# Carbon Sequestration Science

## Focus Area
## Overview Presentation

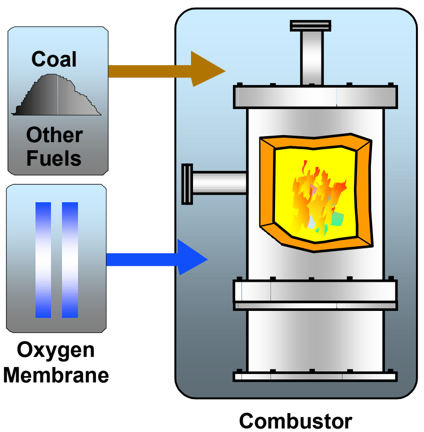
- Mission and Scope
- Program Relationships
- Scientific Challenges
- Research Plans
- Facility Plans

**July 2001**

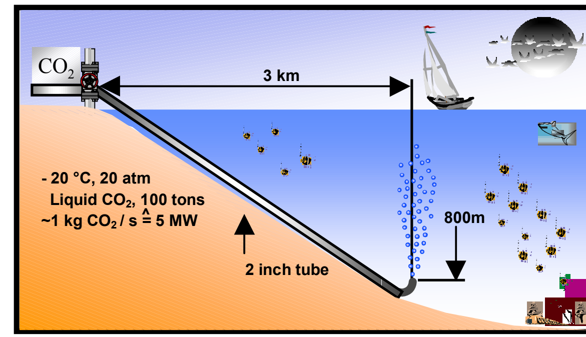
# Carbon Sequestration Science Focus Area

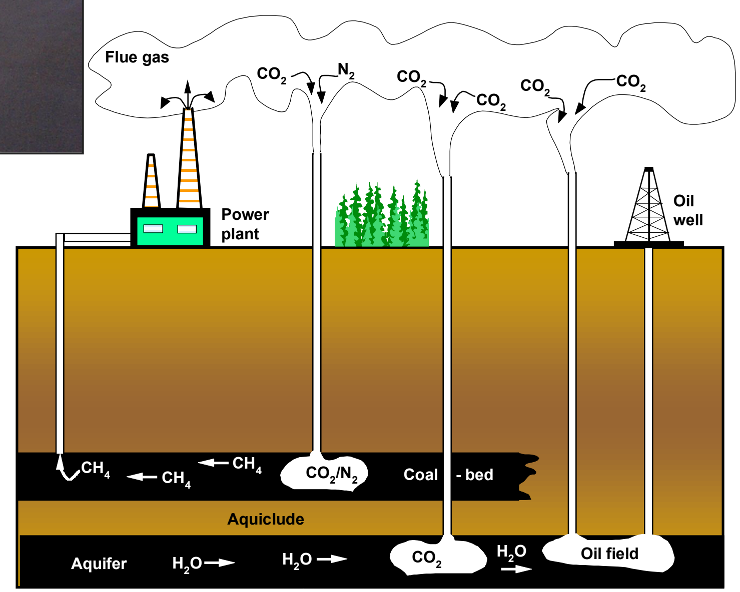
## New Projects Contribute to Sequestration Science

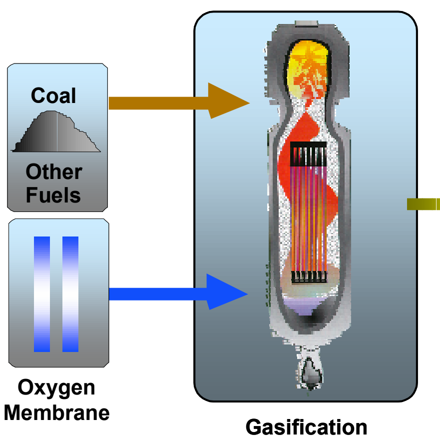
### *Virtual Simulation of $CO_2$ Capture Technologies*



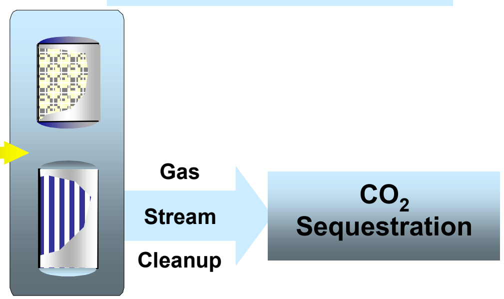

### *Systems Integration*

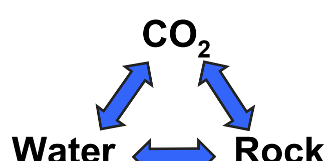



MEA $CO_2$ Capture Facility



# Carbon Sequestration Science Focus Area

## Mission

- Provide scientific basis for carbon sequestration options for large stationary sources of $CO_2$

## Goal

- Produce information that leads to development of economic and environmentally sound $CO_2$ capture and sequestration options

## Scope

- Address:
  - Low-cost capture
  - Long-term storage
  - Beneficial utilization
- Sequestration options include:
  - Geologic (coal seams, deep brine fields, oil and gas reservoirs)
  - Ocean
  - Revolutionary, innovative approaches
- Support for policy development
  - Validation and verification

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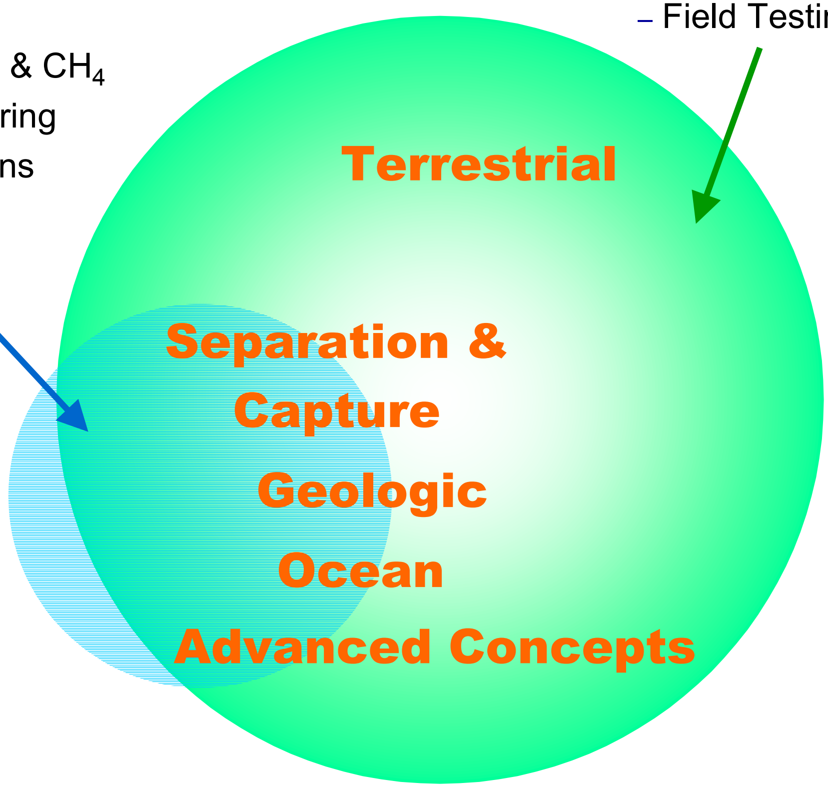
# Carbon Sequestration Science Focus Area Tasks

1 Separation and Capture
2 Oceanic Sequestration
3 Chemical Sequestration
4 Geological Sequestration
5 Geological Sequestration Modeling
6 Process Modeling and Economic Assessment

# Relationship to Office of Fossil Energy/NETL Sequestration Program

**Focus Area**
- Multi-pollutant control
- Hydrate research, $CO_2$ & $CH_4$
- Verification and monitoring
- $CO_2$/water/rock reactions

**External Sequestration Program**
- Field Testing



# Focus Area Planning and Stakeholder Input

## Research partnerships and potential collaborations

AES Corporation Albany Research Center
Alberta Research Council
Battelle Columbus
Dravo
Fluent, Inc.
IMC Chemicals
Los Alamos National Laboratory
Monterey Bay Aquarium Research Institute
Office of Science Center
United States Geological Survey
Sud Chemie

Arizona State University, Clarkson University, Pennsylvania State University, University of Akron, University of Texas, Regional Universities – Carnegie Mellon University, West Virginia University, University of Pittsburgh, and Duquesne University

Burlington Resources
Chung-Ang University
Colorado School of Mines
Dakota Gasification
Energy Information Agency
GoreTex
National Research Council, Canada
OPHIR Corporporation
Selexol

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# Scientific Challenges and Research Plans – Capture and Separation – Task 1

- **Scientific issues**
  - Energy penalties in chemical scrubbing processes
  - Effect of contaminants in gas streams
  - Current processes not suitable for all applications
  - Regenerability of sorbents
  - Degradation of amines
- **Research Plan**
  - Evolutionary and Revolutionary approaches
  - Investigate novel solvents and sorbents
    - Physical solvents for IGCC and ammonia-based solvents for flue gas
    - Dry, regenerable sorbents
      - High and low temperature applications
  - Study multipollutant control
    - $CO_2$, $SO_2$, $NO_x$, PM, Hg
- **Collaborators**
  - IMC Chemicals, AES Corp, Sud Chemie, Regional Universities

Figure 9. Effect of inlet CO2 level on CO2 breakthrough curve.

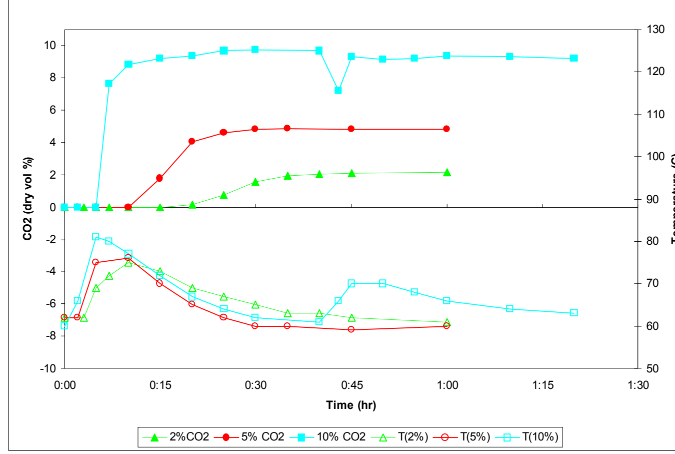
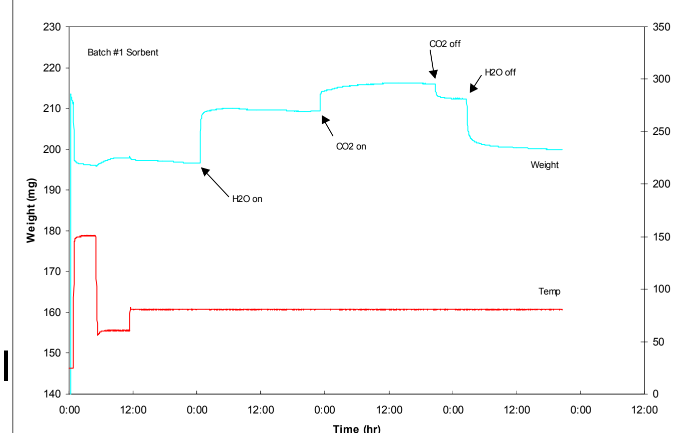



Figure 7. Typical TGA experiment (Batch #1 sorbent @ 80C absorption).

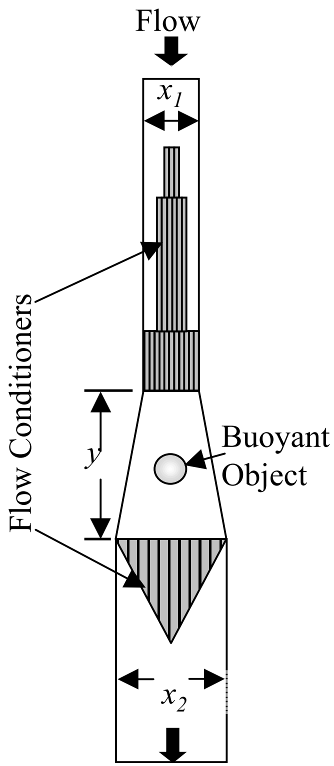


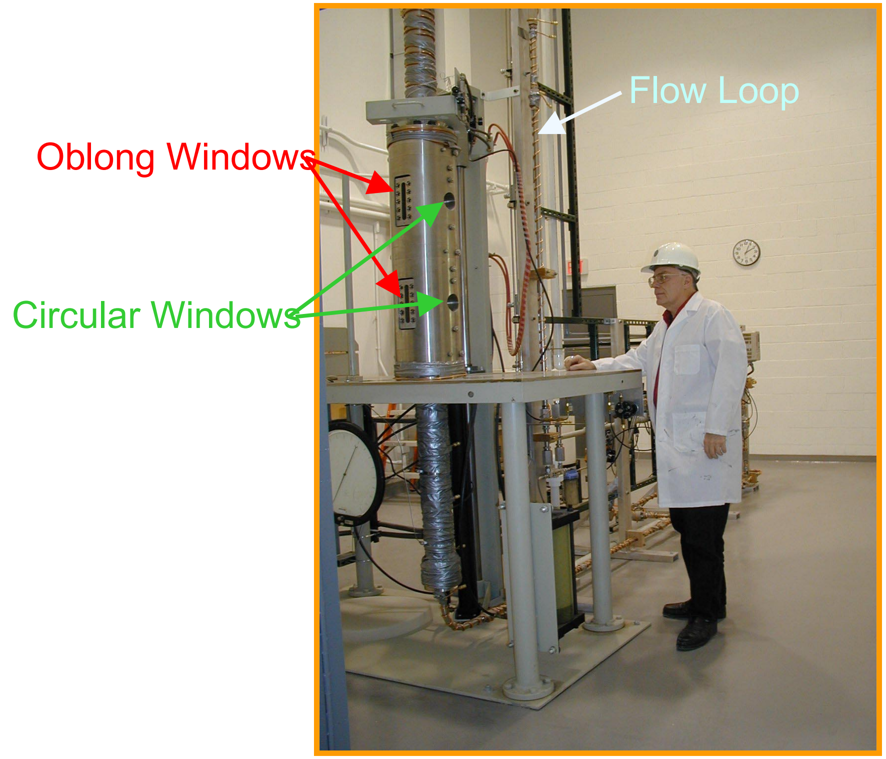
# Scientific Challenges and Research Plans - Ocean Sequestration – Task 2

- **Scientific issues**
  - Physical and chemical behavior of $CO_2$ in deep ocean
  - Impact of ice-like $CO_2$ clathrate hydrate
    - Hydrate particle density
    - Hydrate coating effect on buoyancy and dissolution of $CO_2$
    - Promoter effects
- **Approach**
  - High-pressure, lab-scale research
  - Mathematical simulations
  - Water Tunnel Facility
    - Low pressure facility for design optimization
    - High pressure facility for simulation of oceanic water column
- **Collaborations**
  - University of Pittsburgh, MBARI

**Air bubble stabilized in downward flow of water in low pressure water tunnel**

# Development of a Water Tunnel Facility



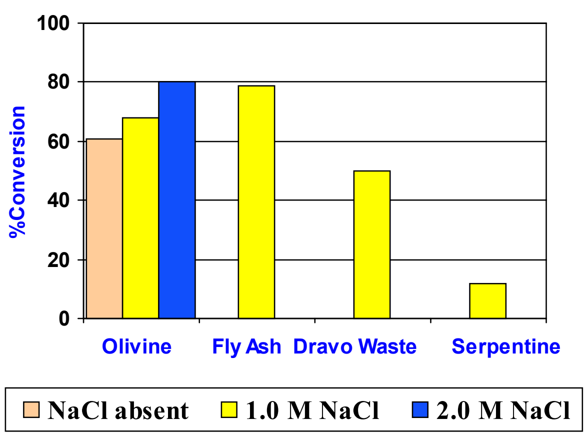

**High-Pressure Water Tunnel Facility in newly renovated laboratory**

# Scientific Challenges and Research Plans - Chemical Sequestration – Task 3

**Kinetics - heat, pressure, stirring requirements for mineral carbonation reactions**

- **Mineral carbonation of Mg-rich mineral silicates**
- **Scientific issues**
  - Kinetics are slow, requires elevated temperatures and pressures as well as fine grinding

**Effect of Solution Chemistry & Reactants on the Extent of Mineral Carbonation**




**Summary of Carbonation Experiments**

| Reactant | $HCO_3^-$ Solution | Pct.Conv., $MgCO_3$ |
|---|---|---|
| Coal Fly Ash | $Na_2CO_3/NaHCO_3/NaCl$ | 80 |
| Olivine | $Na_2CO_3/NaHCO_3/NaCl$ | 70 |
| Dravo Waste | $Na_2CO_3/NaHCO_3/NaCl$ | 50 |
| Serpentine | $Na_2CO_3/NaHCO_3/NaCl$ | 12 |

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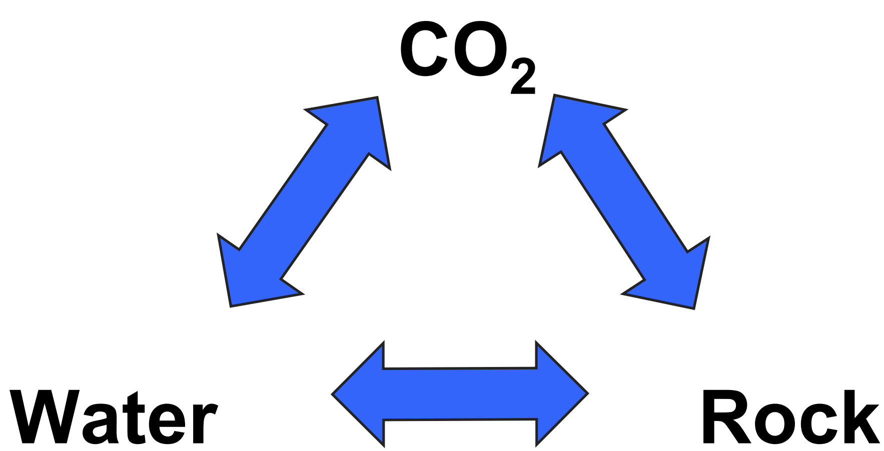
# Scientific Challenges and Research Plans - Chemical Sequestration – Task 3

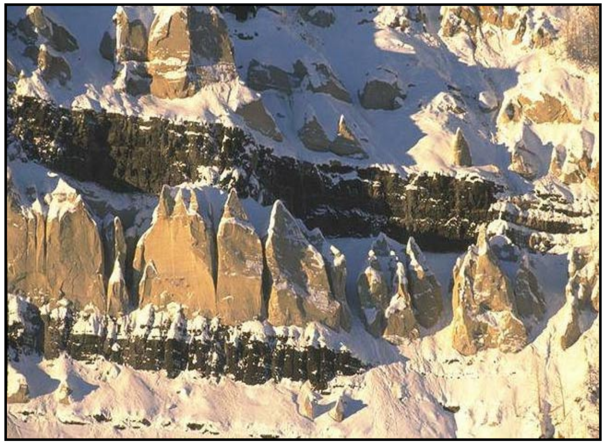
- **Approach**
  - Find other sources of Ca/Mg – rich feedstocks that are waste materials and explore the possibility of using them
  - Study carbonation of mixtures of waste matter and mineral Mg silicates
  - Modify solution chemistry of the mineral carbonation reaction by adding bicarbonate and Group I hydroxides
  - Increase mineral porosity using steam and/or NaOH activation
- **Collaborators**
  - Regional Universities, LANL, Albany Research Center, Arizona State University



# Scientific Challenges and Research Plans - Geological Sequestration – Task 4

- **Unmineable coal seams, deep saline aquifers, active and depleted oil and gas fields, including natural gas hydrates**

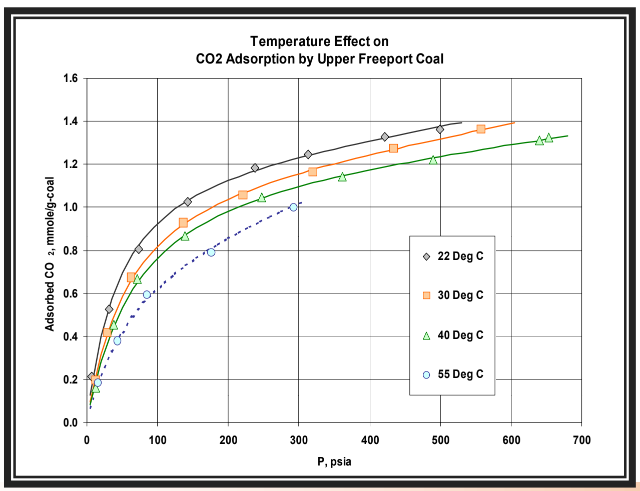
- **Scientific issues**
  - Understanding viscous fingering, gravitational segregation, permeability heterogeneity
  - Understanding-multiphase flow
  - Mineral dissolution and precipitation and their effects on permeability
  - Better defining the kinetics of $CO_2$/water/rock reactions and the factors that influence it



# Scientific Challenges and Research Plans - Geological Sequestration – Task 4

- **Unmineable coal seams, deep saline aquifers, active and depleted oil and gas fields, including natural gas hydrates**

- **Scientific issues**
  - Better understanding of those factors that affect the capacity of a coal seam to absorb $CO_2$ and the stability of the formation
  - Defining factors that determine the optimum conditions for sequestration in each geological formation
  - Developing means to verify and monitor the integrity of sequestration sites
  - Gain increased understanding of the structure of $CO_2$ hydrates




**Summary of Coals Studied to Date**

| Coal | Rank | Heat of Adsorption |
|---|---|---|
| Upper Freeport | Med. Vol. Bit. | 5.65 +/- 0.46 Kcal/mol |
| Illinois No. 6 | High Vol. Bit. | 3.47 +/- 0.20 Kcal/mol |

- **Conclusion:** The heat of adsorption of $CO_2$ is about the same as that of a hydrogen bond. The $CO_2$ is considered to be physically adsorbed. In the pressure range studied, the mechanism of adsorption appears to be physical adsorption into both micro- and meso-pores.

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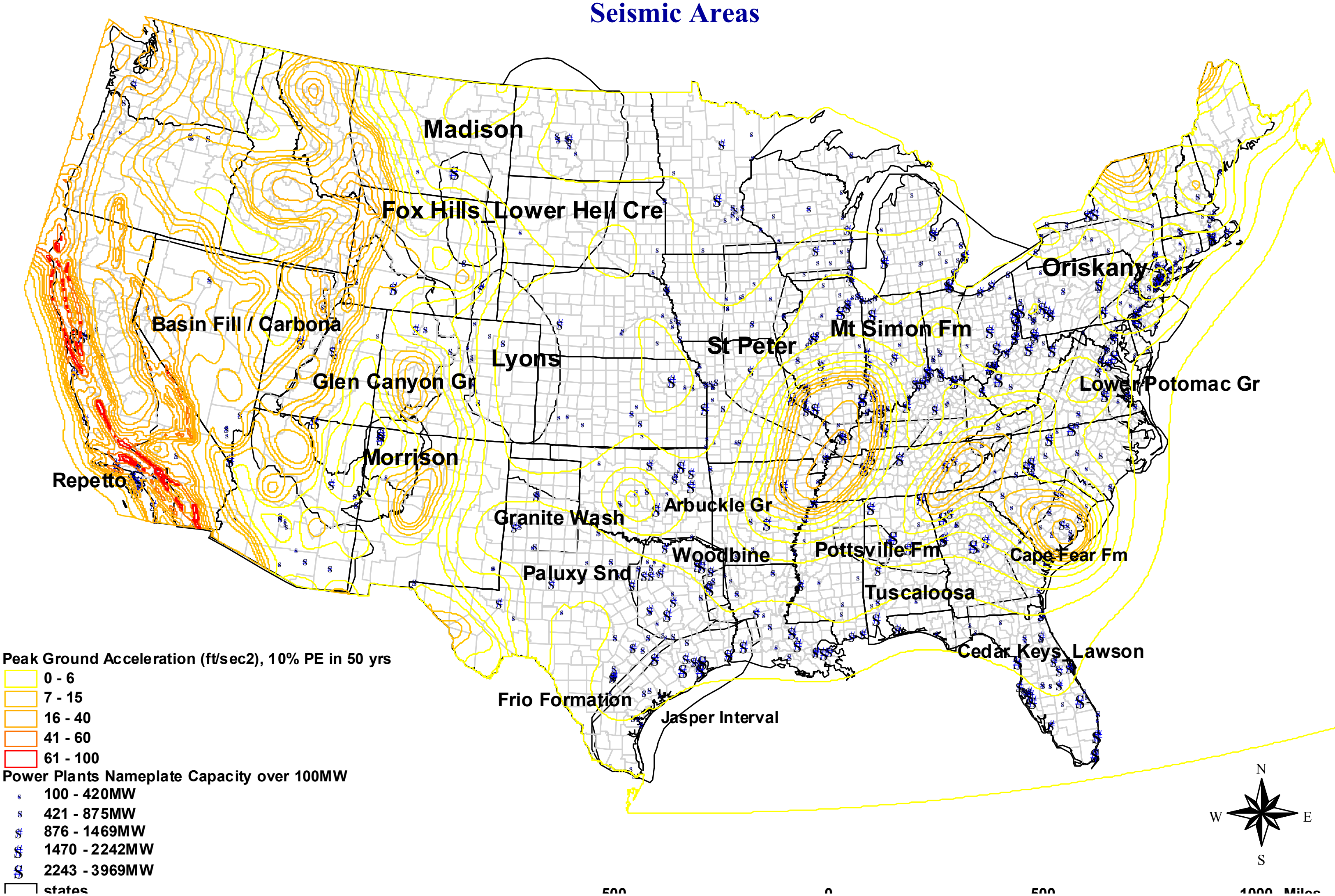
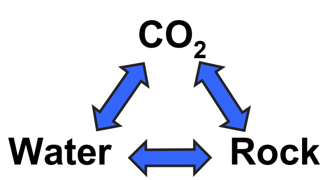
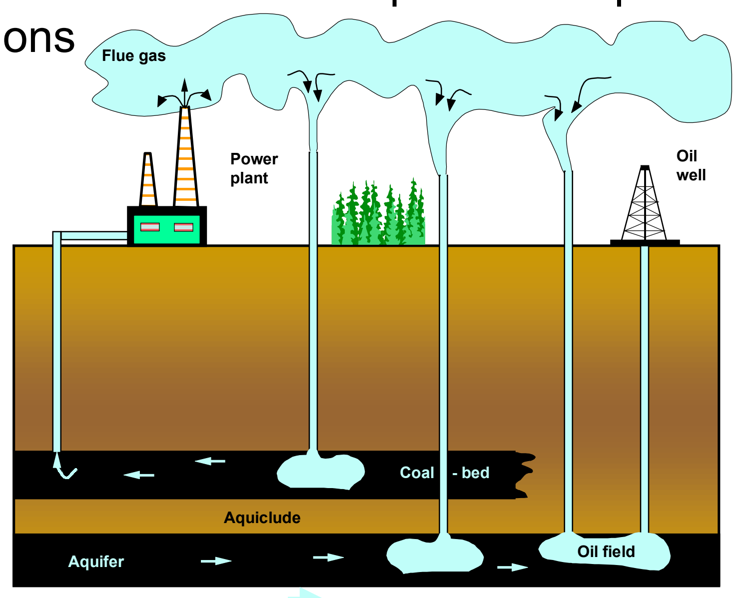
# Geologic Formations
# Conventional Electric Power Generation Facilities >= 100MW
# Seismic Areas



# Scientific Challenges and Research Plans - Geological Sequestration – Task 4

- **Approach**
  - Use phase/volume measurements and high pressure flow calorimetry to study phase behavior and heats of mixing
  - Experiment and model two-phase flow through porous media – measure flow patterns
  - Begin detailed experimental and modeling study of $CO_2$/water/rock chemistry
  - Measure and model adsorption isotherms and heats of sorption/desorption for Argonne coals under various conditions
  - Begin developing ground based monitoring systems for tracers and geological gases



# Scientific Challenges and Research Plans - Geological Sequestration – Task 4

## Potential Collaborators

**Clarkson University, Pennsylvania State University, Colorado School of Mines, University of Texas, Chung-Ang University**

**Regional Universities – Carnegie Mellon University, West Virginia University, University of Pittsburgh, and Duquesne University**

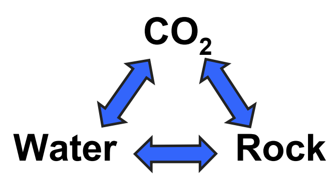
**Battelle Columbus**

**Burlington Resources**

**Fluent, Inc.**

**GoreTex**

**OPHIR Corporporation**




**Alberta Research Council**

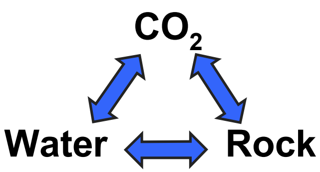
**United States Geological Survey**

**Los Alamos National Laboratory**

**National Research Council, Canada**

# Scientific Challenges and Research Plans - Geological Sequestration Modeling – Task 5

- **Unmineable coal seams, deep saline aquifers, active and depleted oil and gas fields, including natural gas hydrates**




- **Scientific issues**
  - Understanding viscous fingering, gravitational segregation, permeability heterogeneity
  - Understanding-multiphase flow
  - Mineral dissolution and precipitation and their effects on permeability
  - Better defining the kinetics of $CO_2$/water/rock reactions and the factors that influence it
  - Better understanding of those factors that affect the capacity of a coal seam to absorb $CO_2$ and the stability of the formation
  - Defining factors that determine the optimum conditions for sequestration in each geological formation
  - Gain increased understanding of the structure of $CO_2$ hydrates

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# Scientific Challenges and Research Plans - Geological Sequestration Modeling – Task 5

- **Approach**
  - Combine experiments and modeling with traditional methods of petroleum engineering
    - An Iterative interaction between computer simulation and lab experiments
  - Obtain existing models and codes to identify desirable traits that make them good candidates for revision to include sequestration of $CO_2$
    - University of Texas reservoir simulator developed by Gary Pope
    - SOMINEQ – USGS code that models $CO_2$/water/rock interactions
    - EQ6 – code that models $CO_2$/water/rock interactions
    - ACS model for complex ionic equilibria
    - Western Research Institute model for enhanced methane recovery from coal seams
    - FRACGEN and NFFLOW – geological and fluid flow models
    - EIA gas reservoir models
    - PROSIM – $CO_2$/Brine reaction simulator

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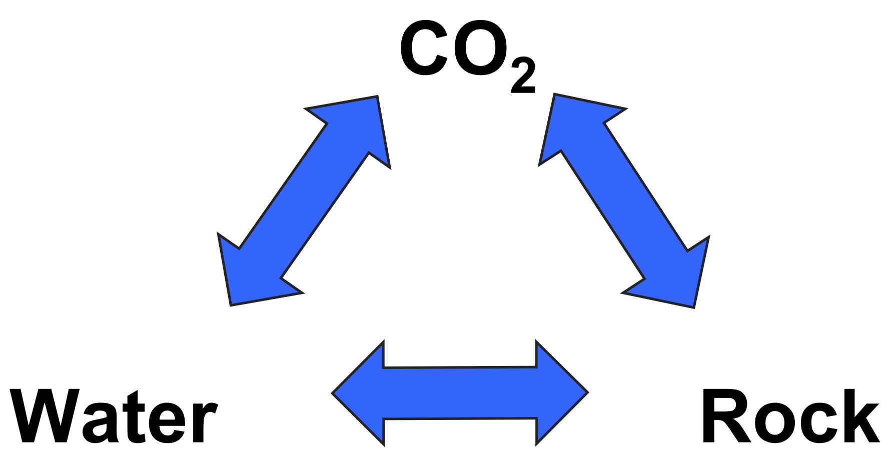
# Scientific Challenges and Research Plans - Geological Sequestration Modeling – Task 5

- **Approach continued**
  - Estimate manpower/resources to amend the codes to include a representation of sequestration in gas, oil, brine and coal fields
  - Begin an iterative set of lab/modeling experiments
  - Revise several codes to include $CO_2$ sequestration



# Scientific Challenges and Research Plans - Geological Sequestration Modeling – Task 5

## Potential Collaborations

Clarkson University, Pennsylvania State University, University of Texas, Chung-Ang University

Regional Universities – Carnegie Mellon University

Alberta Research Council

United States Geological Survey

Energy Information Agency

Battelle Columbus

Western Research Institute

Fluent, Inc.

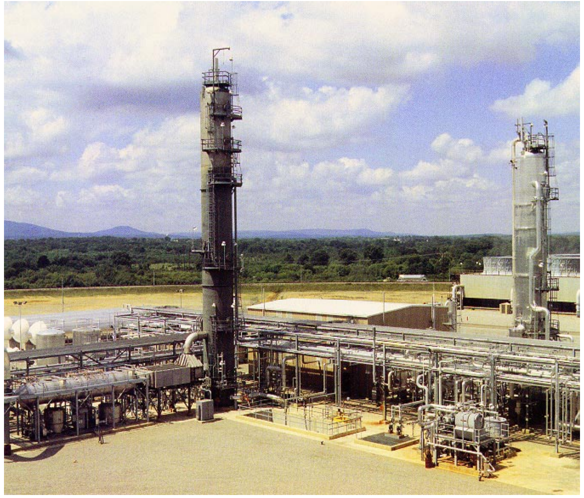
# Scientific Challenges and Research Plans -Process Modeling and Economic Assessment – Task 6

- **Scientific/Technical Issues**
  - What are the economics of existing $CO_2$ capture processes
  - What are the most inefficient steps and process points in each existing capture technology
  - What new technological innovations could be used to improve these inefficient steps
  - How much of an impact will each incorporated innovation make

# Scientific Challenges and Research Plans -Process Modeling and Economic Assessment – Task 6

# Scientific Challenges and Research Plans -Process Modeling and Economic Assessment – Task 6

- **Approach**
  - Using ASPEN and variations thereof, model the existing capture plants
    - AES Corp. – Cumberland, MD
    - Rectisol – Dakota Gasification
  - Convene group of experts from industry, academia and government – incorporate newest technological innovations into the models, determine effects



# Scientific Challenges and Research Plans -Process Modeling and Economic Assessment – Task 6

## Potential Collaborations

IMC Chemicals

AES Corp.

Dakota Gasification

Selexol

# Facility Plans

- **Capture research**
  - Modular facility
    - Advanced instrumentation and diagnostics
- **Geologic sequestration simulation**
  - Multipurpose facility for simulating various geologic formations
    - Highly instrumented, advanced imaging
- **Oceanic sequestration research**
  - High pressure water tunnel
    - Under construction
    - Machine vision, advanced imaging
- **Integrated carbon sequestration research facility**
  - In initial planning stage

**High-Pressure Water Tunnel Facility**

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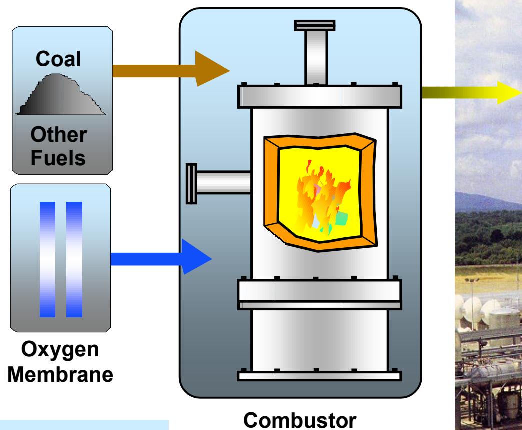
# Carbon Sequestration Science Focus Area

## New Projects Contribute to Sequestration Science

*Virtual Simulation of $CO_2$ Capture Technologies*

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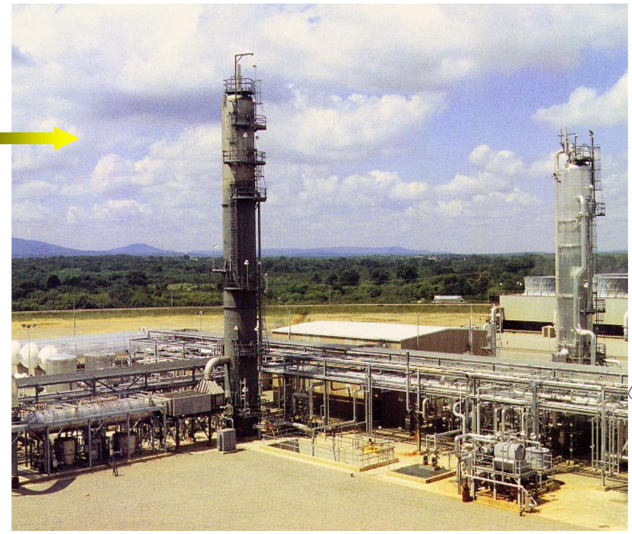
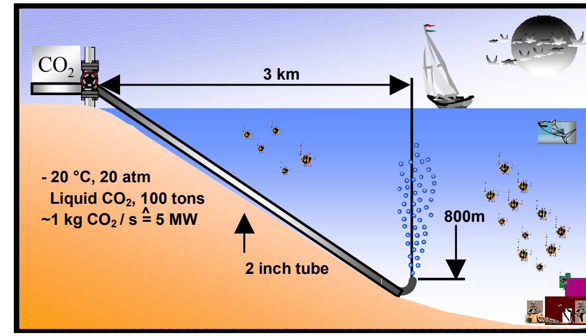
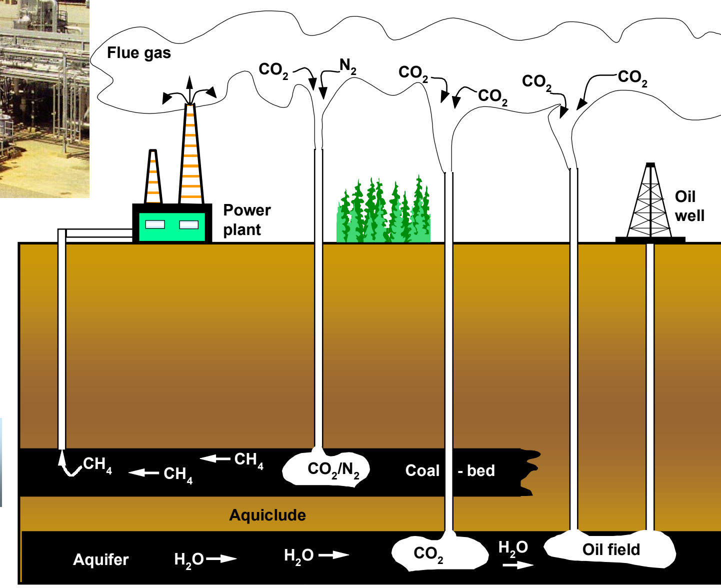


MEA $CO_2$ Capture Facility




*$O_2$ / $CO_2$ Modeling*