

# National Energy Technology Laboratory



**Office of Research and  
Development**

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**Anthony V. Cugini**

**National Energy Technology Laboratory**



**Office of Fossil Energy**



# NETL Research and Development

- DOE's only national lab dedicated to fossil energy R&D
- One lab, three R&D locations, one management structure
  - Government owned and operated
- Conducting research from fundamental science through technology demonstrations



*Oregon*



*Pennsylvania*



*West Virginia*

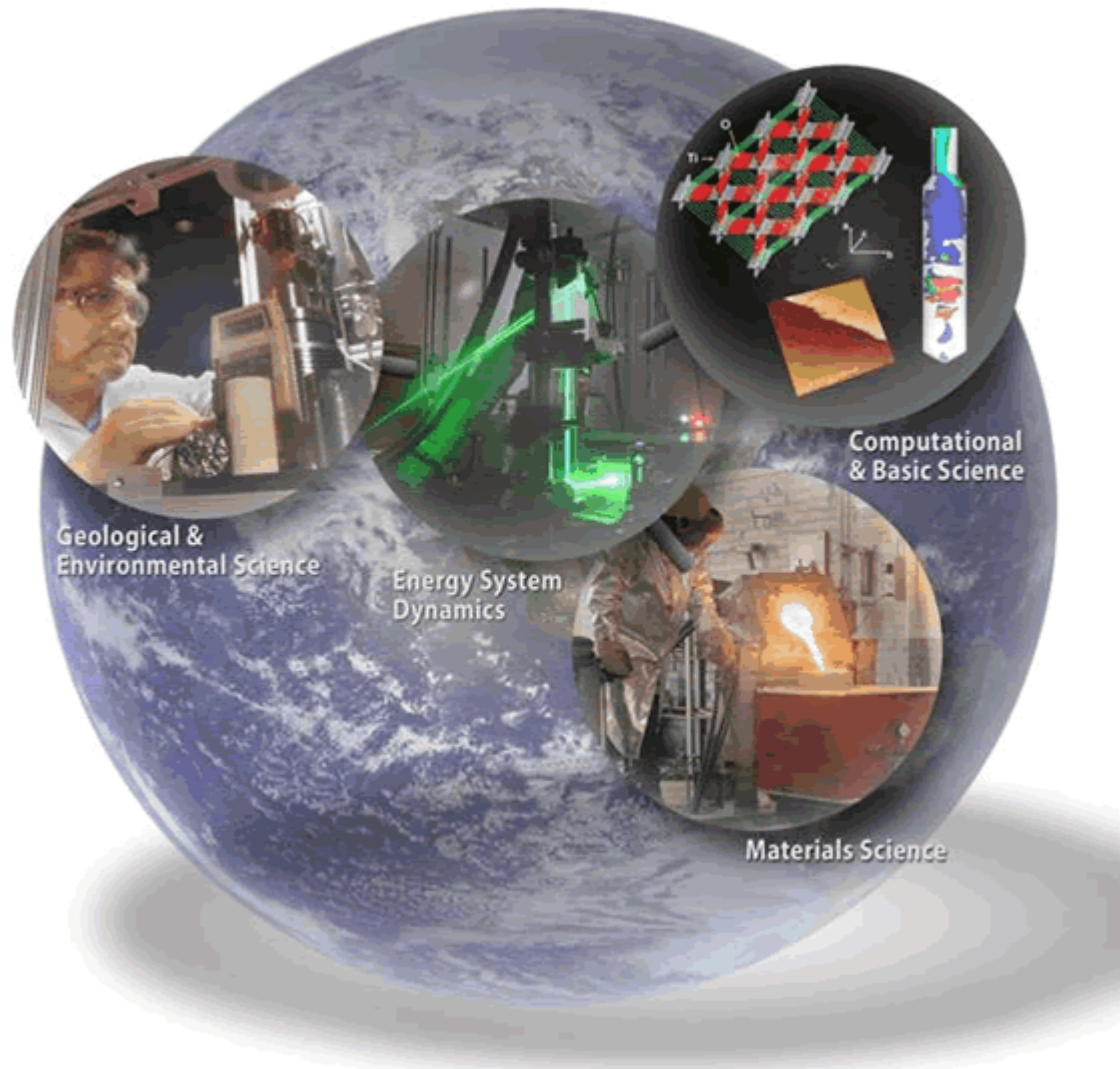


# NETL's Office of Research & Development

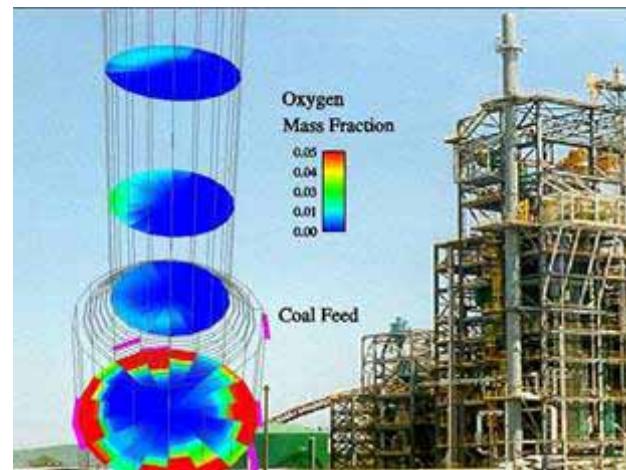
- **Tackling important national energy problems --** CO<sub>2</sub> management, advanced fuels development, hydrogen technology, hybrid cycles, mercury capture, hydrates
- **Capitalizing on unique facilities and capabilities**
- **Achieving breakthrough science-** Computational science and application, hydrogen technologies, combustion science and engineering, sequestration mechanisms
- **Achieving technology successes –** R&D 100 awards, technology transfer awards, publications, licenses, etc.



# Research and Development Focus Areas



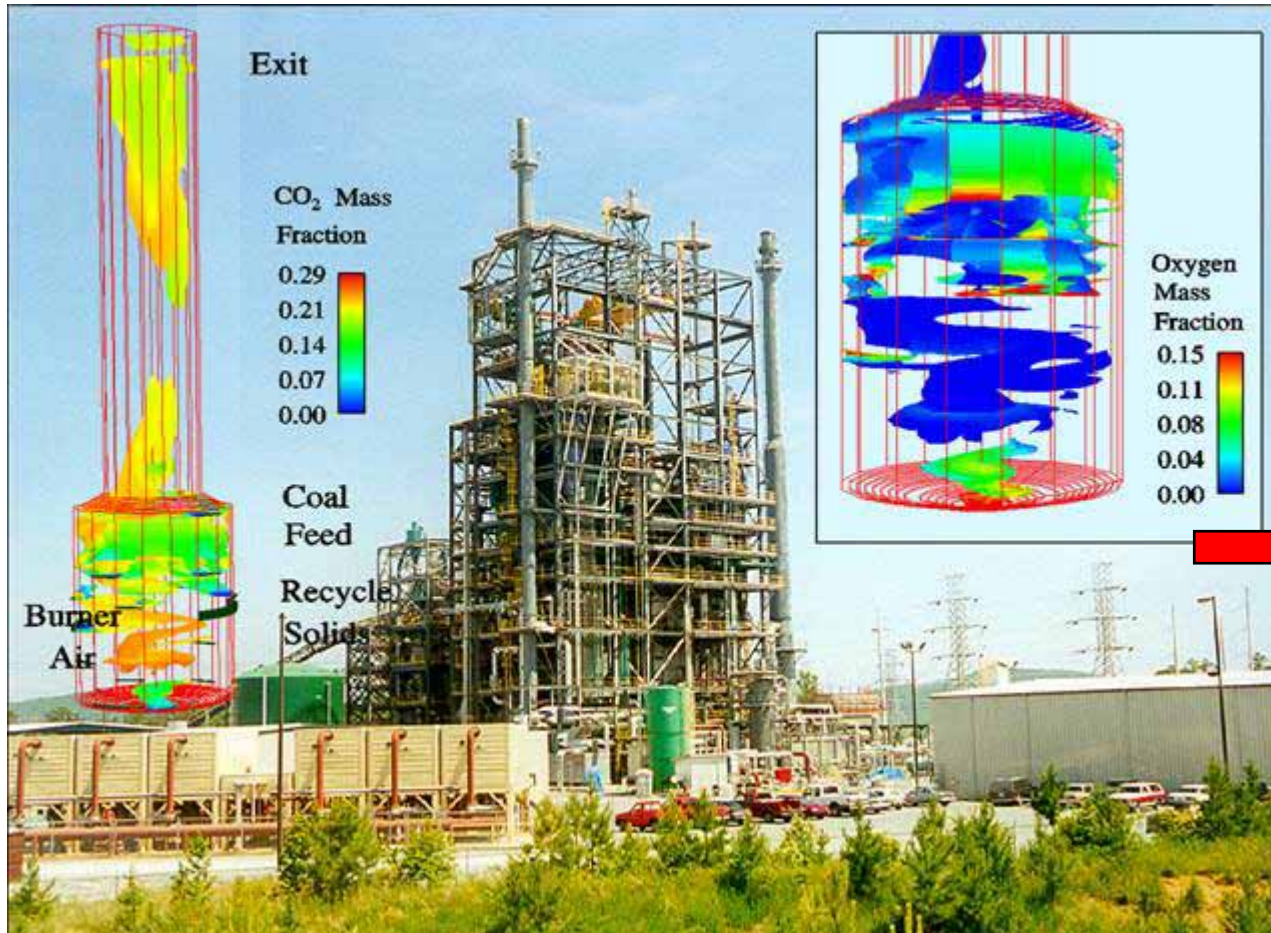
# Computational and Basic Sciences Focus Area



- Fuels Chemistry
- Computational Chemistry
- Device Simulation
- Advanced Fuel Systems
- Gas Hydrates
- Hydrogen and Separation
- Energy Security

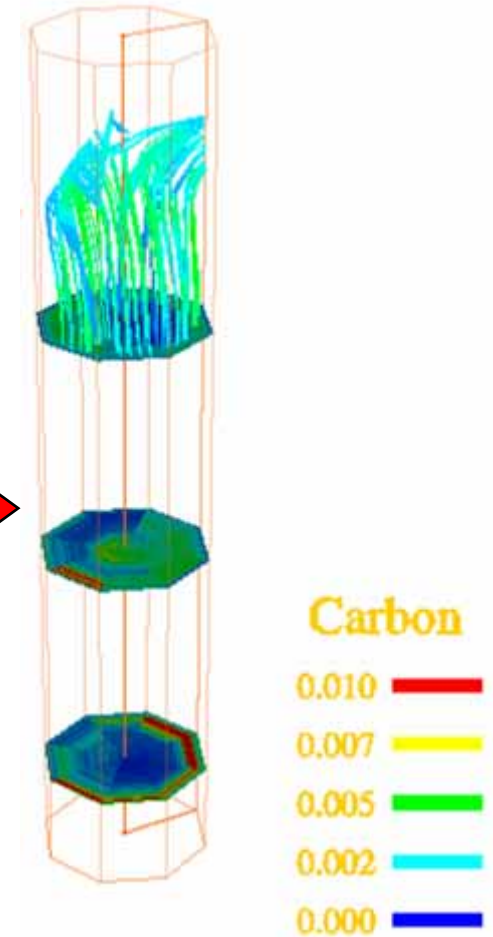


# Gasifier Model Support for IGCC Program



Power Systems Development Facility (PSDF), Wilsonville, AL

O<sub>2</sub> and CO<sub>2</sub> mass fractions superimposed on isosurfaces of at void fraction values of 0.9. Guenther et al. 2002



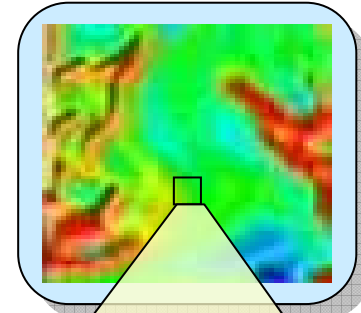
KBR/Southern commercial scale transport gasifier (Guenther 2005)



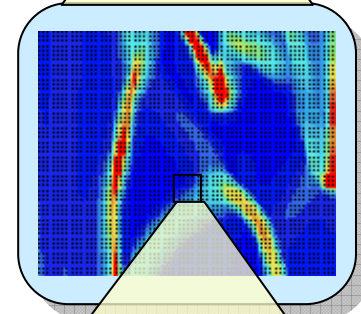
# NETL's MFIX Software

- Discrete/continuum models
- Open source software (2001)
- 1000+ registrations
- 500+ institutions
- 50+ publications
- 20+ graduate theses
- 3 CRADAs (Fluent Inc. and Foster Wheeler)

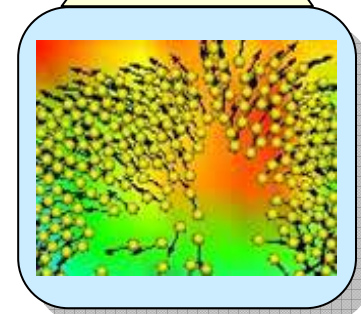
**Device Scale:**  
large flow structures in a CFB



**Meso scale:**  
particle clusters



**Micro Scale:**  
particles in gas



**MFIX**  
[www.mfix.org](http://www.mfix.org)



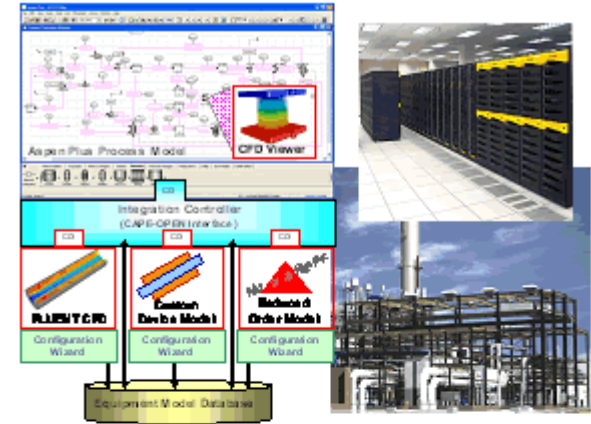
Tech-Transfer  
Award 2006





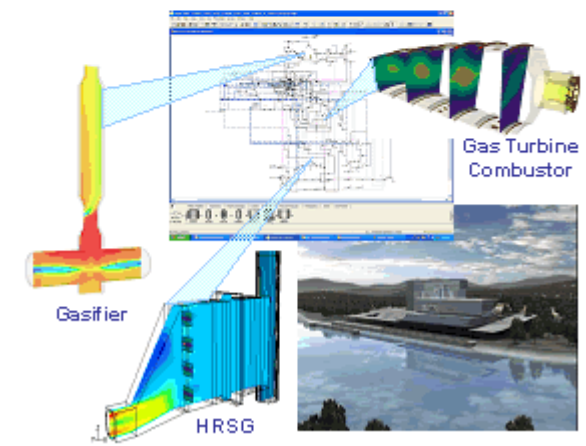
# Advanced Process Engineering Co-Simulator (APECS)

- **APECS** combines process simulation with detailed equipment models, advanced visualization, and high-performance computing
  - First of a kind development by NETL and its R&D technology partners
  - Recognized with **2004 R&D 100 Award**



**APECS Integration Framework**

- **APECS** enables high-fidelity power plant design, analysis, and optimization
  - Provides the necessary level of detail and accuracy essential for advanced power plant simulation
  - Applies to high-efficiency, zero-emission systems, including the **FutureGen** plant



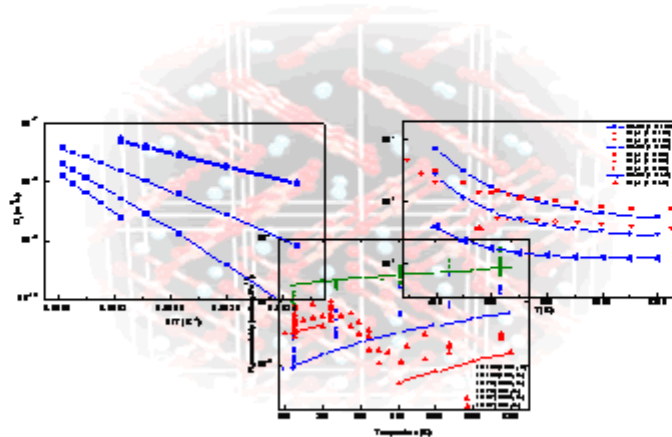
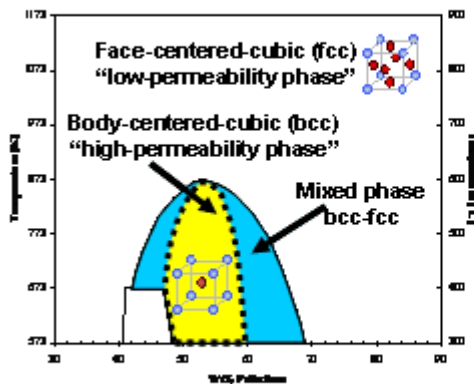
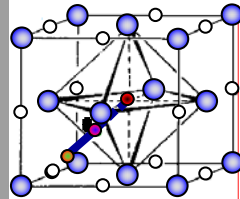
**APECS FutureGen Plant Simulation**



# Computational Modeling and Materials Research

Develop, using nanoscale technologies, advanced materials for extreme environments, hydrogen separation and hydrogen storage

Significance: New materials are needed that enable the high performance expected of a FutureGen plant.



# Energy System Dynamics Focus Area

- **High-pressure Turbine Combustion**
- **Fuel Cells and Fuel Processing for SOFC Power**
- **Hybrid Turbine Fuel Cells**
- **Reciprocating Engines for Stationary Power**
- **Carbon Dioxide Capture for Sequestration**
- **Sensors and Controls for Energy Systems**
- **Humid Gas Cleanup for IGCC**

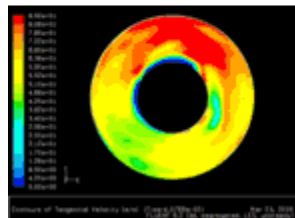
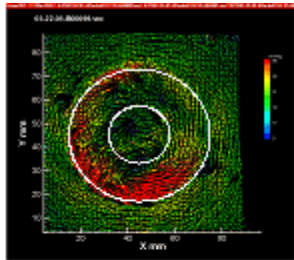


Artist's rendering of the  
Department of Energy's Future Gen Power Plant



# Fuel utilization in turbine combustion

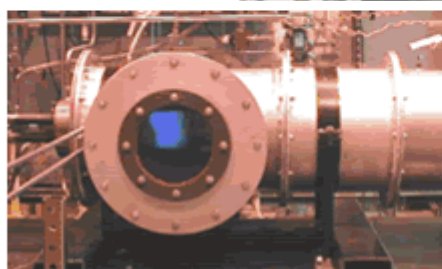
- **NETL on-site research on low-emission combustion with fuel variability**
  - Emission/operability study for FERC assessing LNG versus domestic NG.
  - Flame dynamics/emissions of H<sub>2</sub>, methane + H<sub>2</sub>, and syngas .
  - With Multi-Agency Combustion Coordination Committee:\*
    - Develop *predictive* simulation of fuel blends in engines.
    - Use national cyberinfrastructure to accelerate simulation development (via NSF).
  - Sensors systems for fuel blend variability effects on combustion:
    - Patented flame dynamics sensor (licensed to Woodward Industrial control).



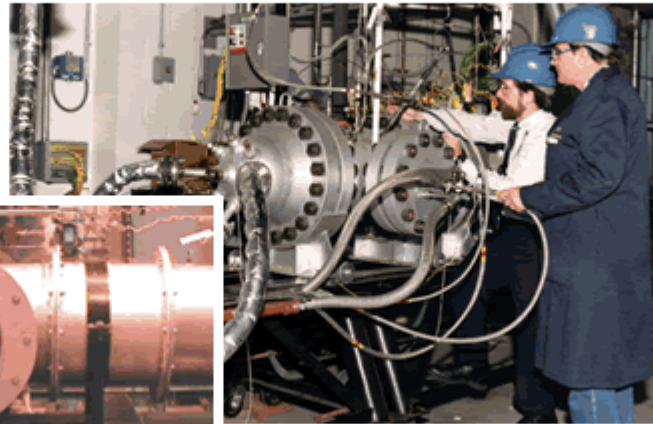
Measured and modeled combustion flow dynamics



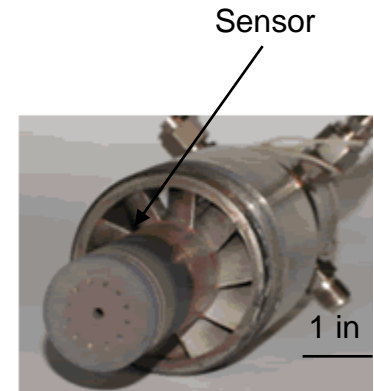
Lab-scale flame dynamics



Low-pressure development combustor



Dynamic Gas Turbine Combustor



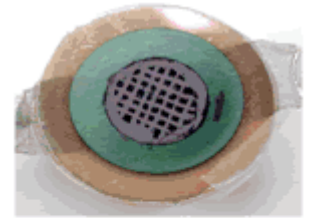
CCADS sensor on prototype fuel injector



\* AFOSR, Edwards AFB, Wright Patt AFB, NASA-Glenn, NIST, NSF, Army, ESTCP/SERDP, DOE-NETL

# Fuel Utilization in Fuel Cells

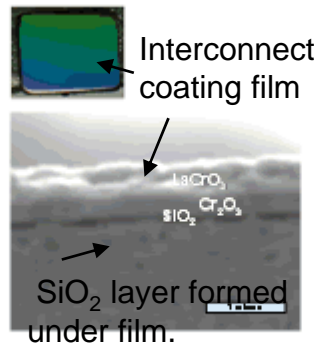
- **Test and evaluation of fuel cell prototypes.**
  - Provides unique SECA (Solid-state Energy Conversion Alliance) program support.
  - Commercial units<sup>1</sup> for evaluation; also open to non-SECA.
- **On-site research for fuel cells and fuel processing**
  - Hydrocarbon reforming for conventional or FT liquid fuels.
  - Low cost interconnect coating & substrate compatibility with coal syngas.
  - Fuel contaminant effects on SOFC cells (Sulfur, Hg, Cl, ....).



Orientation image microscopy shows grain structure in cell after current flow test



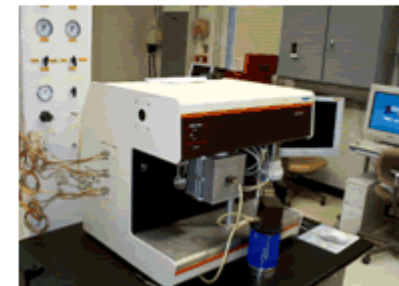
Fuel Cell Test Facility



Interconnect coating and substrate.



Testing with coal-gas slip-stream (planned).



NETL catalyst testing for SOFC reformer

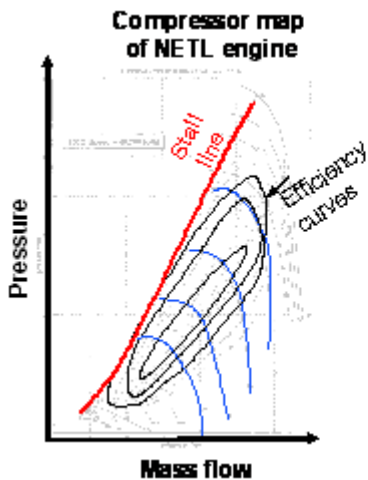
1. GE, Accumentrics, Delphi, SoFCo-Cummins, Siemens-Westinghouse, Fuel Cell Energy

# Fuel Conservation from High Efficiency: Hybrid Turbine Fuel Cell Research

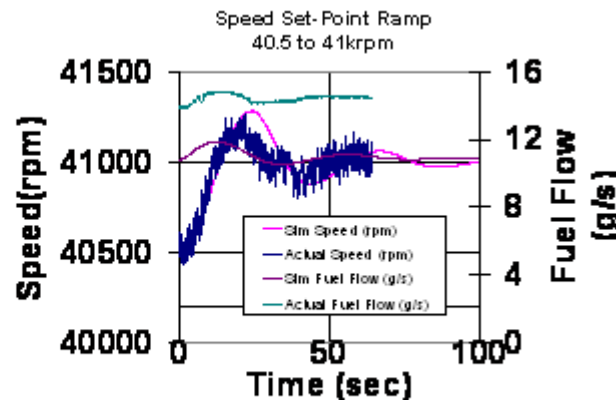
- Hybrid efficiency exceeds turbine & fuel cell efficiencies.
- Technical issues:
  - How to manage energy split (FC vs. GT), load shed, compressor surge?
  - Can fuel cell tolerate plant dynamics?
- NETL HYbrid PERformance (Hyper) facility:
  - Evaluate control architecture to maximize efficiency.
  - Validated models to predict large hybrid performance.
  - Measure real loads expected in fuel cell operation.



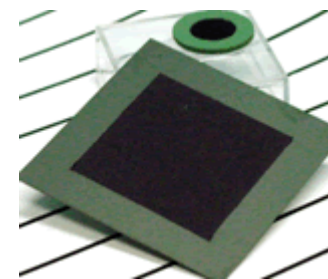
NETL Hyper Facility *simulates* fuel cell dynamics in real turbine environment.



High efficiency occurs near the stall line (red)



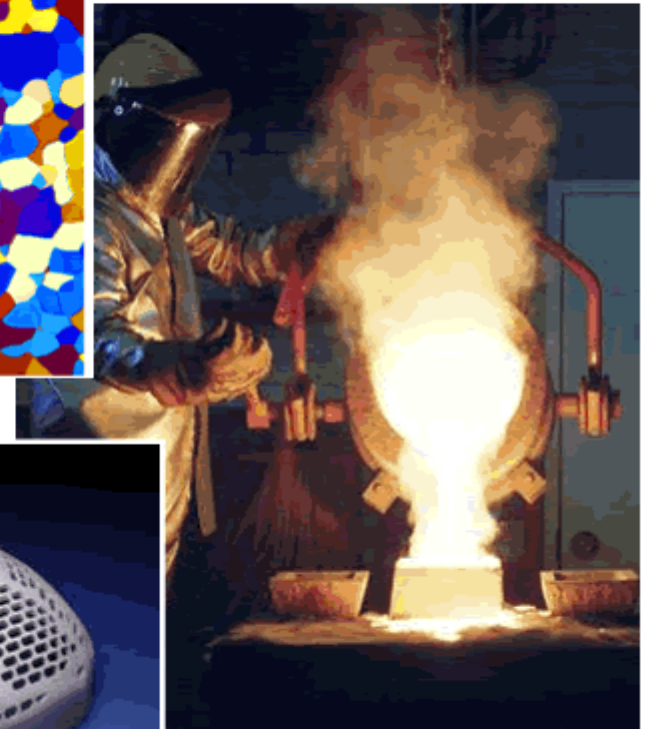
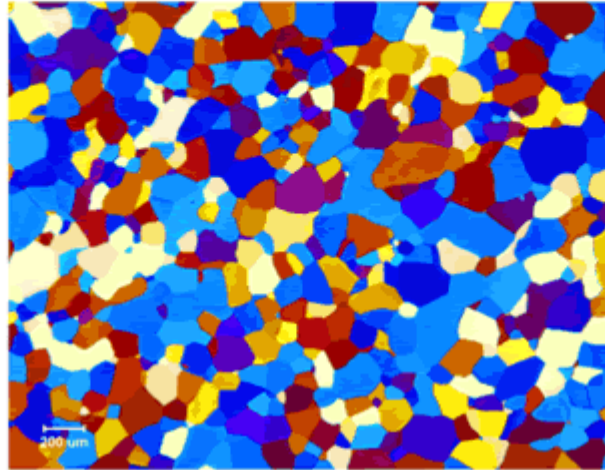
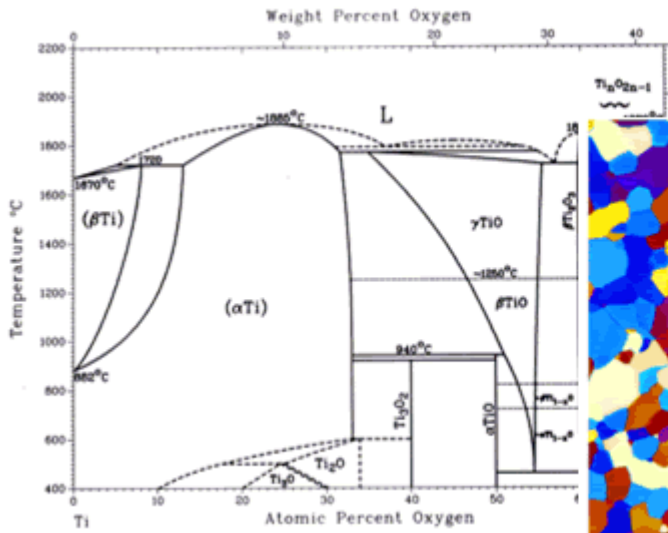
Set-point transients may reverse expected fuel cell flows



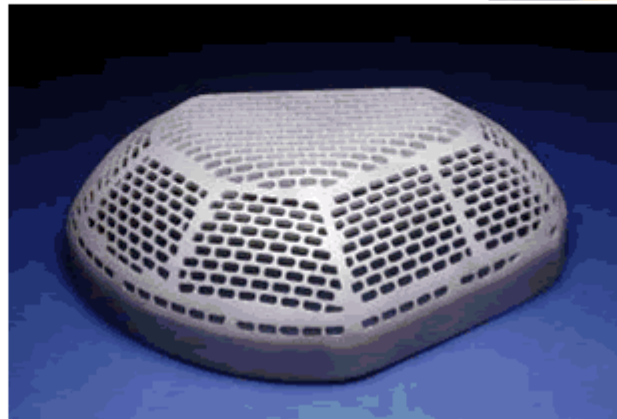
Solid oxide fuel cell can be tested In situ after controlling dynamics



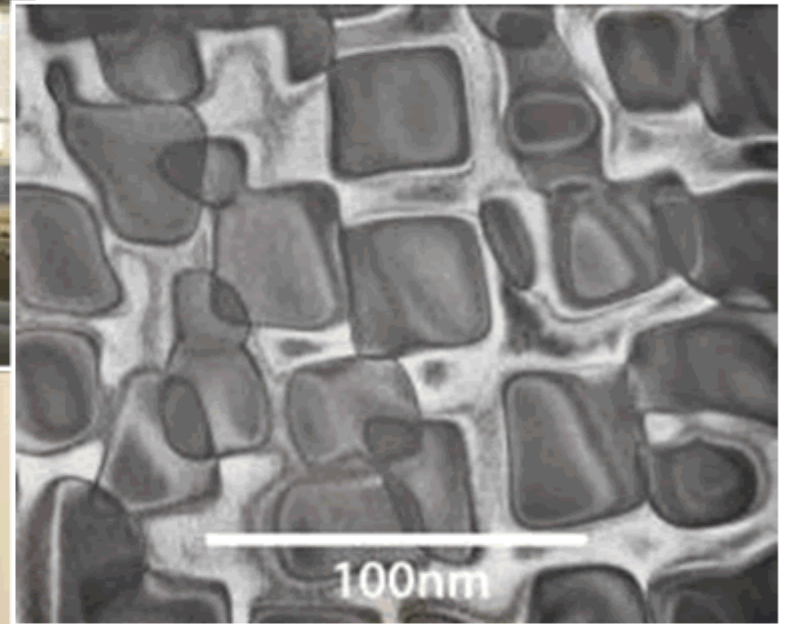
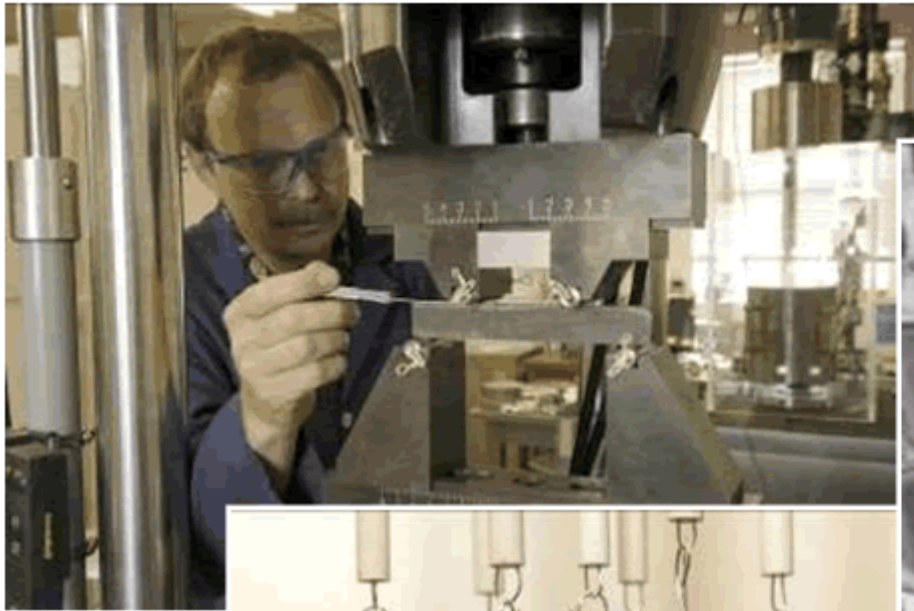
# Materials Science Focus Area



- Fuel Cells
- Advanced Combustion
- Gasification
- FutureGen
- External Partnerships



# Materials Performance Assessment

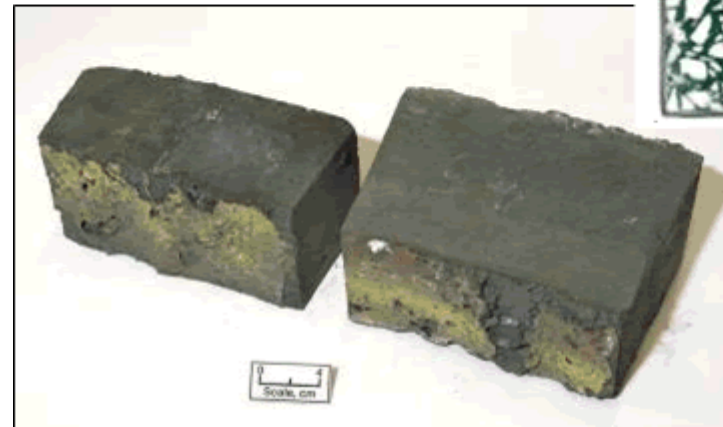
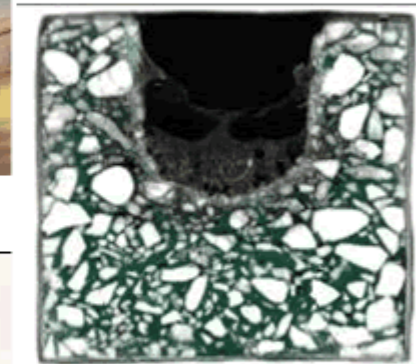
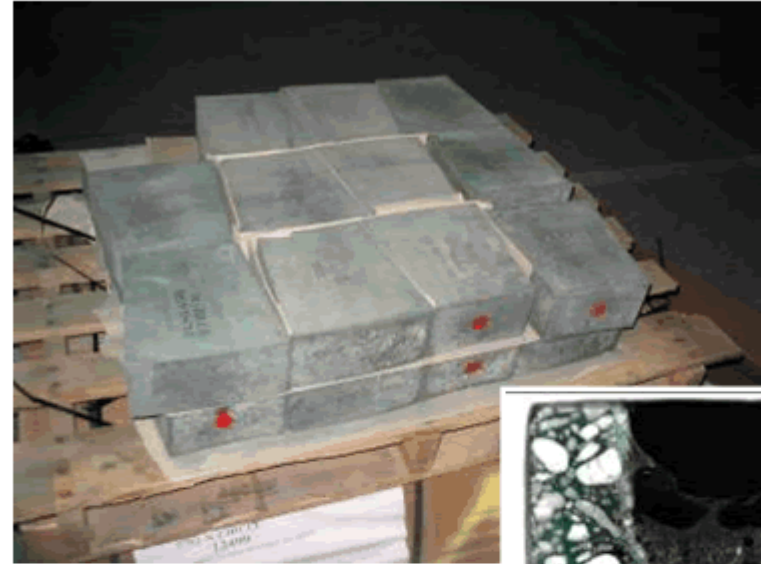


**Corrosion, Wear, Microstructural & Mechanical Stability**

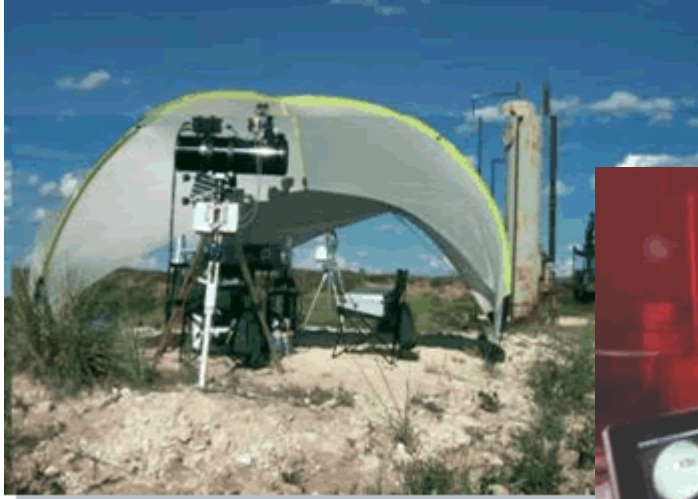


# Materials Performance Improvement

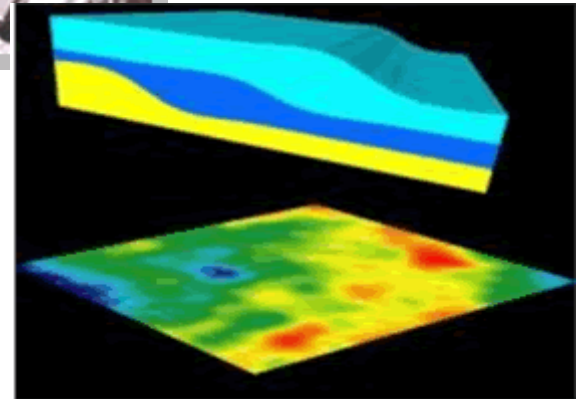
- **Refractories for Gasification**
  - Patent issued
  - Licensing Agreement pending
- **Coating Protection Strategies**
  - Patent pending
- **Surface Treatments for Oxidation Resistance**
  - Patent pending
- **New Iron-Base Alloys for Combustion Systems**
  - Patent pending



# Geological and Environmental Sciences (GES) Focus Area



- Carbon Sequestration
- Water & Coal Utilization
- Coal Byproducts
- Risk Assessment
- Monitoring, Measuring, & Verification



# Carbon Management

- **Reducing the Carbon Footprint**
  - Higher Efficiency
  - Biomass/Coal Gasification and Fuels Production
- **Carbon Capture and Separation**
  - Conventional
  - Unconventional
- **Carbon Storage**
  - Storage Opportunities
  - Interaction with regional partnerships
  - Measurement, monitoring, and verification
- **Risk Assessment**
  - Long-term reactivity
  - Modeling long term behavior
  - Incorporation of other systems analysis



# Carbon Dioxide Capture

**Develop, test, and evaluate sorbents in modular CO<sub>2</sub> capture facility.**

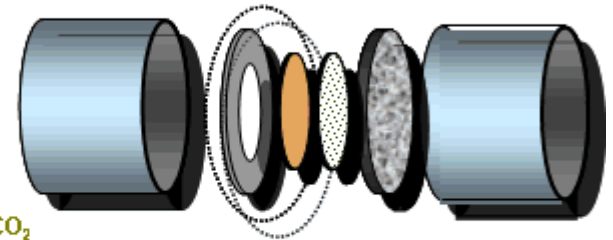
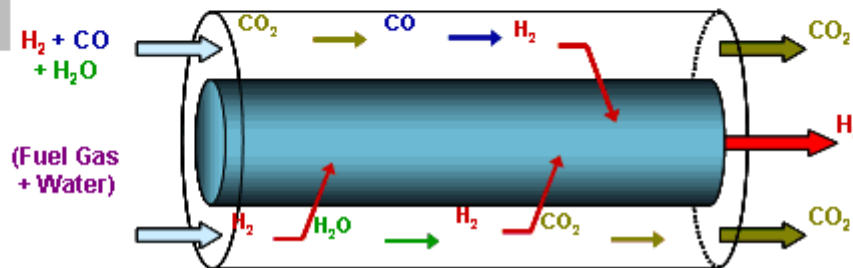
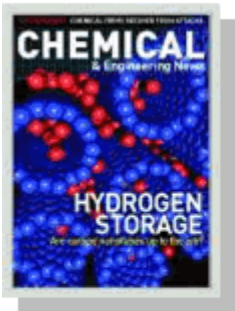
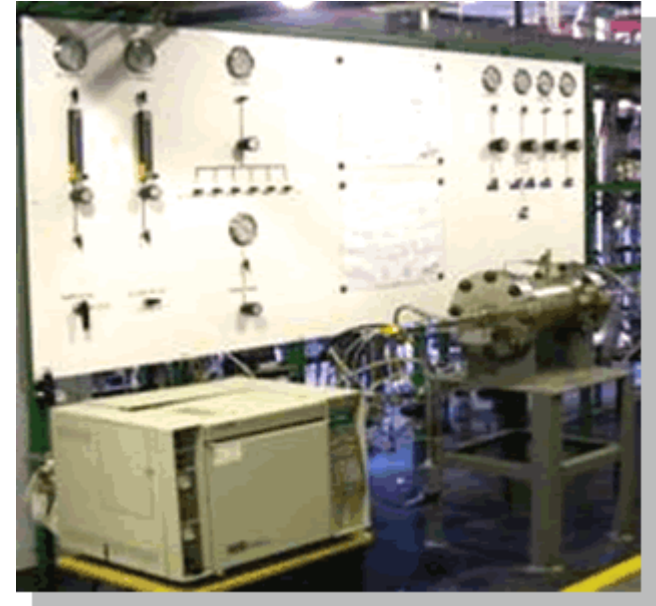
**Significance: Capture and sequestration are key steps on road to the hydrogen economy and existing capture technologies cannot meet cost targets.**



# Carbon Dioxide/Hydrogen Separation Technologies

Investigate sulfur resistant membranes in reactor over range of operating conditions.

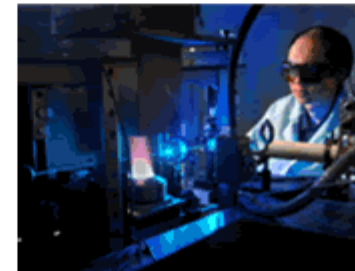
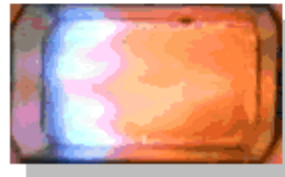
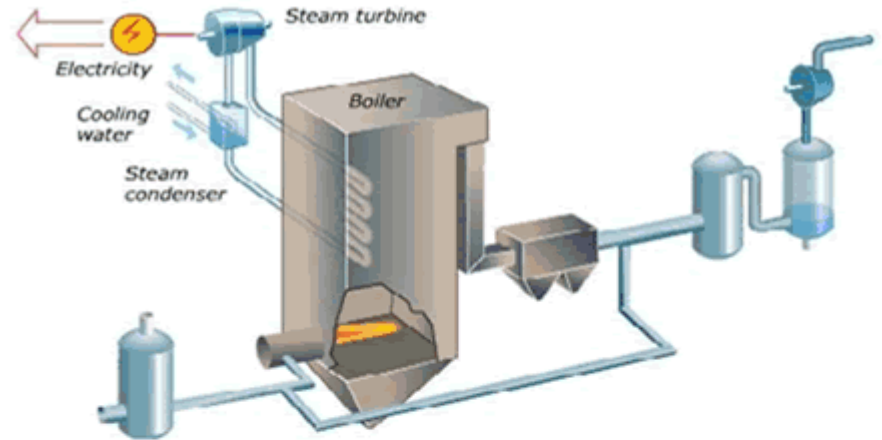
Significance: Hydrogen separation membranes will enhance hydrogen production from coal and reduce hydrogen costs.



# Zero-Emission Oxy-Fuel Combustion

**Develop processes and materials to enable oxy-fuel combustion technologies**

**Significance: Enables CO<sub>2</sub> separation and higher efficiency processes at lower costs than conventional capture methods.**



Zero-emission oxy-fuel combustion

# Storing CO<sub>2</sub> in Geological Formations

**Study internal flows in reservoir materials for model development and validation.**

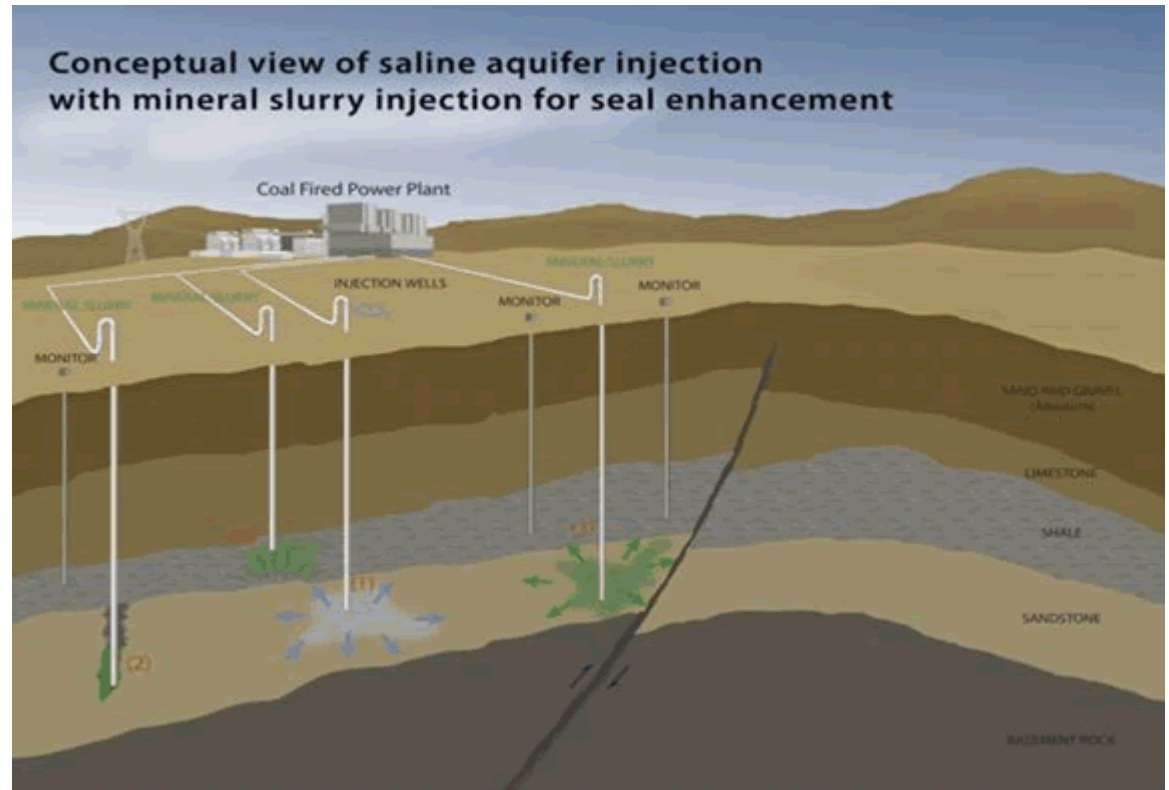
**Significance: Geological sequestration of carbon dioxide and improved oil and gas production.**



*Using infrared spectroscopy to investigate the mechanism by which carbon dioxide will be stored in coal seams, and the storage capacity of the coal seams.*

# Storing CO<sub>2</sub> in Geological Formations

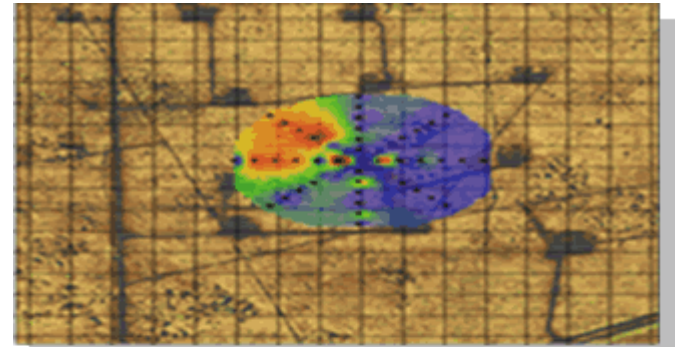
In collaboration with partners from industry, government, and academia, develop processes to capture and sequester green house gas emissions and other industrial pollutants.



# CO<sub>2</sub> Measurement, Monitoring, and Verification

Test CO<sub>2</sub> storage monitoring at Frio geological sequestration site in Texas using tracers and soil gas monitors for CO<sub>2</sub>, methane, and radon flux.

**Significance: Supports Climate Change Initiative. Evaluates methods to monitor CO<sub>2</sub> storage. Goal is refined and improved technologies.**



West Pearl Queen Tracer Tests



Frio Site



# CCS Modeling at NETL

## Capture Modeling

### Plant

- IECM
- Aspen Plus
- APECS

### Device

MFIX  
FLUENT

### Atomic Scale

VASP  
accelrys suite  
GAUSSIAN

## Sequestration Modeling

### Reservoir/coal bed

PSU-COALCOMP  
NFFLOW

## MMV Modeling

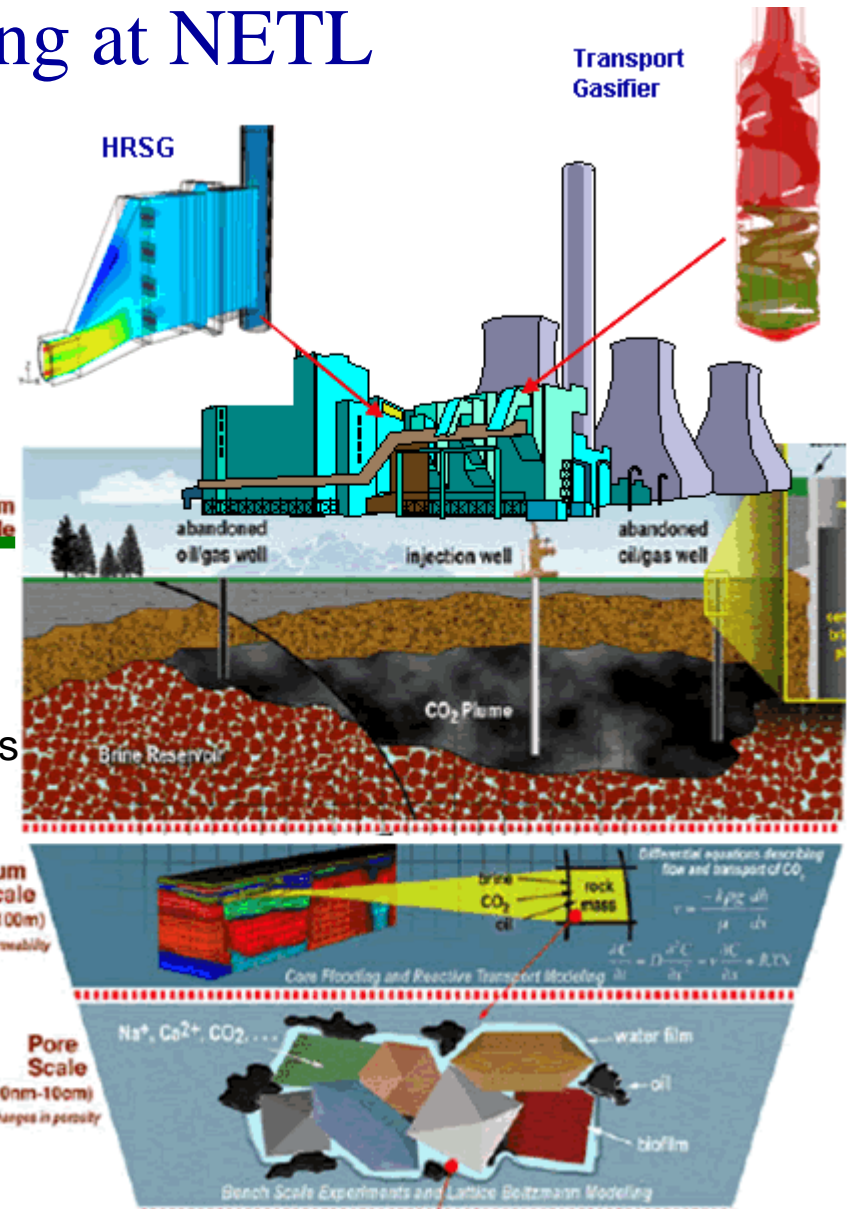
NFFLOW  
TOUGH2  
Statistical methods

## Continuum/Pore scale

FLUENT  
NETFlow

## Geomechanics

SEQURE  
ABAQUS

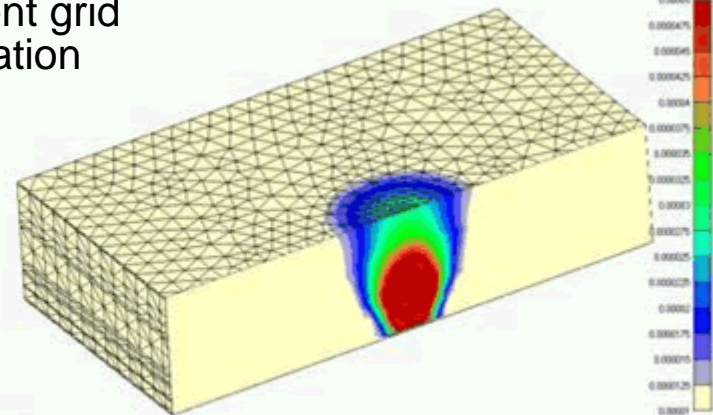


# The SEQUIRE™ geomechanical model has predicted deformations due to CO<sub>2</sub> injection.

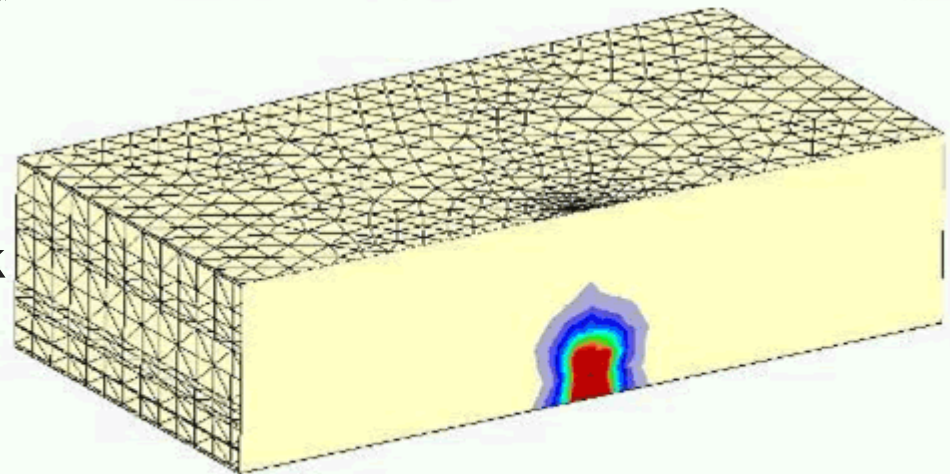
- The finite element analysis allows us to:

- Study the potential for surface deformations (tiltmeters)
- Estimate internal rock stresses, and identify high pressures zones

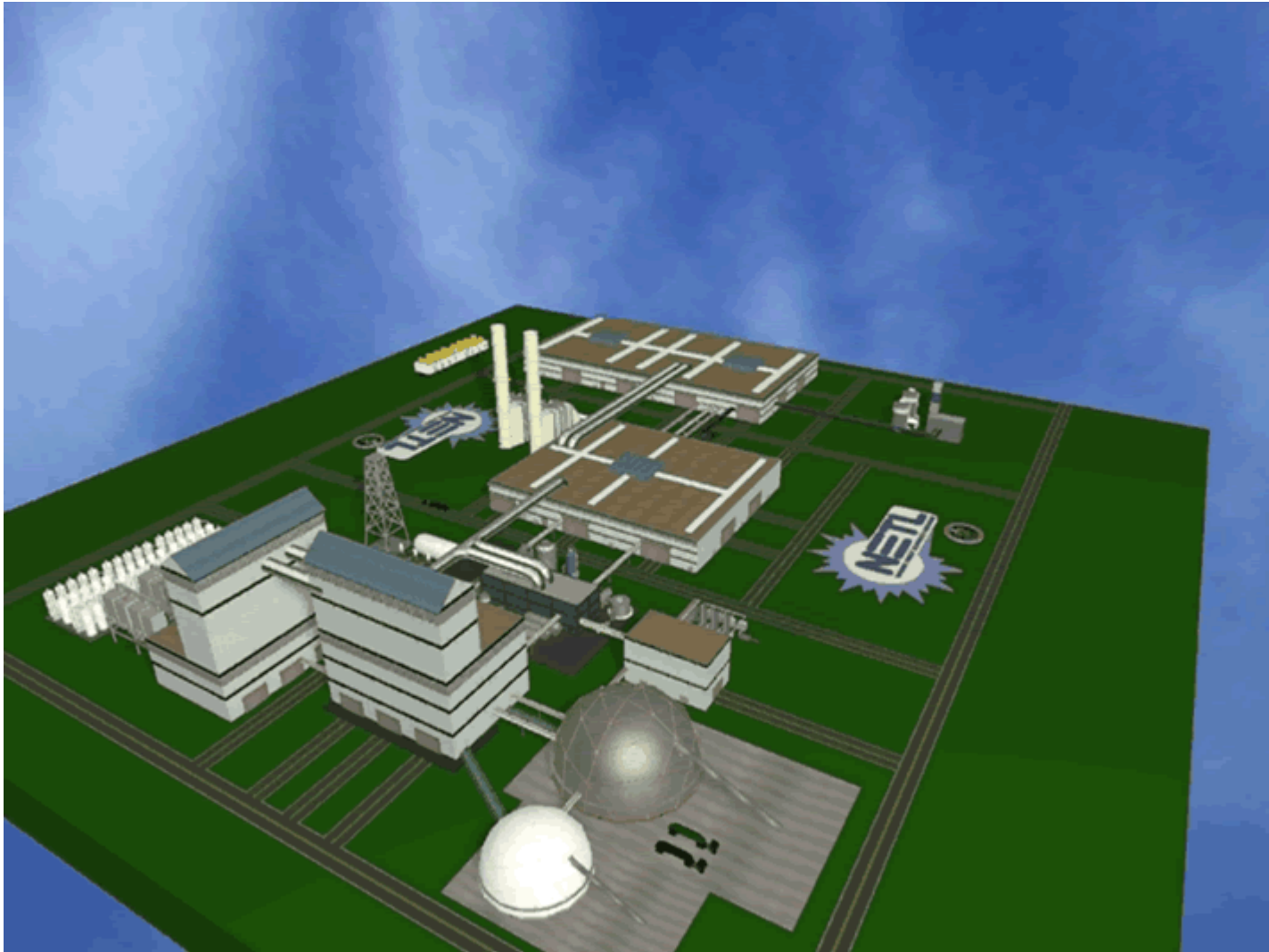
finite element grid deformation



additional stresses deformation



# Virtual Power Plant with Carbon Management



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FOSSIL ENERGY NEWS SPOTLIGHT

**New DOE Report Gauges Future Freshwater Needs for Power Plants**

DOE's National Energy Technology Laboratory has updated its groundbreaking 2004 study estimating future freshwater requirements for the U.S. thermoelectric generation sector. Drawing a much-needed regional focus, the new report identifies a dichotomy between national and local freshwater needs and pinpoints where critical water issues could develop. [Read more >](#)

OFFICE OF FOSSIL ENERGY

Ensuring that we can continue to rely on clean, affordable energy from our traditional fuel resources is the primary mission of DOE's Office of Fossil Energy. Fossil fuels supply 93% of the nation's energy, and we are working on such priority projects as pollution-free coal plants, more productive oil and gas fields, and the continuing readiness of federal emergency oil stockpiles.

Read more about:

- Fossil Energy Organization
- Business & Funding

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[www.fe.doe.gov](http://www.fe.doe.gov)

National Energy Technology Laboratory

Site Map

NETL

THE ONLY U.S. NATIONAL LABORATORY DEVOTED TO FOSSIL ENERGY TECHNOLOGY

ABOUT NETL

KEY ISSUES & MANDATES

ON-SITE RESEARCH

TECHNOLOGIES

SOLICITATIONS & BUSINESS

CAREERS & FELLOWSHIPS

NEWSROOM

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**Tackling U.S. Energy Challenges**

**Secure and Reliable Energy**

Domestic coal, oil, and natural gas resources can contribute enormously to our Nation's economic strength, energy security, and quality of life through the 21st century.

View Secure & Reliable Energy Supplies

2005 NETL Accomplishments Report

We are pleased to announce the release of NETL's [2005 Accomplishments Report](#), a summary of the result of NETL's work over the past fiscal year.

A Certification in order to ensure that the public is presented a clear understanding of the U.S. Department of Energy's perspective on the current status of mercury control technologies for coal-fired power plants and their associated costs, DOE/NETL, in cooperation with the PA Federation of Spent Mercuric Chloride, has issued the subject certification to the EPA's April 18 press release titled U.S. Department of Energy Says Mercury Control Technology Available, Costs Low; Spent Mercuric Chloride to Protect Pennsylvania's Chesapeake Bay.

NEWS & FEATURES // [All >](#)

- [Preliminary Economic Analysis of Advanced Carbon Injection \(PFI-1\) MFC](#)
- [Solicitation for "Novel Technology & Commercial Feasibility Assessments for CO2 Capture & Separation for Coal-fired & Pulverized Coal-fired Electric Generation Power Plants"](#)
- [Solicitation for "Clean, Clean Transportation Sector: Petroleum Refining Technology Commercial Deployment"](#)
- [NETL's 2005 Energy, ETL, Research & Cost Analysis](#)
- [Tax Credit Certification Guidelines](#)

EVENTS CALENDAR // [All >](#)

- [21st International Technical Conference on Coal Utilization & Fuel Systems](#)
- [2006 International Coalbed Methane Symposium](#)
- [Teaching With Confidence 2006](#)
- [Society of Petroleum Engineers 2006 Annual Technical Conference & Exhibition](#)
- [2006 Environmental Controls Conference](#)

PUBLICATIONS &

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[www.netl.doe.gov](http://www.netl.doe.gov)

