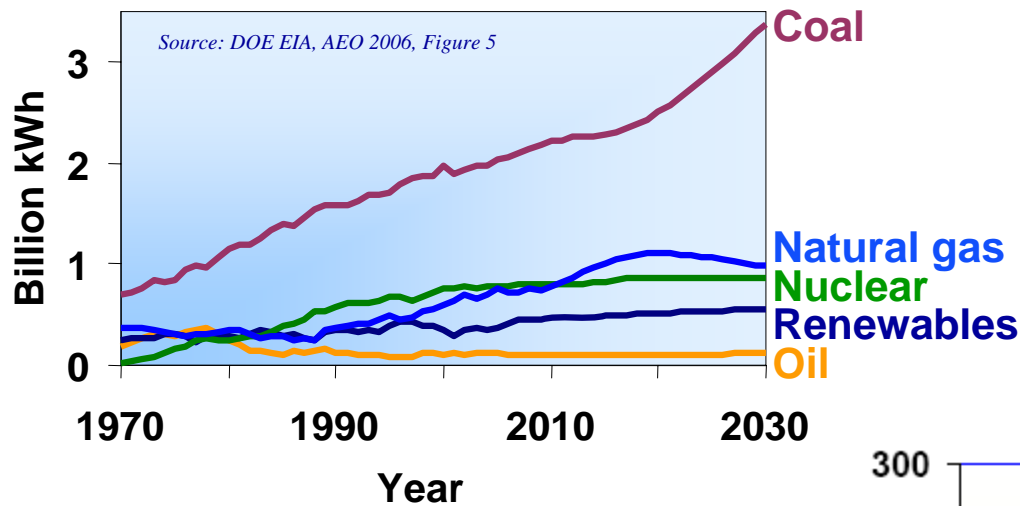**Albany, Oregon (2006)**

Growing U.S. Energy Demand
Fossil Fuels Dominate Energy Consumption

U.S. "Electricity Generation" Outlook by Fuel Type

Source: DOE EIA, AEO 2006, Figure 5

(Chart axes: Billion kWh vs. Year 1970–2030; curves labeled Coal, Natural gas, Nuclear, Renewables, Oil)

Coal dominates electricity generation

Over 50% of U.S. electricity from coal.

Over 250 year supply of coal at current demand levels!

U.S. Fossil Fuel Reserves / Production Ratio

Coal ($1-2 per MBtu)*
Oil ($6-12 per MBtu)*
Natural Gas

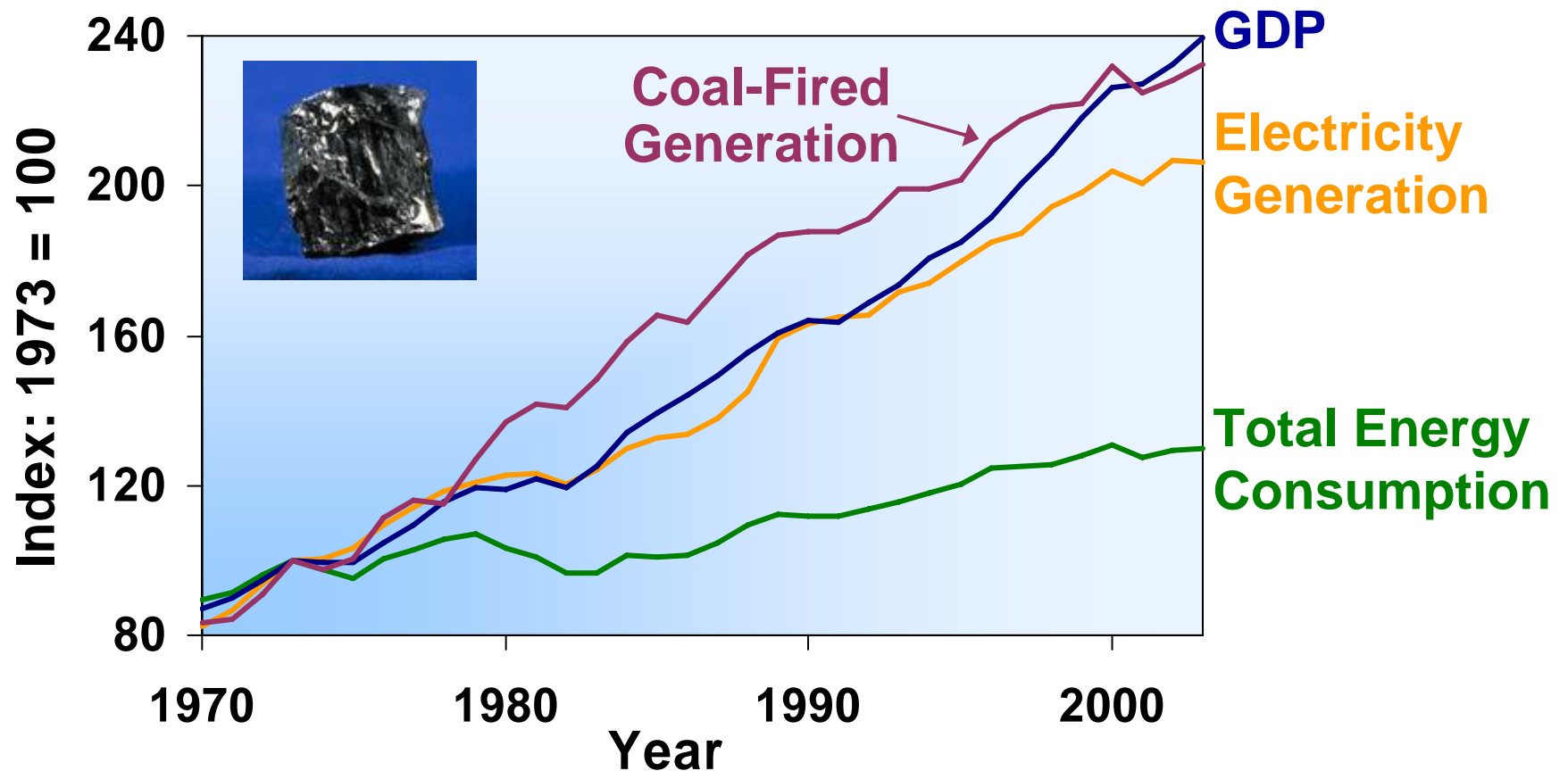258 Sub-Bituminous & Lignite / Anthracite & Bituminous
11.7
9.7
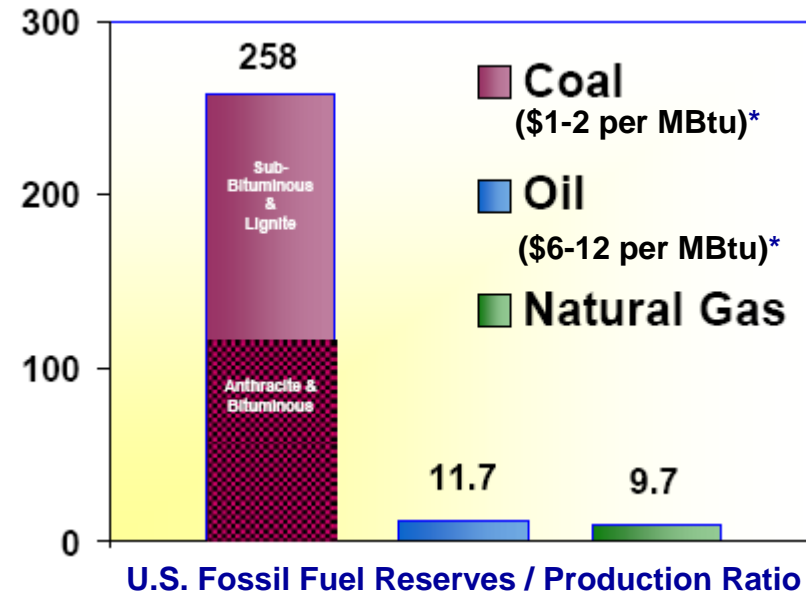
Sources: BP Statistical Review, June 2004, - for coal reserves data - World Energy Council; EIA, Advance Summary U.S. Crude Oil, Natural Gas, and Natural Gas Liquids Reserves, 2003 Annual Report, September 22, 2004 - for oil and gas reserves data

*Source – The Future of Coal, MIT, 2007

NETL

U.S. Coal Use Linked to Economic Growth

Index: 1973 = 100

- GDP
- Coal-Fired Generation
- Electricity Generation
- Total Energy Consumption

Year: 1970, 1980, 1990, 2000

Index values: 80, 120, 160, 200, 240

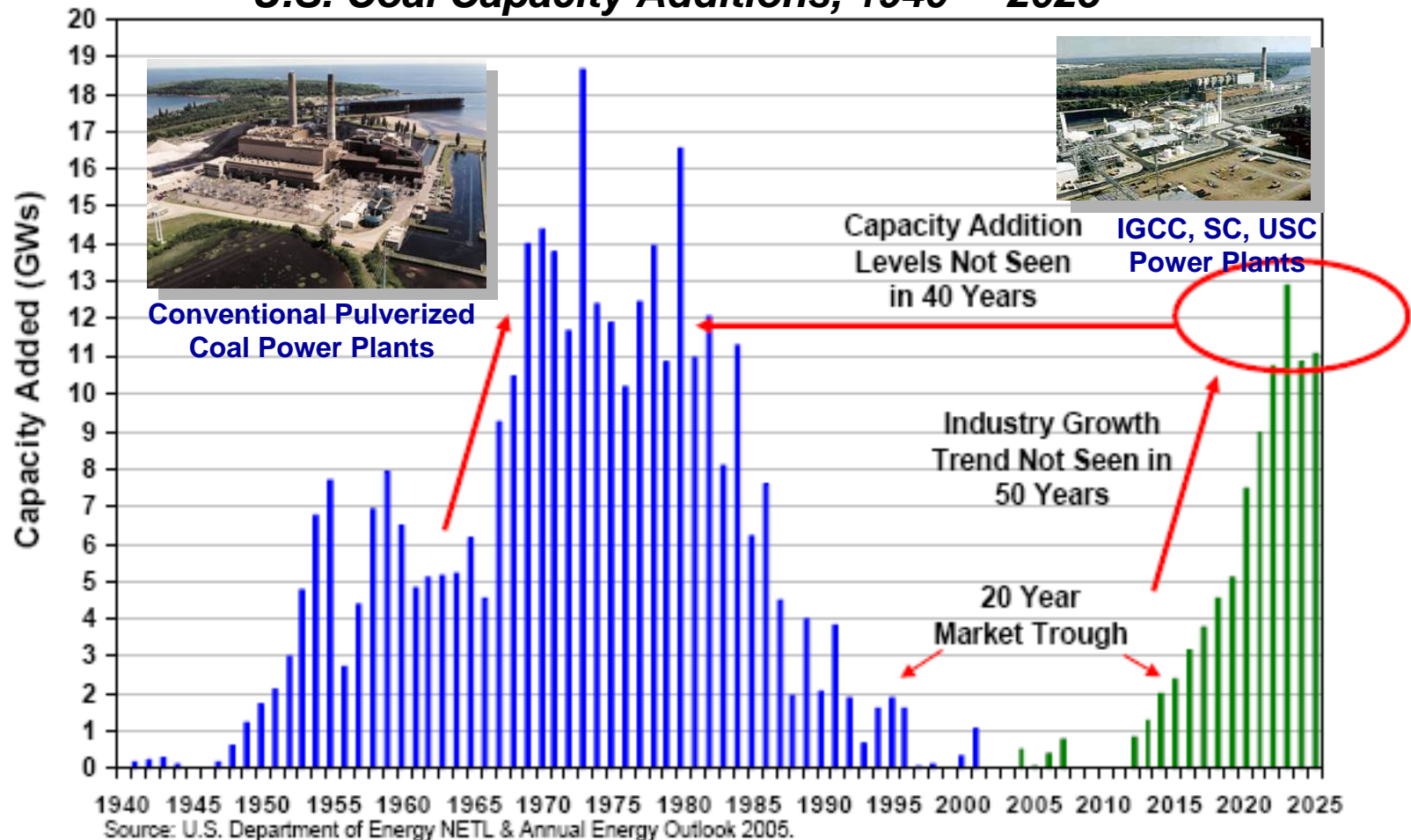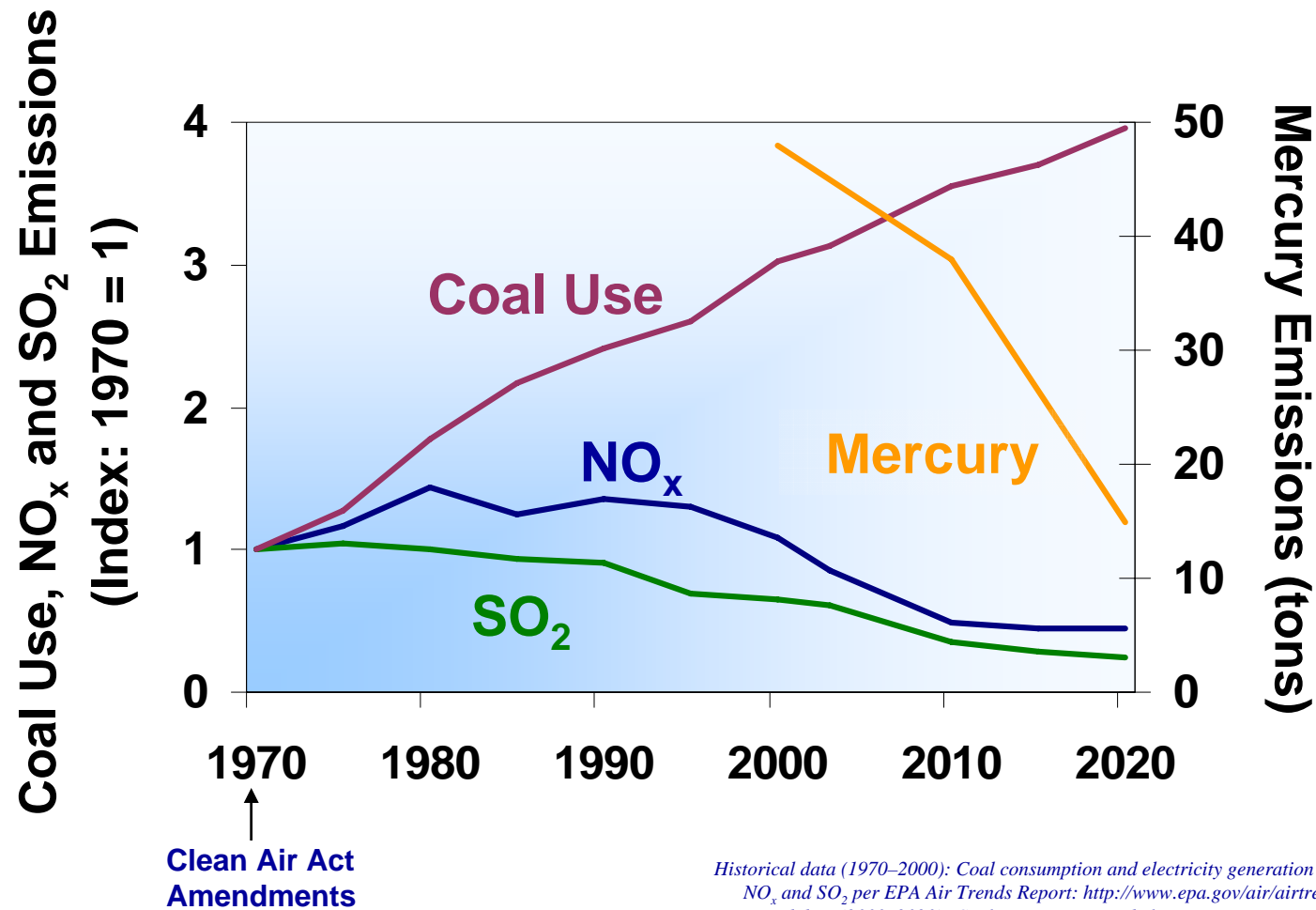*Coal-fired generation and GDP have grown at nearly the exact same pace over last 30 years*

NETL

U.S. Forecasts Largest Coal Generation Capacity Installation in 40 Years

U.S. Coal Capacity Additions, 1940 —2025

Conventional Pulverized Coal Power Plants

IGCC, SC, USC Power Plants

Capacity Addition Levels Not Seen in 40 Years

Industry Growth Trend Not Seen in 50 Years

20 Year Market Trough

Source: U.S. Department of Energy NETL & Annual Energy Outlook 2005.

Air Emission Trends and Projections
Annual U.S. Air Emissions and Coal Use

Coal Use

NO$_x$

Mercury

SO$_2$

Coal Use, NO$_x$ and SO$_2$ Emissions (Index: 1970 = 1)

Mercury Emissions (tons)

1970 1980 1990 2000 2010 2020

Clean Air Act Amendments

NETL

U.S. CO_2 Emissions from Fossil Power Generation
Forecast - Annual Energy Outlook 2006
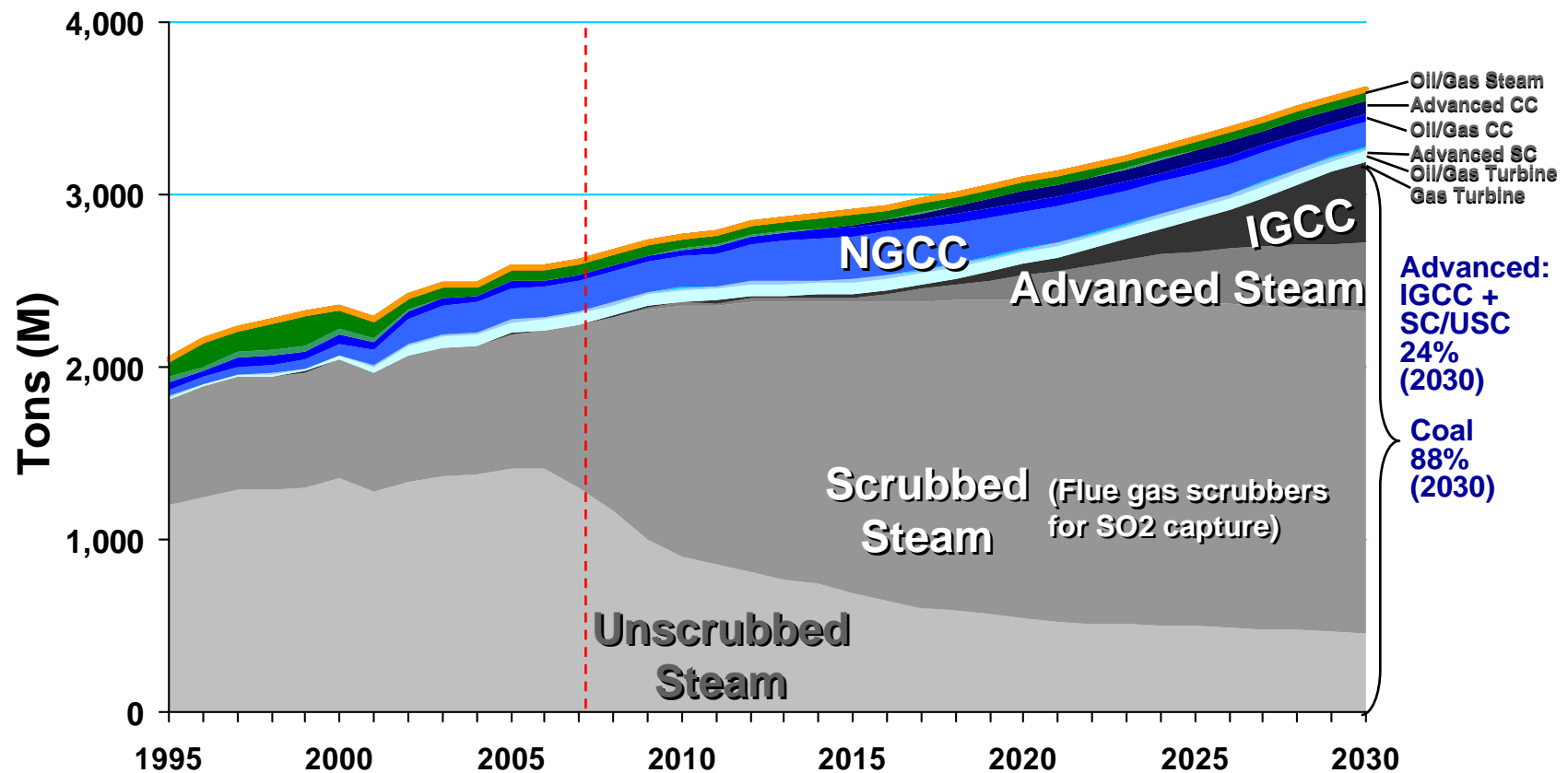
Need for CO_2 Capture and Storage (CCS) as Coal Dominates CO_2 Emissions from Fossil Power Generation

Fossil Energy Power Generation
Industry Challenges

- *Short-term:* **Manage existing fleet of combustion power plants**

  - Plant optimization and control

  - Improve efficiency

  - Reduce carbon intensity

- *Long-term:* **Design next generation of high-efficiency, zero-emission coal-fired power plants**

  - Oxy-fuel PC combustion plants

  - Integrated gasification combined cycles (IGCC)

  - Polygeneration systems

  - CO_2 capture and storage (CCS)

  - Chemical looping

Coal-Fired Power Plant

IGCC Power Plant
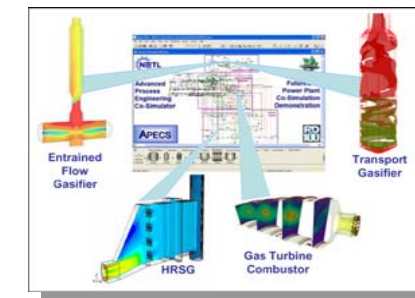
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FutureGen **Plant**

NETL Onsite R&D

APECS Co-Simulation

NETL Mission

Conduct R&D from fundamental science to technology demonstration for resolving the environmental, supply, and reliability constraints of producing and using fossil resources
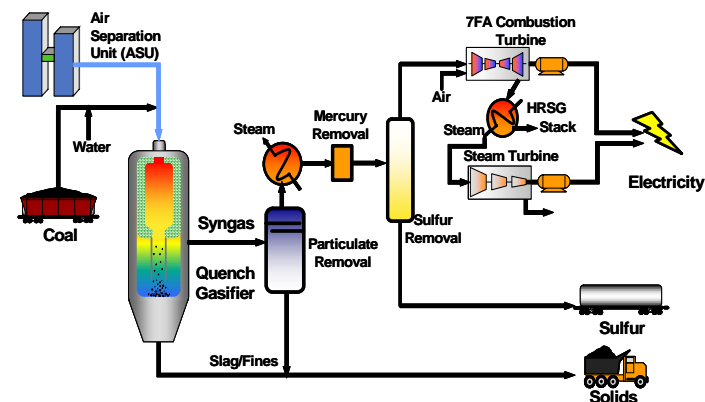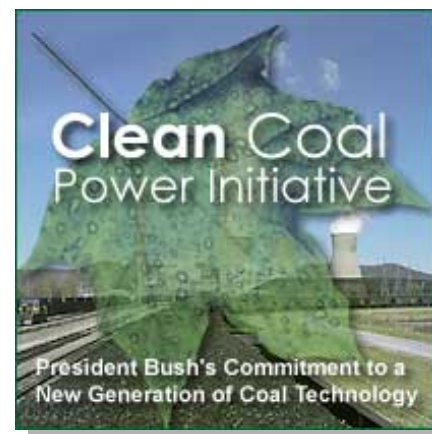
Accomplishing Our Mission

- **Support energy policy development**
  - Presidential Initiatives
    - Clear Skies
    - Climate Change
    - Hydrogen Fuels
    - Energy Security
  - Demonstration Programs
    - Clean Coal Power Initiative (CCPI)
    - *FutureGen* R&D Initiative

FUTURE GEN

Clean Coal Power Initiative

President Bush's Commitment to a New Generation of Coal Technology

NETL

Clean Coal Power Initiative (CCPI)

- **$2B, 10-year program to demonstrate a new generation of power plant technologies**

- **Government / industry partnership**

- **Industry cost share of at least 50%**

- **Anticipate four rounds of solicitations**

- **Round 1 (January 2003)**
  - Eight projects selected; two withdrawn
  - $315M DOE / $1B industry cost share

- **Round 2 (October 2004)**
  - Four projects, including two IGCCs:
    - Southern Co., Orlando, FL – 285MW with KBR transport gasifier
    - Excelsior Energy, MN – 531MW with CoP entrained-flow gasifier

- **Round 3 (May 2007)**
  - NETL published Notice of Intent to issue a funding opportunity announcement
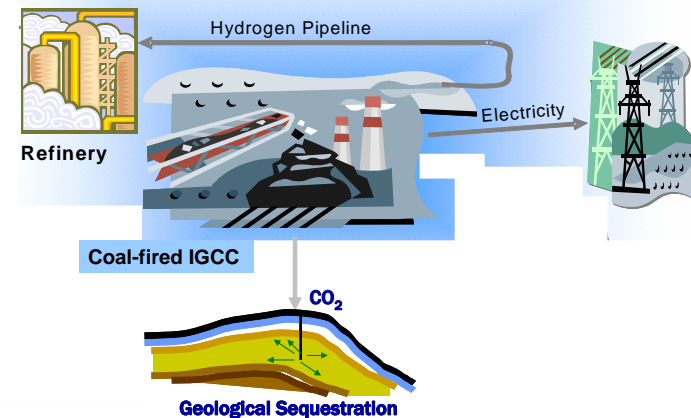

IGCC Process

U.S. DOE *FutureGen* Initiative
Pathway to Zero Emissions

- 10-year, $1B DOE project

- Commercial-scale, coal-fired, gasification-based plant

- Co-production of H_2 and electricity (275 MWe)

- Sequester >90% CO_2 with potential for ~100%

- Minimum 1-million tons/year CO_2 captured and stored

- "Living R&D laboratory" for cutting-edge technologies

- FutureGen Alliance

- On-line 2012

FutureGen™ ALLIANCE

Refinery
Hydrogen Pipeline
Electricity
Coal-fired IGCC
CO_2
Geological Sequestration

Accomplishing Our Mission

- **Support energy policy development**
  - Presidential Initiatives: Clear Skies, Climate Change, Hydrogen Fuels, Energy Security
  - Demonstration Programs: *FutureGen,* Clean Coal Power Initiative (CCPI)

- **Implement and manage extramural RD&D**
  - R&D activities in U.S. and around the world
  - States, industry, academia, and others
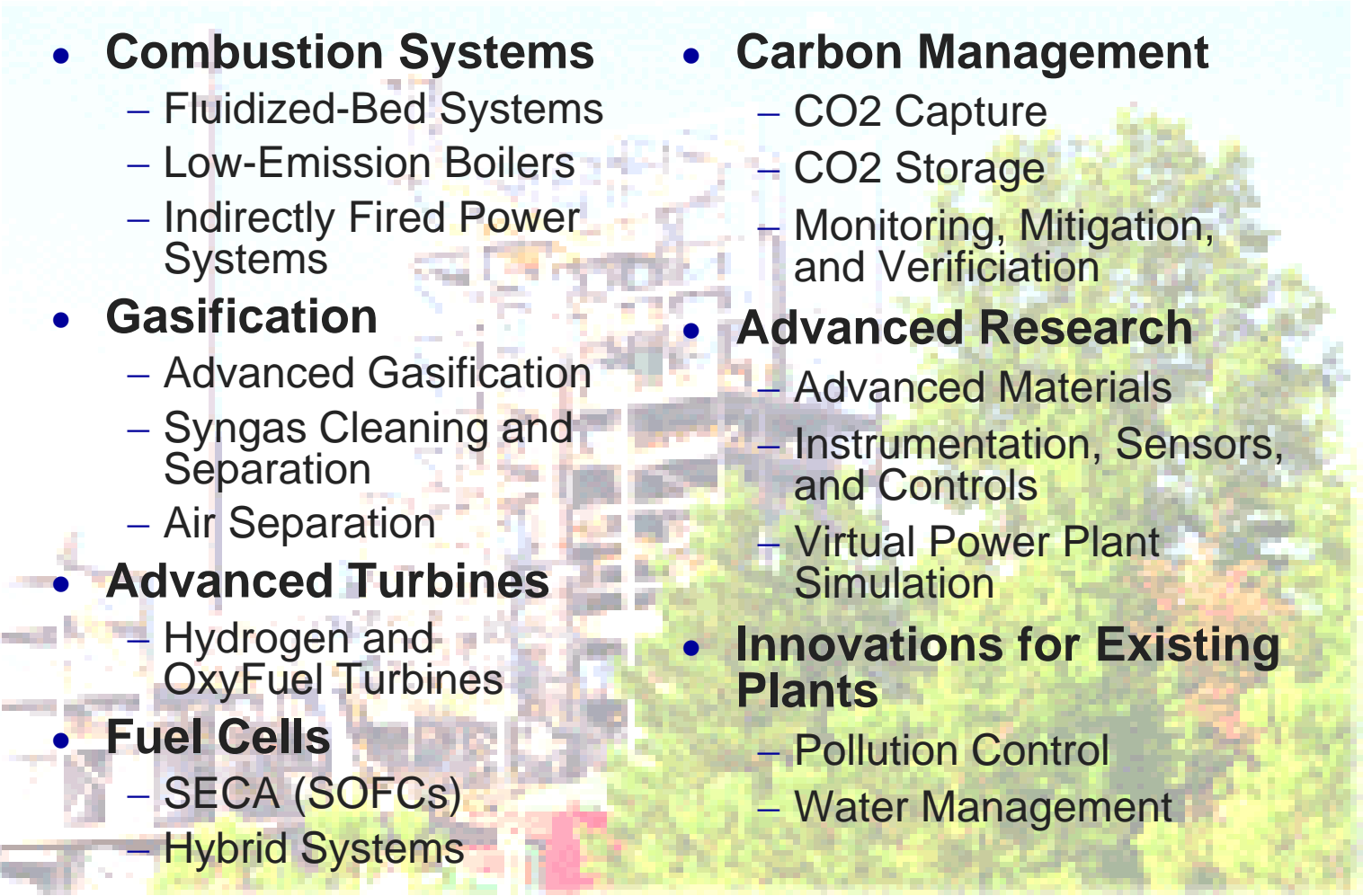 - Private sector cost-sharing

NETL Implements and Manages Extramural RD&D

- **Over 1,800 research and deployment activities in U.S. and more than 40 foreign countries**
- **Total award value over $9 billion**
- **Private sector cost-sharing over $5 billion**
  - Leverages DOE funding
  - Ensures relevance
  - Accomplishes mission through commercialization

Number of Projects
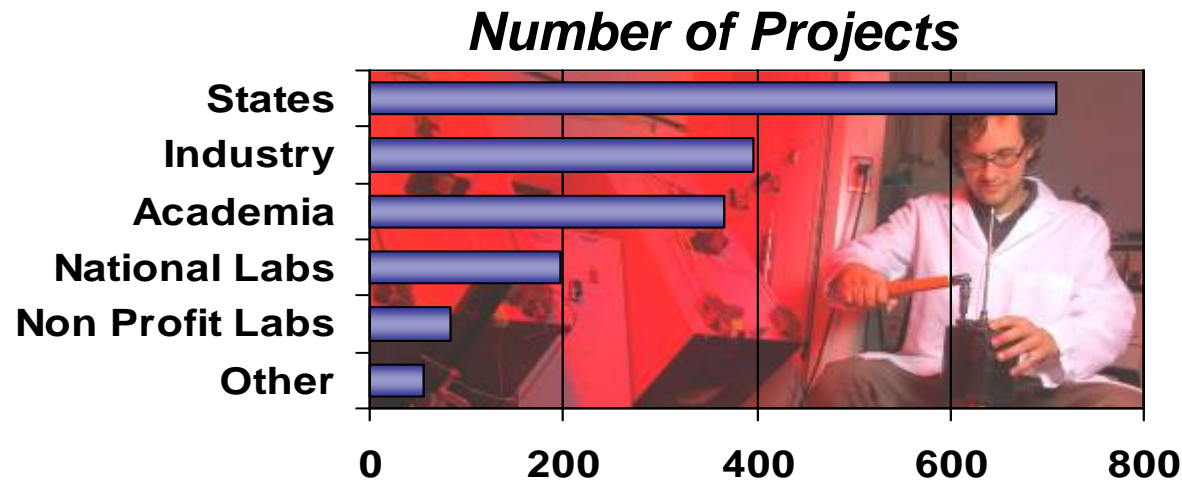
Clean Coal - Core R&D Programs

- **Combustion Systems**
  - Fluidized-Bed Systems
  - Low-Emission Boilers
  - Indirectly Fired Power Systems
- **Gasification**
  - Advanced Gasification
  - Syngas Cleaning and Separation
  - Air Separation
- **Advanced Turbines**
  - Hydrogen and OxyFuel Turbines
- **Fuel Cells**
  - SECA (SOFCs)
  - Hybrid Systems

- **Carbon Management**
  - CO2 Capture
  - CO2 Storage
  - Monitoring, Mitigation, and Verificiation
- **Advanced Research**
  - Advanced Materials
  - Instrumentation, Sensors, and Controls
  - Virtual Power Plant Simulation
- **Innovations for Existing Plants**
  - Pollution Control
  - Water Management

Accomplishing Our Mission

- **Support energy policy development**
  - Presidential Initiatives: Clear Skies, Climate Change, Hydrogen Fuels, Energy Security
  - Demonstration Programs: *FutureGen,* Clean Coal Power Initiative (CCPI)

- **Implement and manage extramural RD&D**
  - Over 1,800 research activities in U.S. and more than 40 foreign countries
  - Total award value over $9B
  - Private sector cost-sharing over $5B

- **Conduct onsite research and analysis**
  - More than 550 engineers and scientists
  - Over 150 with Ph.D. and 300 with M.S.
  - Office of Systems, Analyses & Planning
  - Office of Research and Development

Office of Systems, Analyses and Planning
Employing an Interdisciplinary Approach to Guide R&D and Support Energy Policy Development

- **Systems analysis**
  - Technical and economic feasibility
  - Integrated operation requirements
  - Setting cost and performance targets
- **Life cycle analysis**
- **Benefits quantification**
  - Advanced technologies deployment
- **Forecasts and trend analysis**
- **Technology-regulatory implications**
- **Assessment of natural resource requirements**

Office of Systems, Analyses and Planning
Cost and Performance Baselines

- **Baseline Cases**
  - PC, Oxyfuel PC
  - NGCC, IGCC
  - *FutureGen*
  - Polygeneration
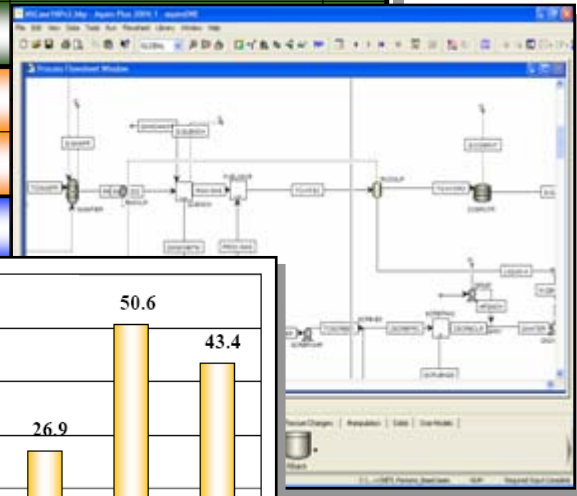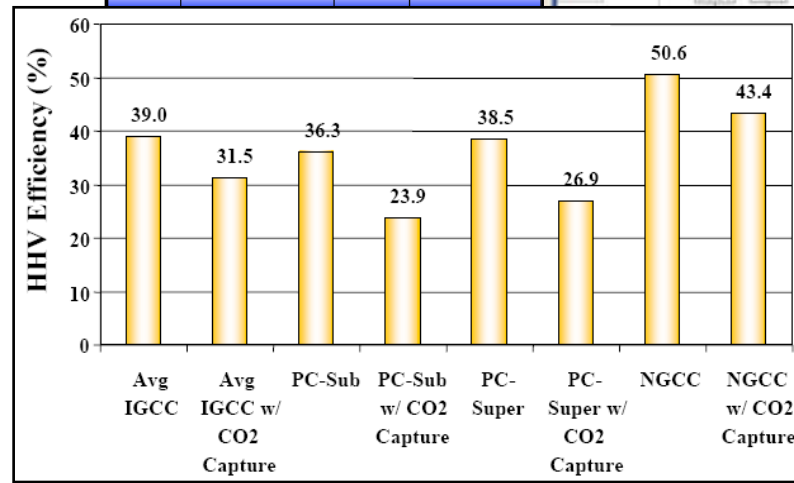 - Coal/Bio-to-Liquids
- **Cost/Performance**
  - Efficiency
  - Capital cost
  - Cost of electricity
- **Simulation Tools**
  - Steady State
    - Aspen Plus
    - GateCycle
  - Costing
    - Spreadsheets
    - ICARUS

Plant Type	ST Cond. (psig/°F/°F)	GT	Gasifier/ Boiler	Acid Gas Removal/ CO_2 Separation / Sulfur Recovery		CO_2 Cap
IGCC	1800/1050/1050	F Class	GE	Selexol / - / Claus		
				Selexol / Selexol / Claus		90%
			CoP E-Gas	MDEA / - / Claus		
				Selexol / Selexol / Claus		90%
			Shell			
PC	2400/1050/1050		Subcritical			
	3500/1100/1100		Supercritical			
NGCC	2400/1050/950	F Class	HRSG			

HHV Efficiency (%) bar chart:
- Avg IGCC: 39.0
- Avg IGCC w/ CO2 Capture: 31.5
- PC-Sub: 36.3
- PC-Sub w/ CO2 Capture: 23.9
- PC-Super: 38.5
- PC-Super w/ CO2 Capture: 26.9
- NGCC: 50.6
- NGCC w/ CO2 Capture: 43.4

NETL

Office of Research and Development
Creates and Transfers Innovative
Fossil Energy Technologies

Focus Areas

- **Energy System Dynamics**
- **Geological & Environmental Science**
- **Materials Science**
- **Computational & Basic Science**
  - Computational Chemistry
  - Multiphase Flow
  - Device-Scale Simulation
  - Model Validation
  - Process & Dynamic Systems
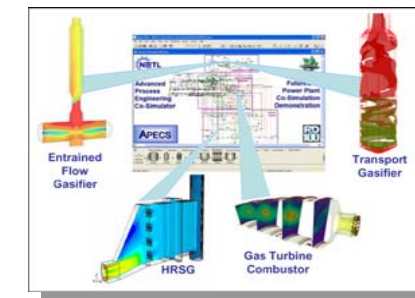
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*FutureGen* **Plant**

NETL Onsite R&D

APECS Co-Simulation

Fossil Energy Power Generation Industry
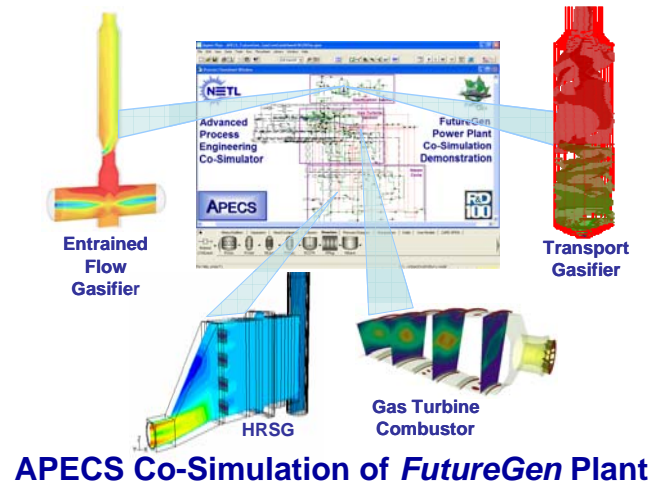## *Process Systems Engineering R&D Challenges*

- Wide range of potential plant configurations with heat/water network management

- Large, complex, highly-integrated, and multipurpose designs

- Limited number of demo plants

- Aggressive design goals
  - Zero emissions
  - Unprecedented efficiency

- Uncertain cost fluctuations for raw materials / finished products

- Growing demand for experience with plant operations and control

- Optimization across plant lifecycle

FutureGen Power/Hydrogen Generation Plant with CCS
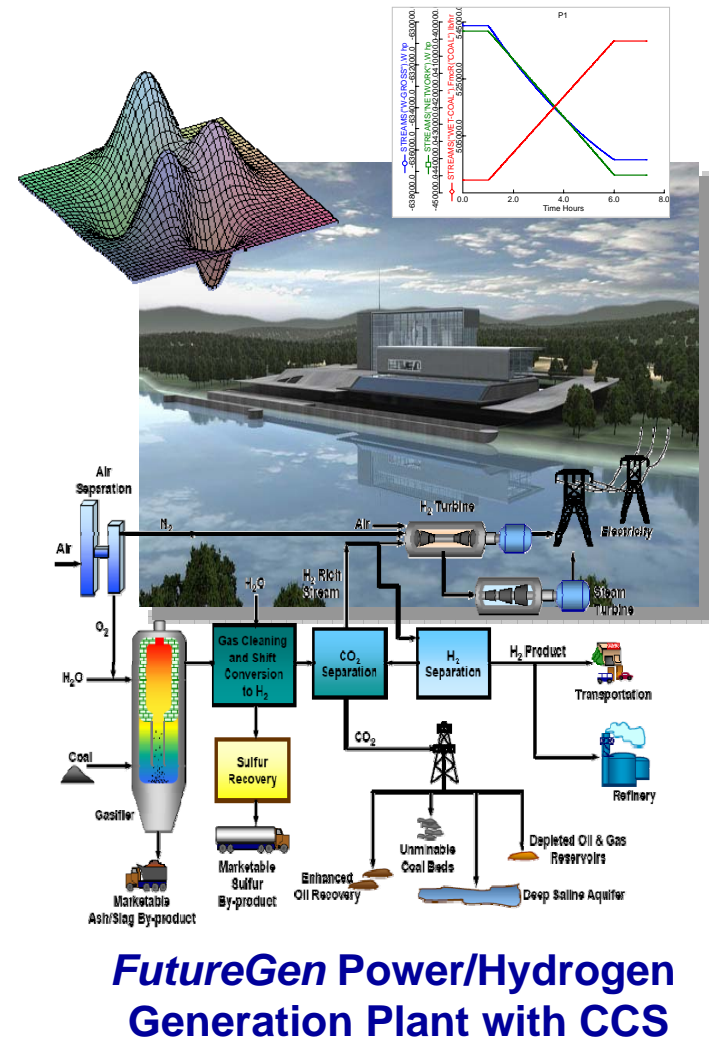
Process Systems Engineering R&D at NETL
Goals and Objectives

- Reach beyond traditional steady-state systems analysis

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

  – High-fidelity modeling

  – Dynamic modeling

  – Systems optimization

- Apply to existing and emerging fossil energy systems

- Establish strong RD&D collaborations

- Transfer technology to process and energy industries

Entrained Flow Gasifier

Transport Gasifier

HRSG

Gas Turbine Combustor

APECS Co-Simulation of *FutureGen* Plant

NETL Collaboratory for Process & Dynamic Systems Research

NETL
Carnegie Mellon
University of Pittsburgh
West Virginia University

APECS- 2006/07 Federal Laboratory Consortium Awards for Excellence in Technology Transfer
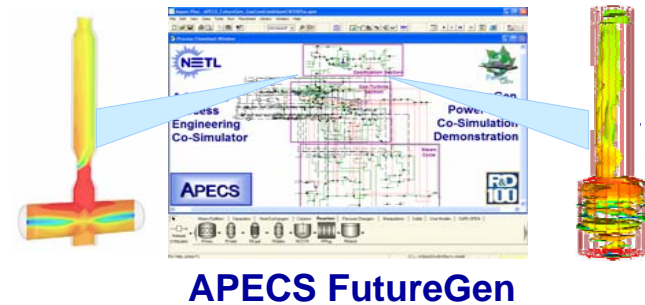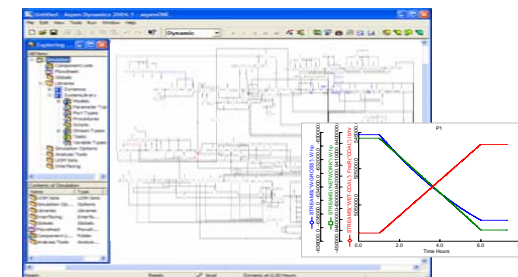
Process Systems Engineering R&D
Focus Areas

- **High-Fidelity Systems**
  - Advanced process engineering co-simulation (APECS)
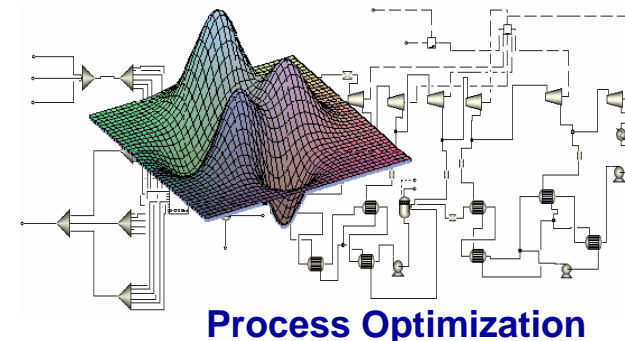 - Virtual power plant simulation

APECS FutureGen

- **Dynamic Systems**
  - Dynamic simulation
  - Process control
  - Real-time applications

IGCC Dynamic Simulation

- **Systems Optimization**
  - Plant-wide optimization
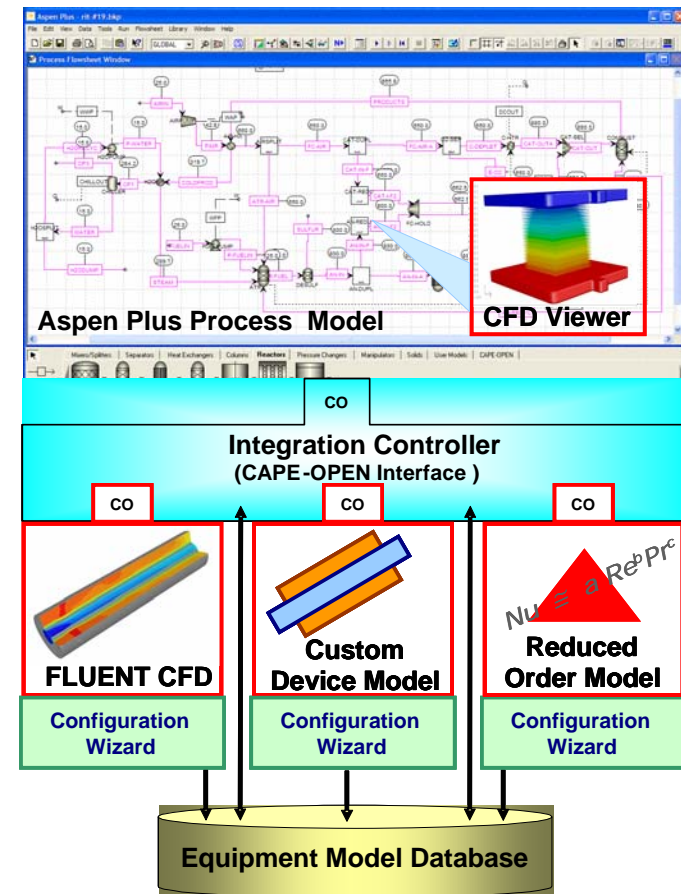 - Stochastic simulation for uncertainty/risk analysis
  - Cost estimation

Process Optimization

Advanced Process Engineering Co-Simulator (APECS)

- **Co-simulation** software framework for integration of:
  - Process simulation
  - Equipment simulations
    - Computational fluid dynamics (CFD)
    - Custom engineering models (CEMs)
    - Reduced-order models (ROMs)
- Enables analysis and optimization of overall plant performance with respect to complex thermal and fluid flow phenomena
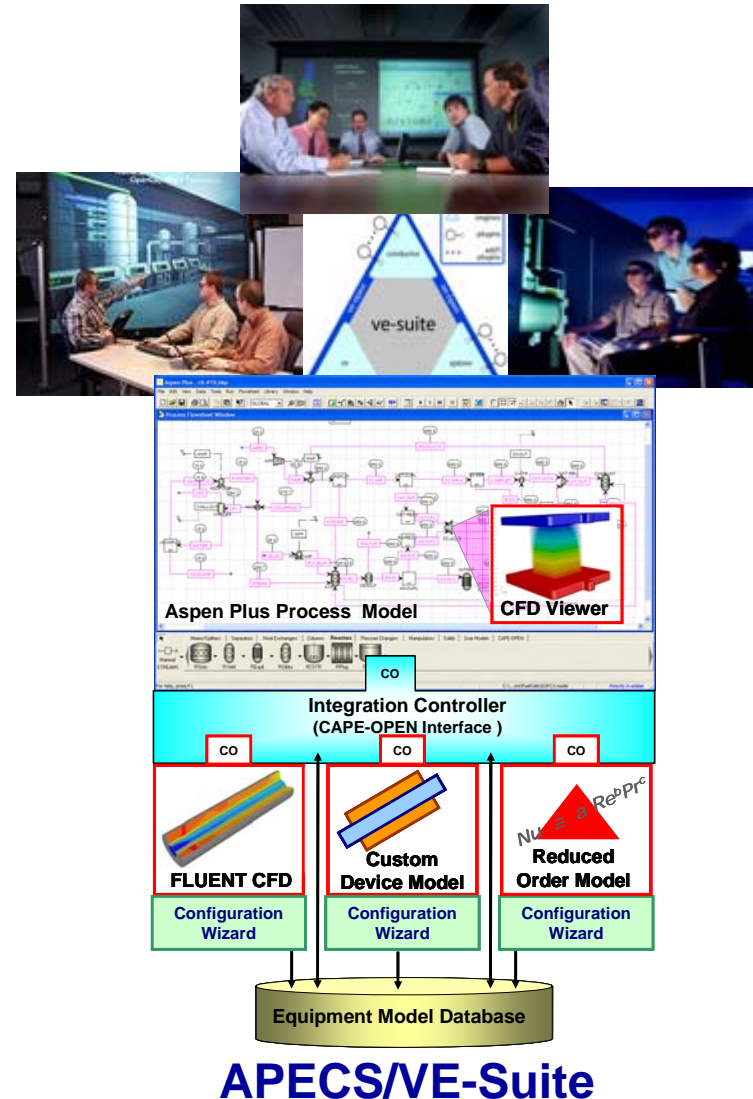

Aspen Plus Process Model | CFD Viewer

CO

Integration Controller
(CAPE-OPEN Interface)

CO   CO   CO

FLUENT CFD | **Custom Device Model** | **Reduced Order Model**

Configuration Wizard | Configuration Wizard | Configuration Wizard

Equipment Model Database

APECS Software Integration Framework

APECS Software Components and Features

- **Process Simulators**
  - CAPE-OPEN compliant
  - Aspen Plus®, HYSYS®, gPROMS®
- **Equipment Models and Database**
  - CAPE-OPEN compliant
  - CFD: FLUENT®
  - Custom Models: e.g., INDVU
  - ROMs: LR, NN, PCA, POD
- **Integration Controller**
  - CAPE-OPEN v1.0 Interfaces
  - Unit Ops, Phys Props, Reactions
- **Configuration Wizards**
  - FLUENT®, Custom Model, and ROM
- **Solution/Analysis Tools**
  - CAPE-OPEN compliant
  - Hybrid: Speed (ROM), Accuracy (CFD)
  - Stochastic, Multi-objective Optimization
- **Distributed Execution**
  - CAPE-OPEN COM/Corba Bridge
  - Windows/Linux, Serial/Parallel
- **Virtual Engineering**
 - CFD Viewer (2D), Paraview (3D)
  - VE-Suite

Aspen Plus Process Model — CFD Viewer

CO

Integration Controller
(CAPE-OPEN Interface)

CO   CO   CO

FLUENT CFD | Custom Device Model | Reduced Order Model

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Equipment Model Database

APECS/VE-Suite
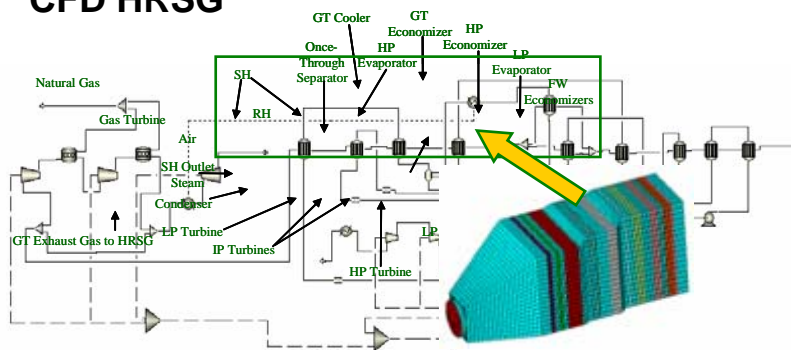
APECS Power Generation Applications

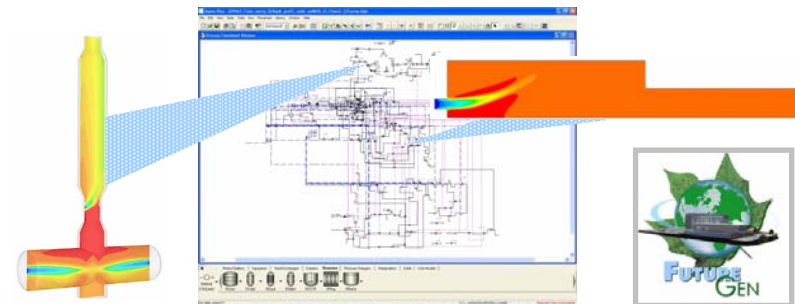- **Fuel Cell Auxiliary Power Unit (APU) with 3D CFD SOFC**
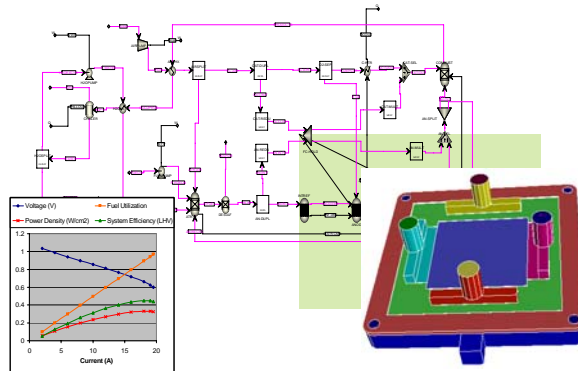
- **ALSTOM Conventional Steam Plant (250MWe) with 3D CFD Boiler**
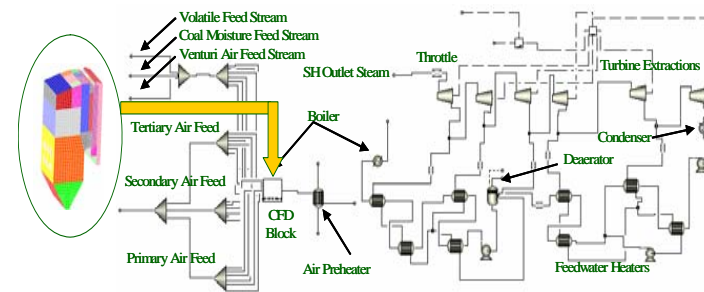
- **ALSTOM NGCC (250MWe) with 3D CFD HRSG**

- **FutureGen Plant (250MWe) with 3D CFD Gasifier and 2D CFD Turbine Combustor**

US-UK Collaboration on Virtual Plant Simulation
Fossil Energy R&D

- **Major Goal**
  - Develop compatible process/CFD co-simulation software platforms for application to advanced FE systems

- **Leverages On-Going R&D Projects**
  - US DOE/NETL APECS
  - UK Virtual Plant Demonstration Model (VPDM)
  - CAPE-OPEN Software Standard

- **Didcot A coal-fired power station**
  - Plant: PSE (gPROMS)
  - Equipment Items:
    - Furnace – RWE; APECS for CFD (FLUENT) / ROM (ANN)
    - Boiler – MBEL; Turbine – ALSTOM
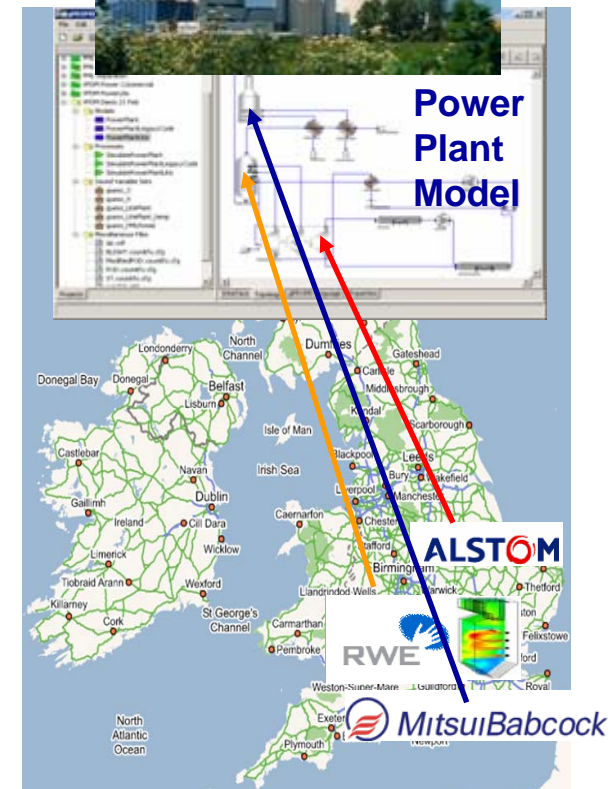
Power Plant Model

Distributed Equipment Models

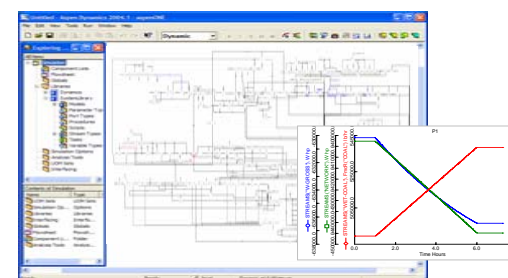# Process & Dynamic Systems Research
Focus Areas

- **High-Fidelity Systems**
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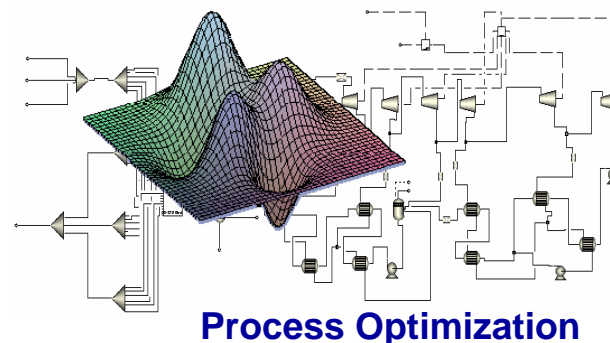 - Virtual power plant simulation

APECS FutureGen

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  - Dynamic simulation
  - Process control
  - Real-time applications

IGCC Dynamic Simulation

- **Systems Optimization**
  - Plant-wide optimization
  - Stochastic simulation for uncertainty/risk analysis
 - Cost estimation

Process Optimization

IGCC Dynamic Simulator & Research Center
Project Objectives

- Full-scope, high-fidelity, real-time, generic IGCC simulator

- IGCC DS&R Center at WVU's National Research Center for Coal & Energy (NRCCE)

- NETL Collaboratory for Process & Dynamic Systems Research

- Strong R&D collaborations
  - Enginomix, EPRI, FCS, Bechtel, Software/services vendor, …

- Industry participation
  - CoalFleet (AEP, BP, GRE, …)

- Custom, site-specific IGCC dynamic simulators

- Extension to *FutureGen* and other advanced FE systems
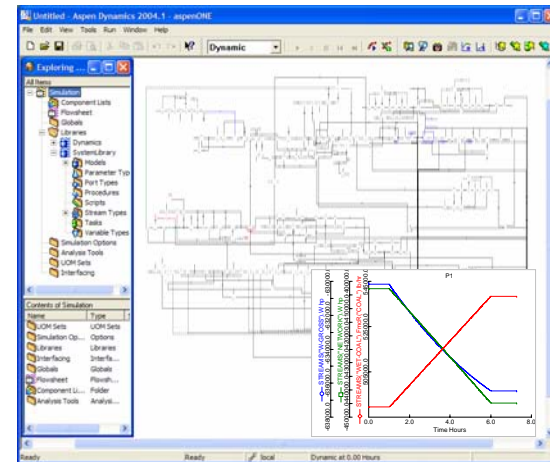

IGCC DS&R Center
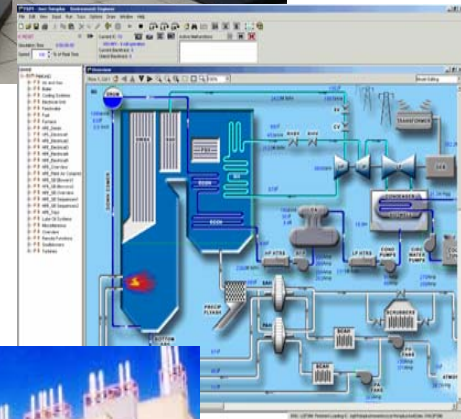
WVU's NRCCE

Process & Dynamic Systems Research
R&D Projects – Dynamic Systems

- Dynamic IGCC Model for Industry Cluster (Turton - WVU)

- Plant-wide IGCC Control and RT-Optimization (Ydstie - CMU)

- Plant-wide IGCC Model Predictive Control (Bequette - RPI)

- Nonlinear Model Predictive Control for IGCC (Biegler - CMU)

- Gas Turbine/Fuel Cell Hybrid Systems (NETL)

Plantwide IGCC Simulation in Aspen Dynamics
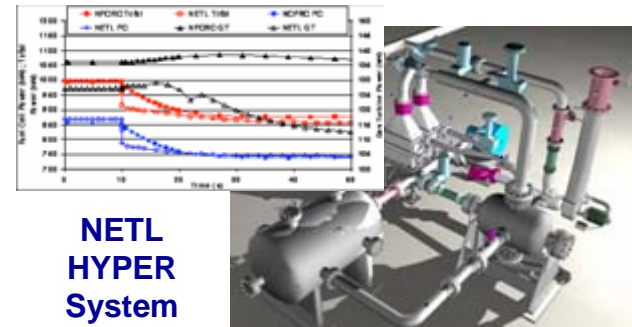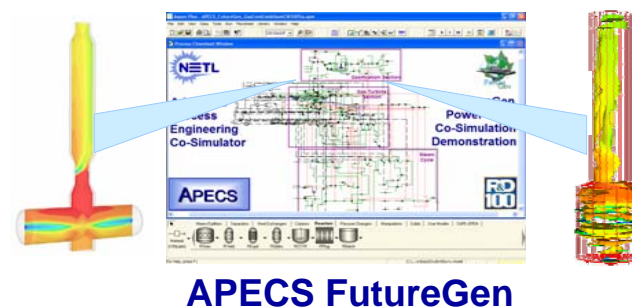

NETL HYPER System

Process & Dynamic Systems Research
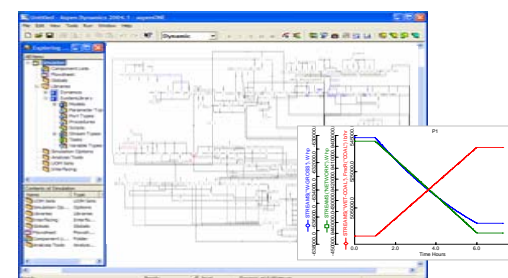## *Focus Areas*

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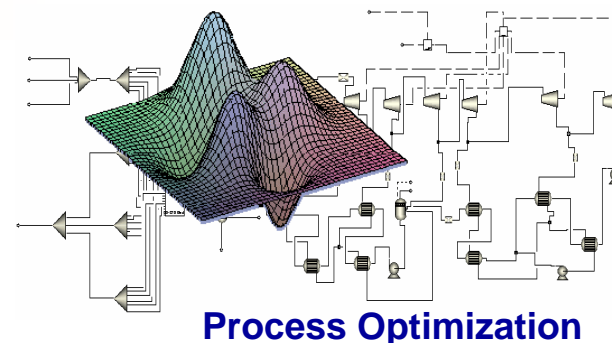 - Virtual power plant simulation

- **Dynamic Systems**
  - Dynamic simulation
  - Process control
  - Real-time applications
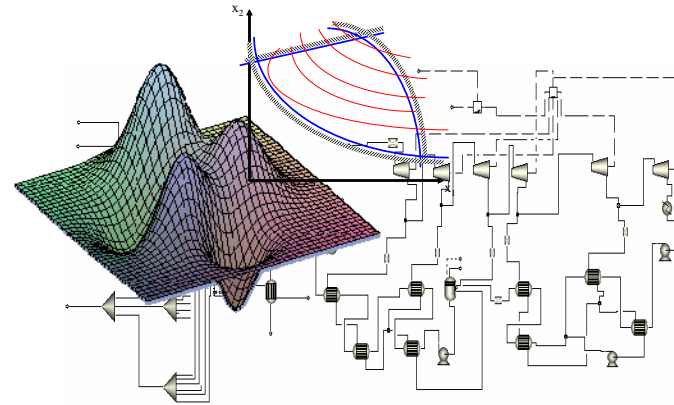
- **Systems Optimization**
  - Plant-wide optimization
  - Stochastic simulation for uncertainty/risk analysis
  - Cost estimation

APECS FutureGen

IGCC Dynamic Simulation


Process Optimization

Process & Dynamic Systems Research
R&D Projects – Optimization

- IGCC Process Synthesis (Grossmann – CMU)

- Integrated Optimization Strategies for Zero-Emission Power Plants (Biegler - CMU)

- Stochastic Analysis and Multi-objective Optimization (Diwekar – VRI)

- Aspen-based Performance and Cost Models for Power Systems Analysis (Rubin - CMU)

Process Optimization
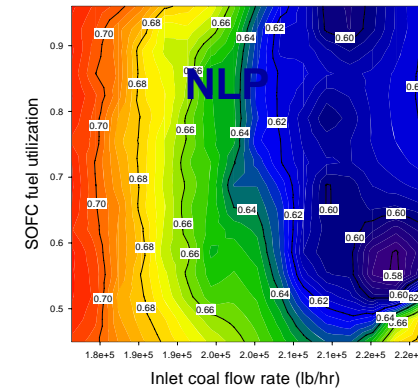
Stochastic Simulation of Advanced Power Plant
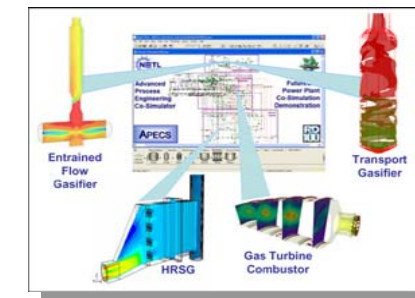
Outline of Presentation

- **Introduction**

- **US Fossil Energy Outlook**

- **NETL's Fossil Energy Mission**

  – Energy Policy Support

    • Clean Coal Power Initiative

    • *FutureGen*

  – Extramural RD&D

  – Onsite Research and Analysis

- **Process Systems Engineering**

  – Industry R&D Challenges

  – NETL R&D Activities

- **Concluding Remarks**

FutureGen Plant

NETL Onsite R&D

APECS Co-Simulation

Concluding Remarks

- U.S. energy challenges are daunting

- Fossil fuels, including coal, will continue to play a major role for decades

- IGCC emerging as an attractive technology option for next-generation, coal-fired plants

IGCC Plant

- *FutureGen* is a pathway to zero-emission, coal-fueled, power generation

- NETL supports DOE's Fossil Energy mission with broad spectrum of R&D from fundamental science to technology demonstrations

FutureGen **Plant**

- NETL's process systems engineering R&D is aimed at reducing the time, cost, and risk of developing advanced power generation plants

- Optimization challenges across the power plant lifecycle offer considerable potential for collaborative research

NETL Onsite R&D

Visit Fossil Energy, NETL, and *FutureGen* Websites

http://fossil.energy.gov/

www.netl.doe.gov

www.futuregenalliance.org

Thank You

Questions?

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