NATIONAL ENERGY TECHNOLOGY LABORATORY

Accelerating Carbon Capture and Storage Technology Development with the help of Modeling and Simulation

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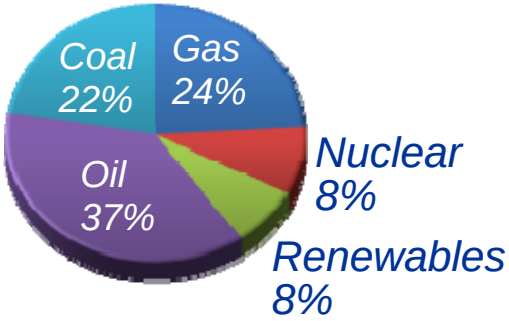
2011 Fall Creek Falls Conference, Gatlinburg, TN, September 14-16, 2011.

Energy Demand 2008

Energy Demand 2035

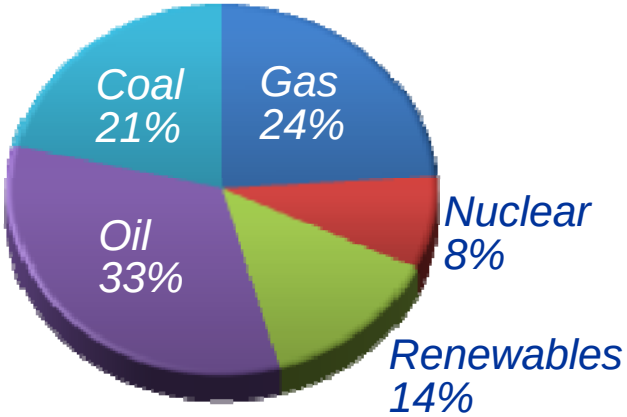
100 QBtu / Year
84% Fossil Energy



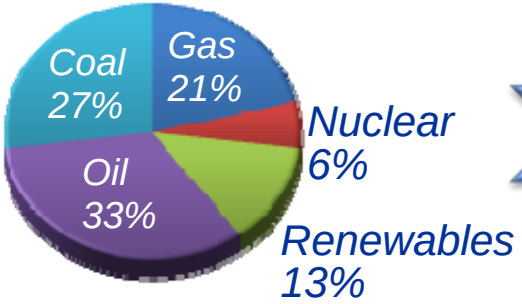
+ 14%

United States

114 QBtu / Year
78% Fossil Energy



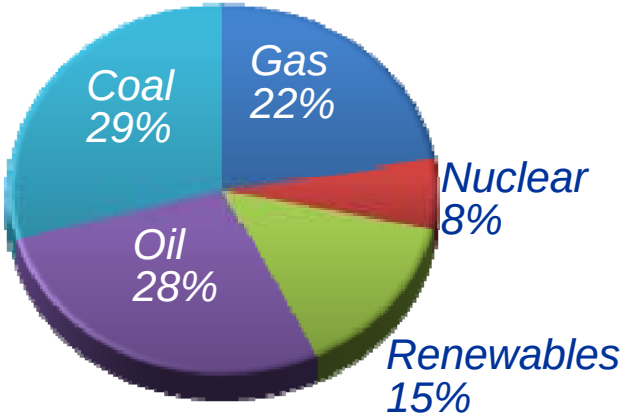
487 QBtu / Year
81% Fossil Energy



+ 47%

World

716 QBtu / Year
79% Fossil Energy



U.S. data from EIA, Annual Energy Outlook 2011; World data from IEA, World Energy Outlook 2010, Curren Policies Scenario

Pathways to CO_2 Emission Reduction

- **Energy efficiency (14 $GtCO_2e/yr$)[1]**
  - Vehicles, Buildings, industrial equipment
- **Low-carbon energy supply (12 $GtCO_2e/yr$)**
  - Wind, Nuclear, Solar Energy
  - Biofuels for transportation
  - Fossil fuels with CCS
- **Terrestrial carbon (12 $GtCO_2e/yr$)**
  - Reforesting, halting deforestation
  - CO2 sequestration in soils through changing agricultural practices
- **Behavioral change (~4 $GtCO_2e/yr$)**

1. CO_2 Reduction opportunities by 2030 from Pathways to a Low-Carbon Economy, McKinsey & Company, 2009.

What is Carbon Capture and Storage?

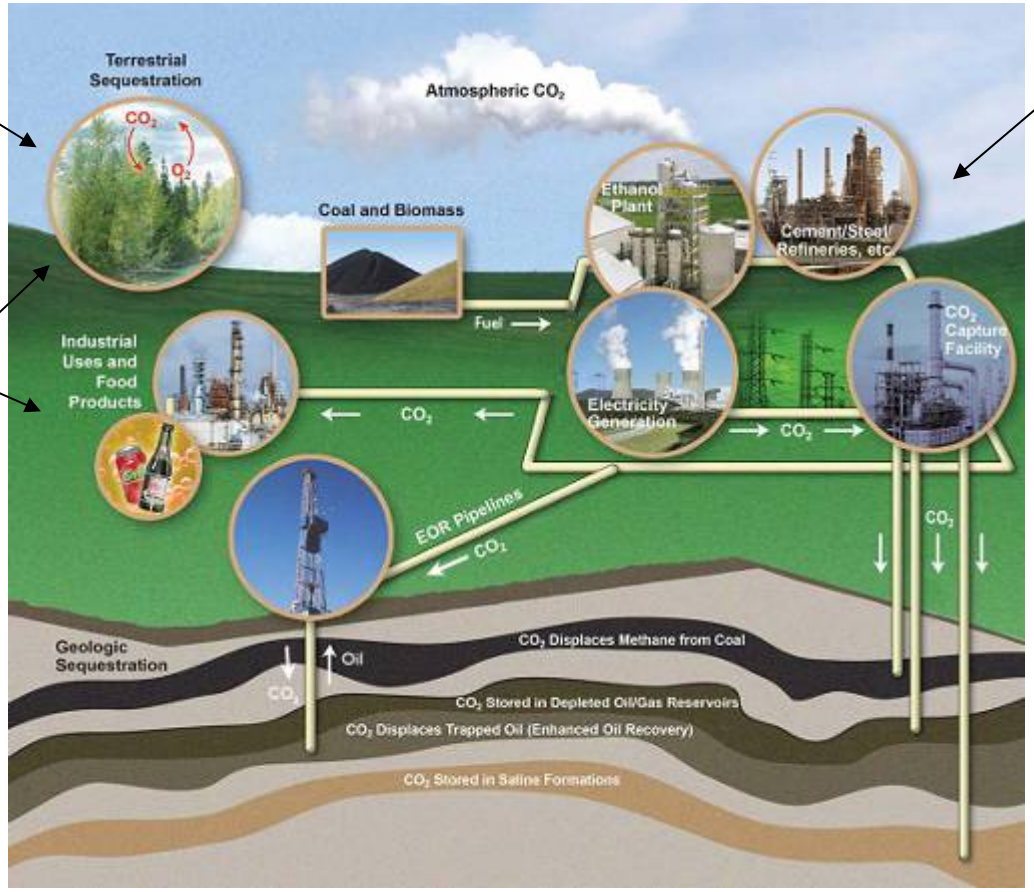
Capture and storage of CO_2 and other Greenhouse Gases that would otherwise be emitted to the atmosphere

Terrestrial Capture

CO_2 absorbed from air

Terrestrial Storage

Trees, grasses, soils



Point Source Capture

Power Plants

Ethanol Plants

Cement, Steel, Refineries

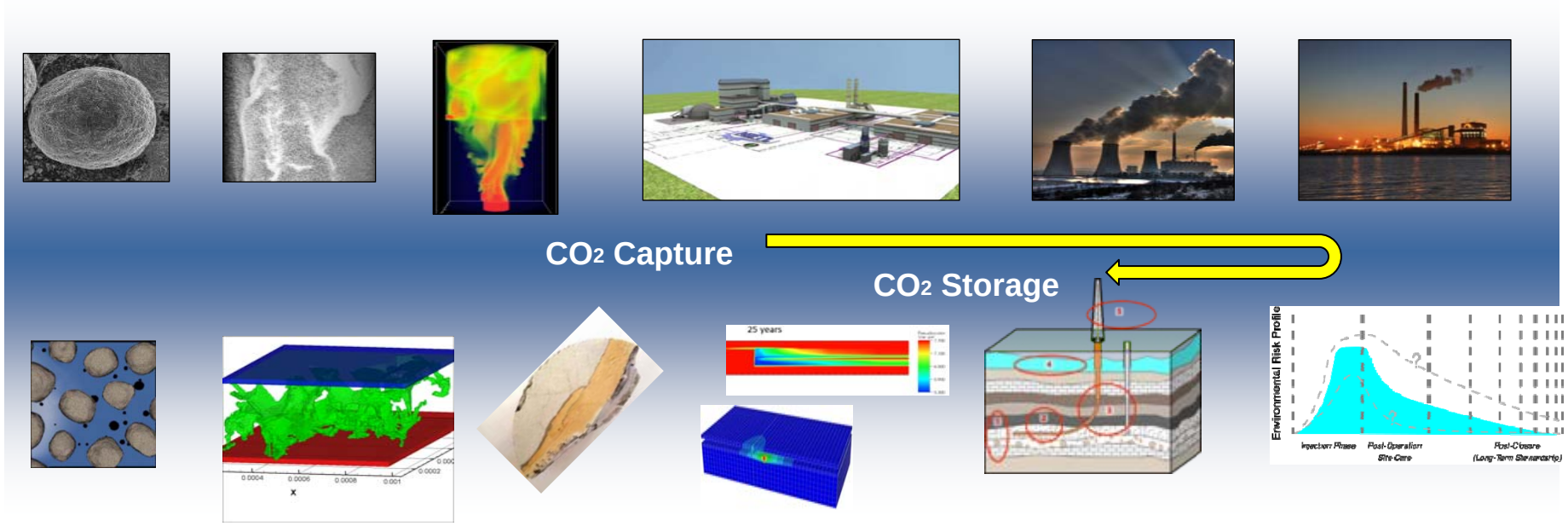
Natural Gas Processing

Geologic Storage

- ***saline formations***
- ***depleted oil/gas***
- ***unmineable coal***
- ***other: basalts, shales***

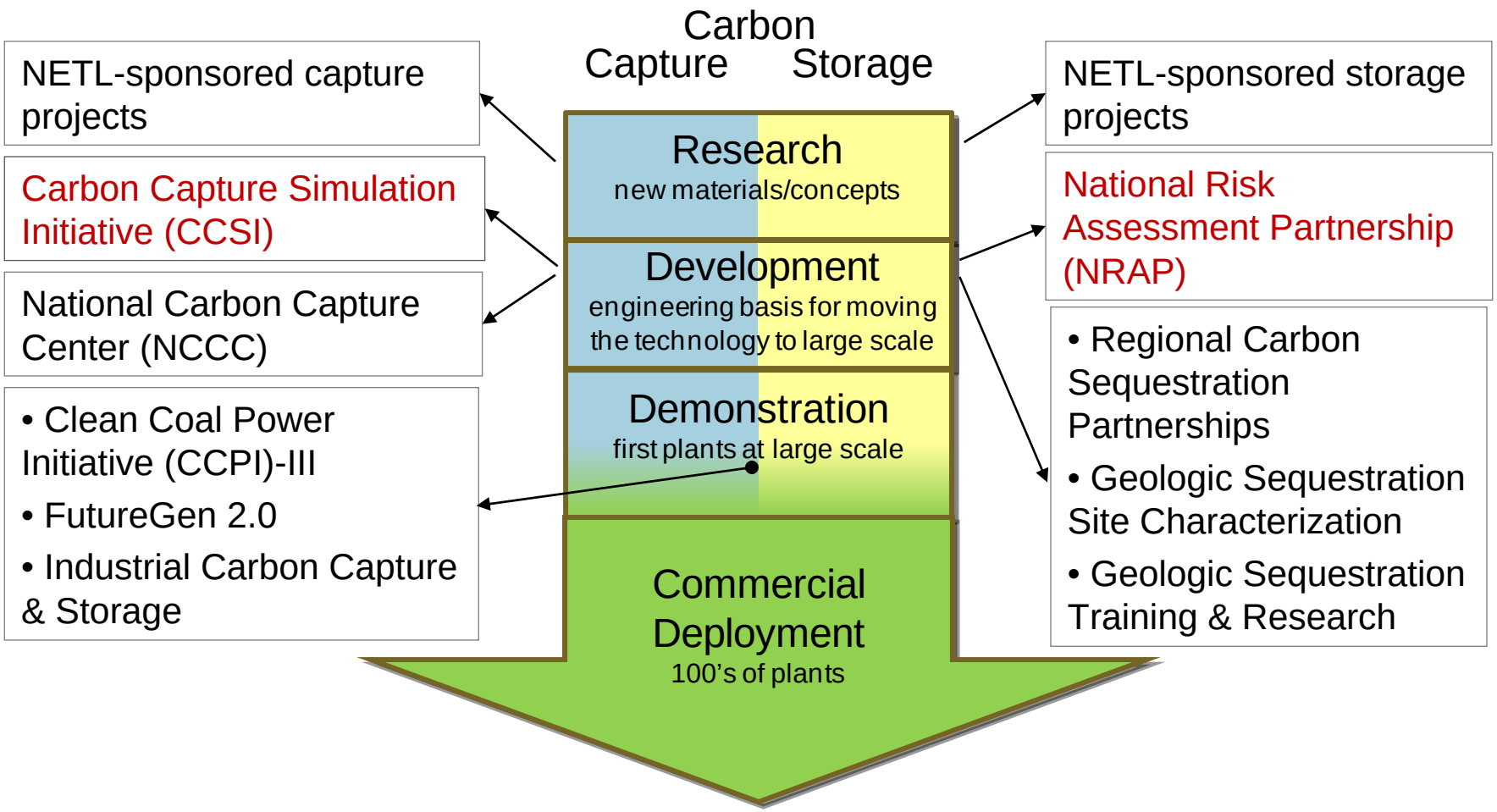
DOE-FE is leveraging science-based predictive capabilities to accelerate deployment of CCS

Carbon Capture Simulation Initiative (CCSI)



National Risk Assessment Partnership (NRAP)

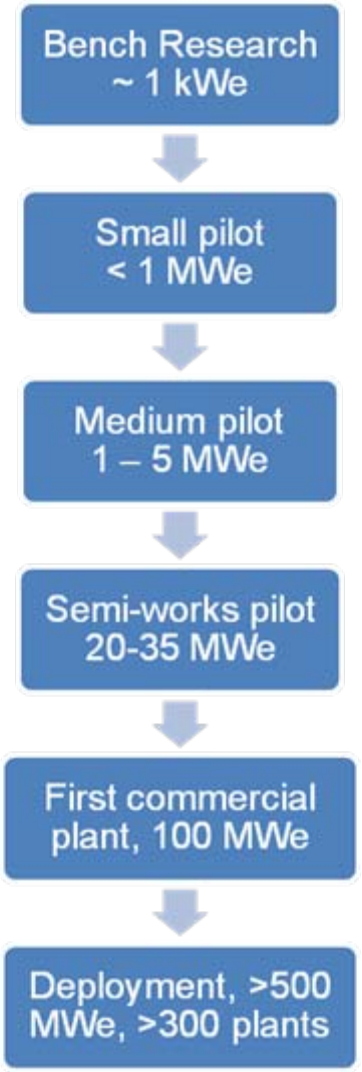
CCSI and NRAP on DOE CCS RD&D roadmap



http://www.netl.doe.gov/publications/press/2011/110106-DOE-NETL_CO2_Capture_and_Storage_RDD_Roadmap.html

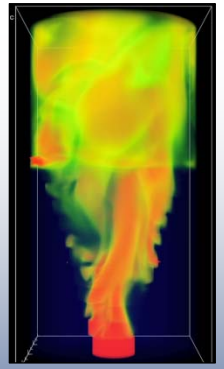
Carbon capture challenge

- **The traditional pathway from discovery to commercialization of energy technologies can be quite long, i.e., ~ 2-3 decades**
- **President's plan requires that barriers to the widespread, safe, and cost-effective deployment of CCS be overcome within 10 years**
- **To help realize the President's objectives, new approaches are needed for taking CCS concepts from lab to power plant, quickly, and at low cost and risk**
- **CCSI will accelerate the development of CCS technology, from discovery through deployment, with the help of science-based simulations**



CCSI
Carbon Capture Simulation Initiative

CCSI will develop M&S tools to accelerate the commercialization of CCS



Identify promising concepts → Reduce the time for design & troubleshooting → Quantify the technical risk, to enable reaching larger scales, earlier → Stabilize the cost during commercial deployment

National Labs

Berkeley Lab
Pacific Northwest National Laboratory
NETL
Los Alamos National Laboratory EST. 1943
Lawrence Livermore National Laboratory

Academia

Carnegie Mellon
Virginia Tech
Penn State 1855
Princeton University
West Virginia University
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Industry

ADA Environmental Solutions
Ameren
B&W
Babcock Power Inc.
Air Products
Alstom
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GE
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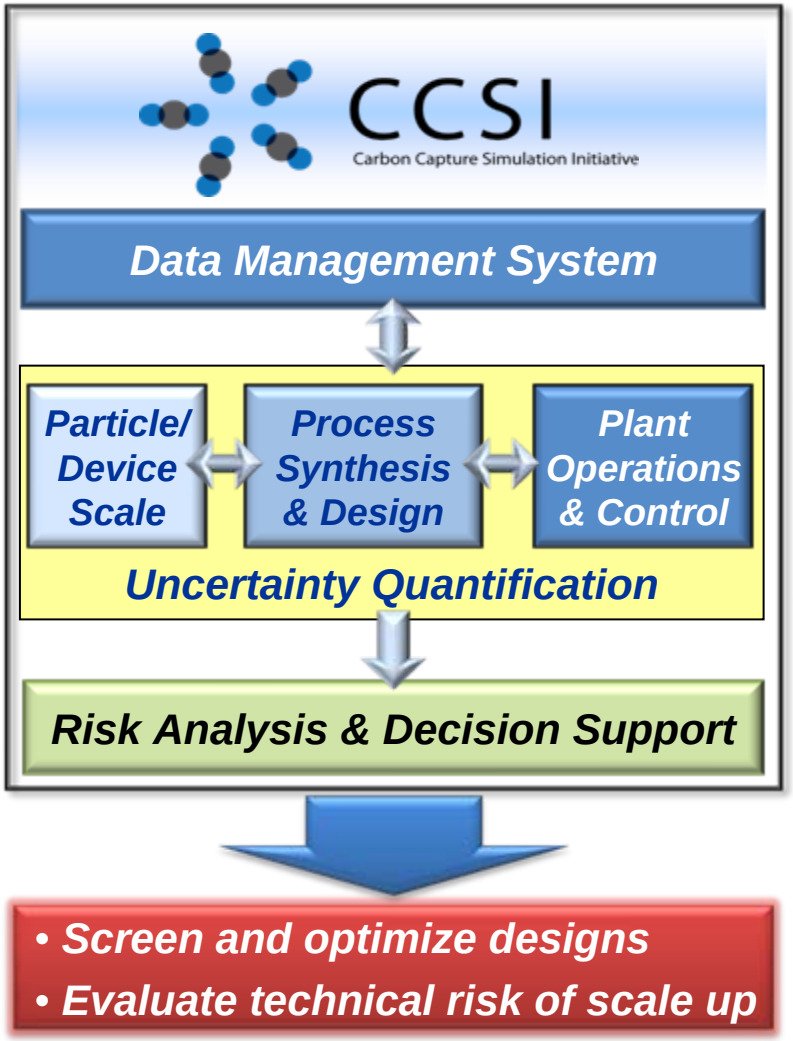
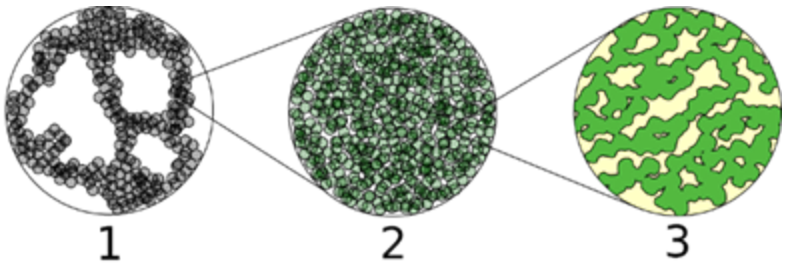
Southern California Edison An Edison International Company San Onofre Nuclear Generating Station
Southern Company
Chevron
Eastman
EPRI Electric Power Research Institute
WorleyParsons resources & energy
URS

Toolset will integrate M&S with uncertainty quantification & technical risk analysis



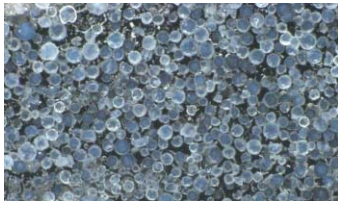
Particle-scale models describe CO_2 uptake kinetics

- Assimilate the fundamental thermo-chemical data into a form that can be used by device and process models
- Models range from detailed single particle scale reaction-diffusion models to ROMs

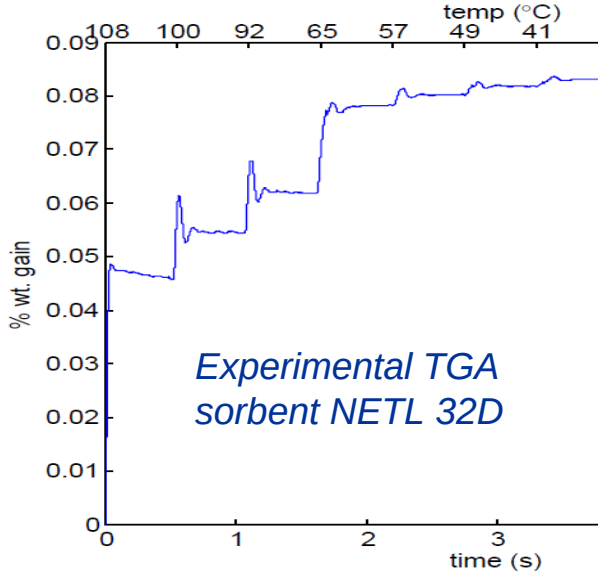


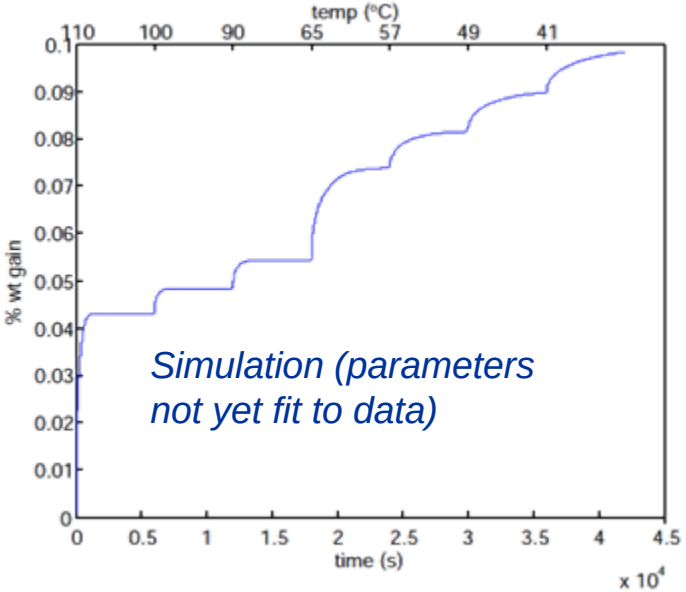
$$R_2NH + CO_2 \rightleftharpoons R_2NH^+ : CO_2^-$$
$$R_2NH^+ : CO_2^- + R_2NH \rightleftharpoons R_2NH_2^+ + R_2NCO_2^-$$

zwitterion mechanism (anhydrous)



PEI on CARiACT Q10 (100 to 350 µm dia.)

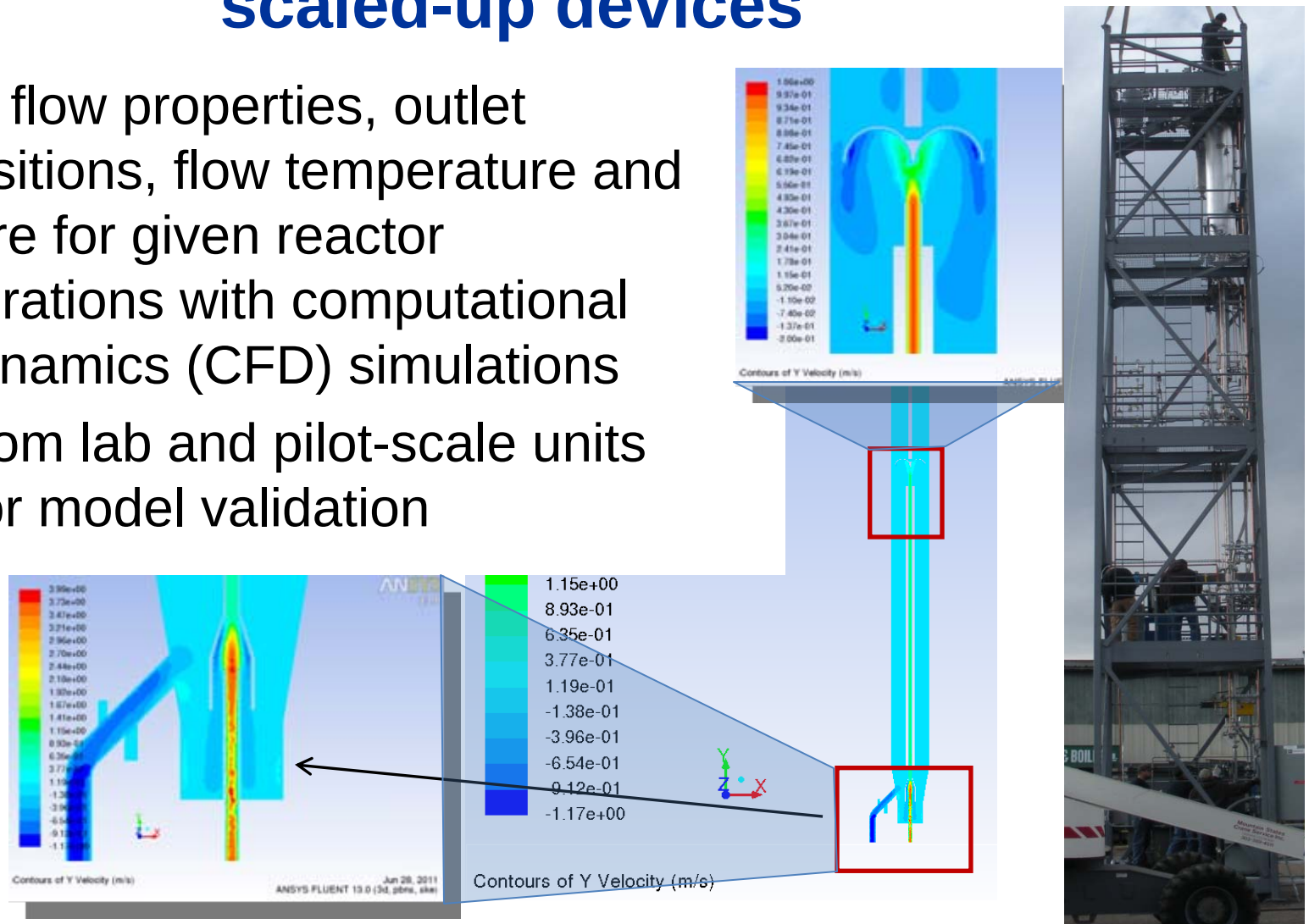




Validation of PEI-Silica sorbent reaction model

CFD models predict the performance of scaled-up devices

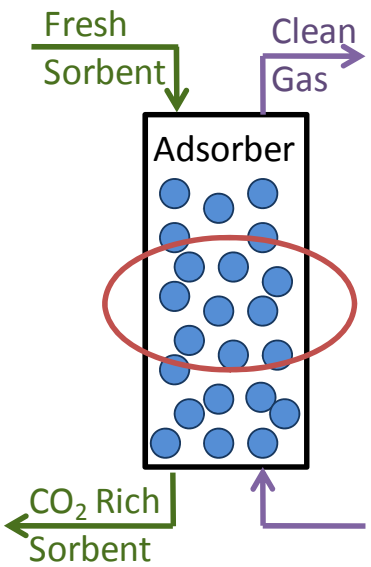
- Predict flow properties, outlet compositions, flow temperature and pressure for given reactor configurations with computational fluid dynamics (CFD) simulations
- Data from lab and pilot-scale units used for model validation

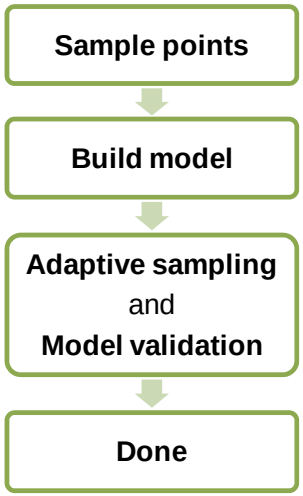


Validation of adsorber model with ADA-ES 1 kWe pilot-scale data

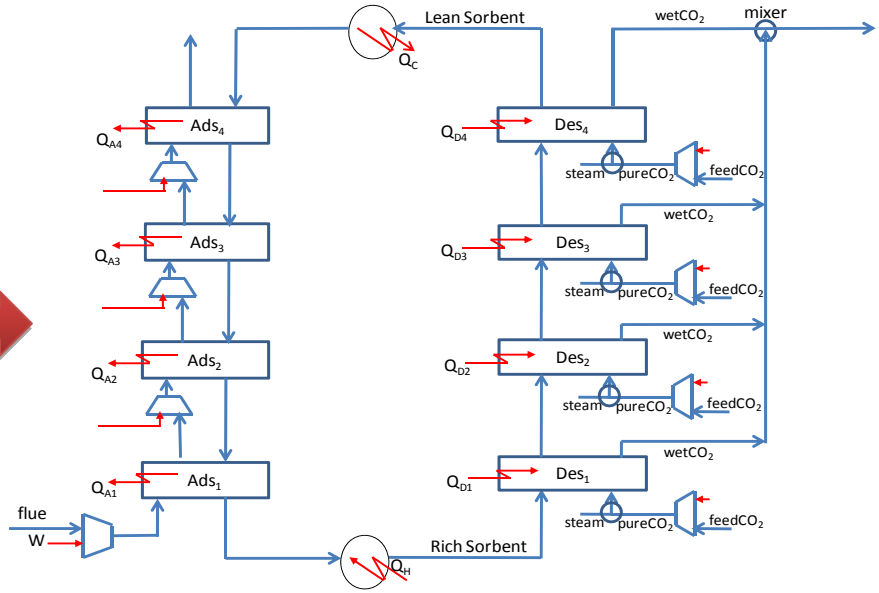
Process simulation for optimizing design and reducing costs and risk of scale-up

- Develop capabilities for process synthesis, design and optimization for carbon capture technologies
- The integrated multi-scale design, scale-up, and risk analysis will facilitate retrofitting existing plants



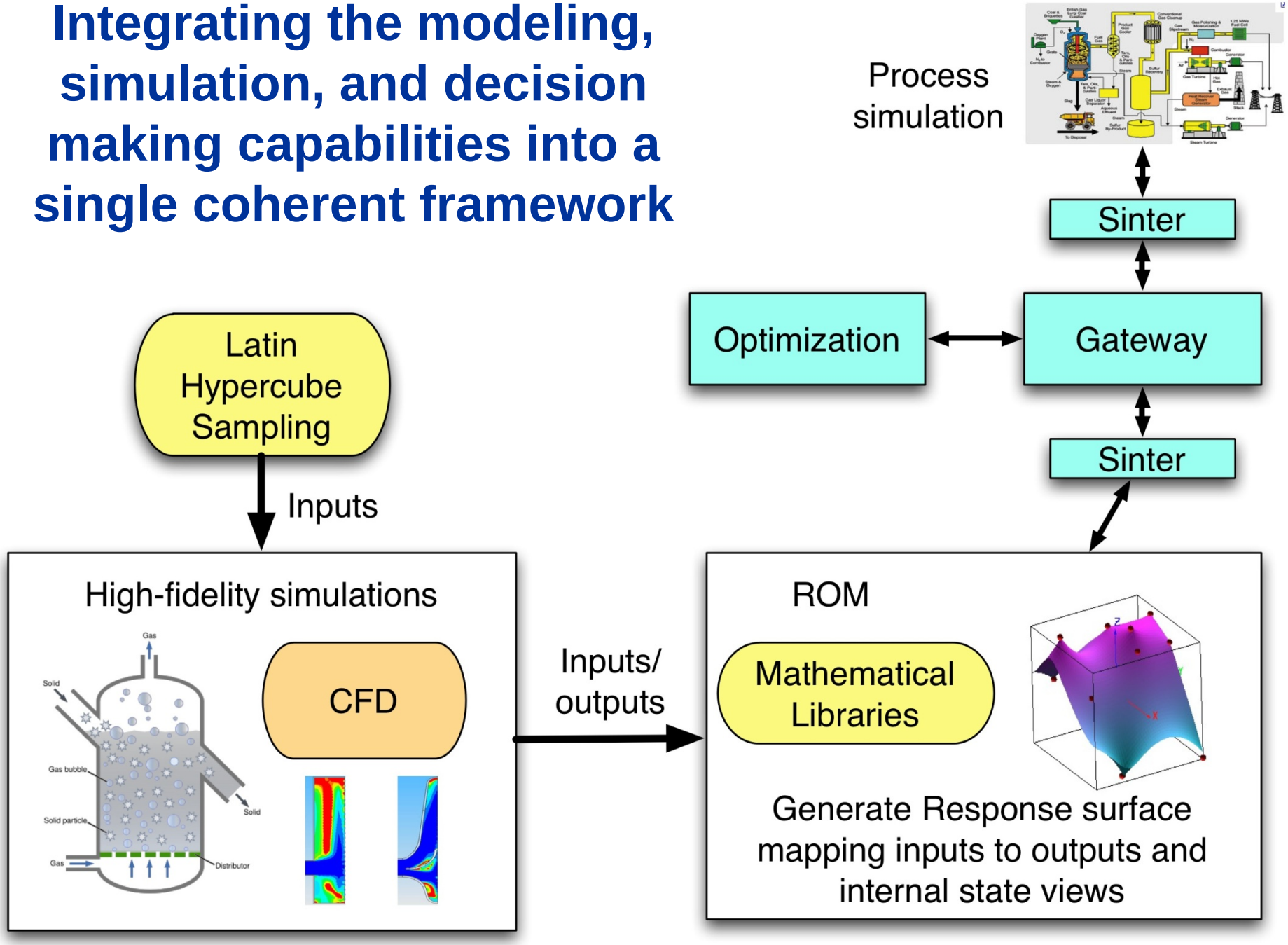


$$f(x)$$

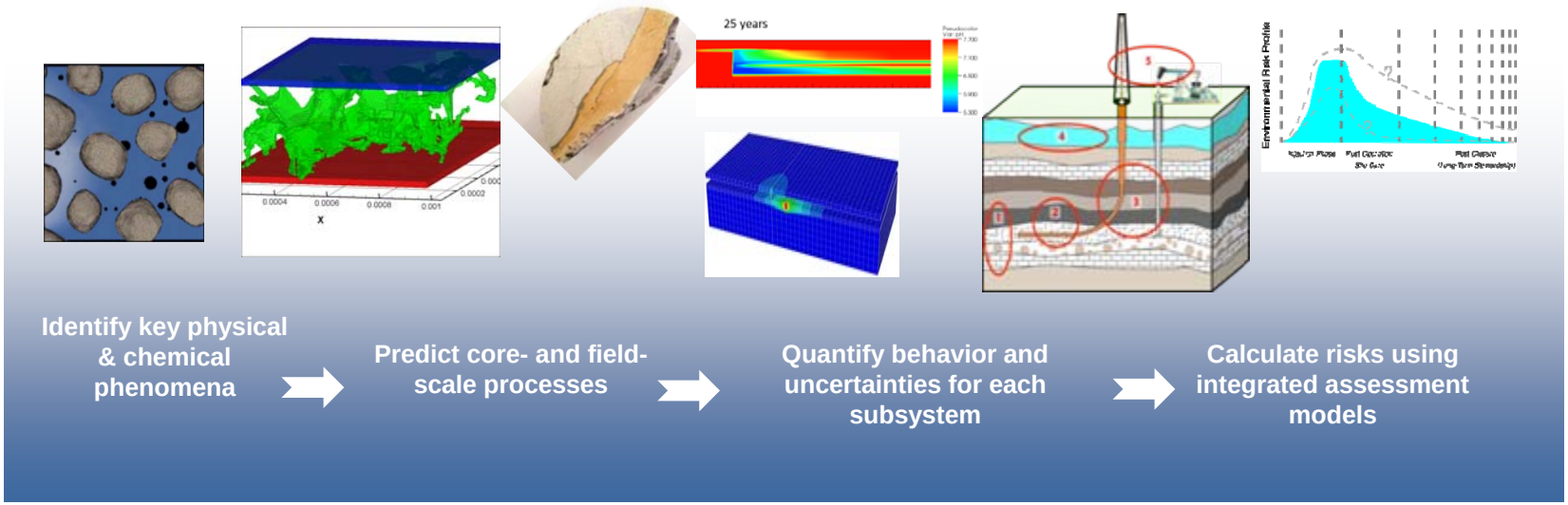


Superstructure with algebraic ROMs used for determining optimal process configuration

Integrating the modeling, simulation, and decision making capabilities into a single coherent framework

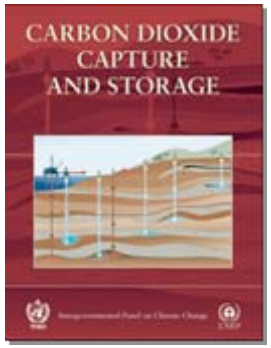


National Risk Assessment Partnership



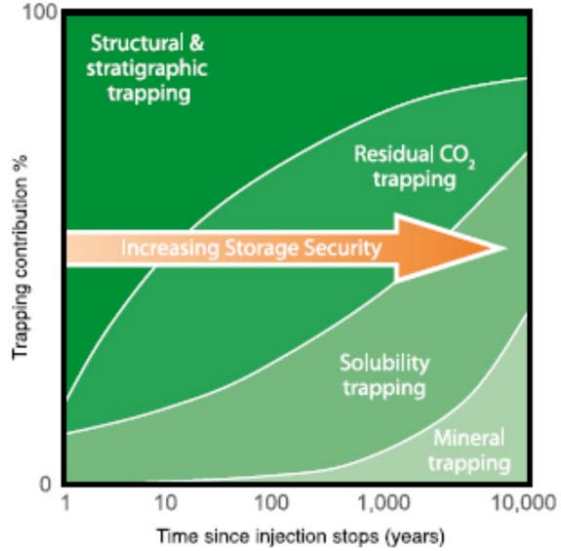
- **Overall NRAP goal: To develop and demonstrate a methodology for generating long-term quantitative risk profiles for carbon storage to support widespread commercial deployment.**
  - Develop framework and computational tools needed to generate quantitative risk profiles (long-term liability)
  - Use laboratory and field data to fill gaps in the science base as needed to confirm model validity, to reduce uncertainty, and to direct model development
  - Develop risk-based monitoring and mitigation strategy that lowers uncertainty and risk

Security/permanence is expected to be high for CO_2 storage in geologic reservoirs.



IPCC (2005)

Schematic evolution of trapping mechanisms over time (IPCC, 2005)



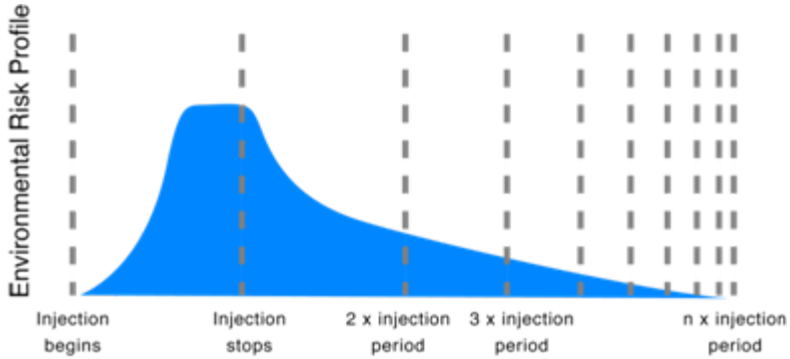
Multiple trapping mechanisms reduce CO_2 mobility over time

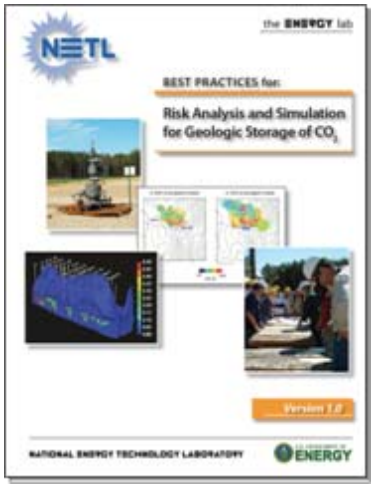
- structural/stratigraphic
- residual
- solubility
- mineralization; sorption

Risk profiles are expected to decline over time

Site characterization, site operations, and monitoring strategies will work to promote storage security (e.g., DOE Best-Practices documents)

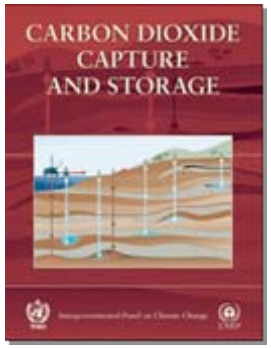
Schematic profile of environmental risk (Benson, 2007)





"Observations from engineered and natural analogues as well as models suggest that ***the fraction retained in appropriately selected and managed geological reservoirs is very likely to exceed 99% over 100 years and is likely to exceed 99% over 1,000 years."***

NRAP focus is on addressing technical needs related to confirming geologic storage security.

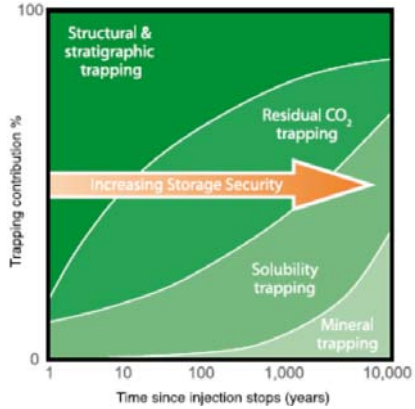


IPCC (2005)

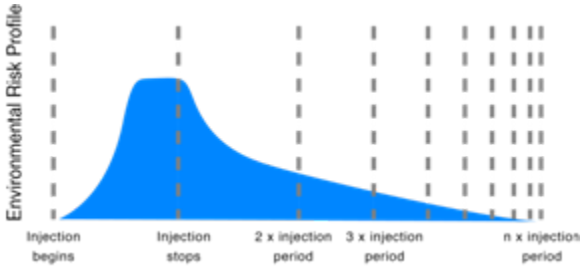
"Observations from engineered and natural analogues as well as models suggest that ***the fraction retained in appropriately selected and managed geological reservoirs is very likely to exceed 99% over 100 years and is likely to exceed 99% over 1,000 years."***

"With appropriate site selection informed by available subsurface information, a monitoring program to detect problems, a regulatory system, and the appropriate use of remediation methods to stop or control CO_2 releases if they arise, the local health, safety and environment risks of geological storage would be comparable to risks of current activities such as natural gas storage, EOR, and deep underground disposal of acid gas."

Schematic evolution of trapping mechanisms over time (IPCC, 2005)

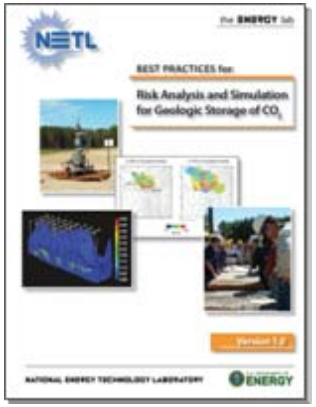


Schematic profile of environmental risk (Benson, 2007)



Needs

- *Quantify common storage security relationships*
- Assess validity *and nature of relationships over variety of geologic environments*
- Quantify & reduce uncertainty in risk assessments



Some Key Risk-Related Issues

probability that an event will occur

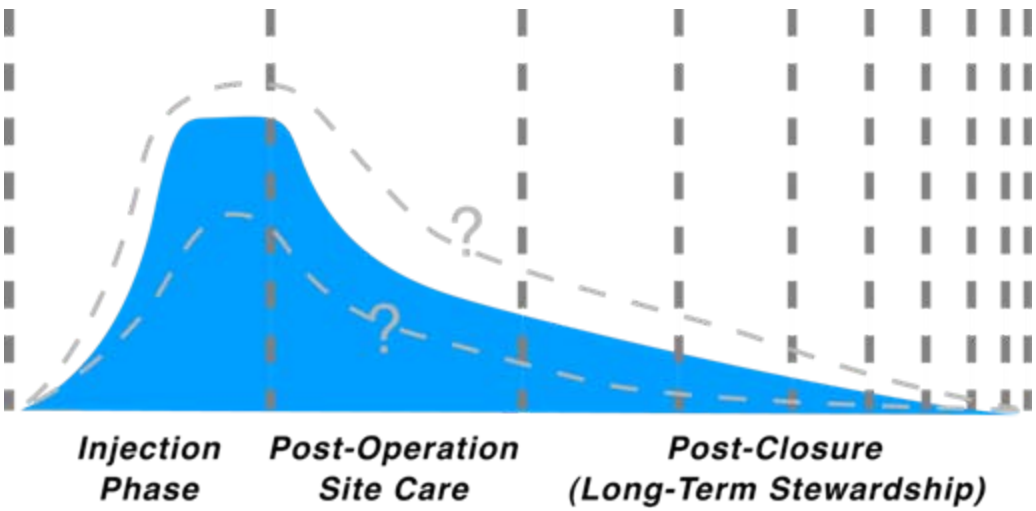
consequence of an event

$$Risk = P_{event} \times C_{event}$$

Liability can occur when a consequence is declared a harm.

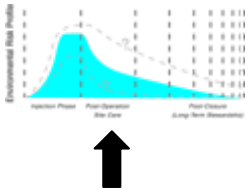
operator ⟷ ***regulator***

NRAP results will benefit/inform both sides



- **Quantification of long-term risk (liability) & uncertainty**
- **Definition of post-operation site-care**
  - *time period*
  - key monitoring needs (signals to monitor; size of area-of-review)

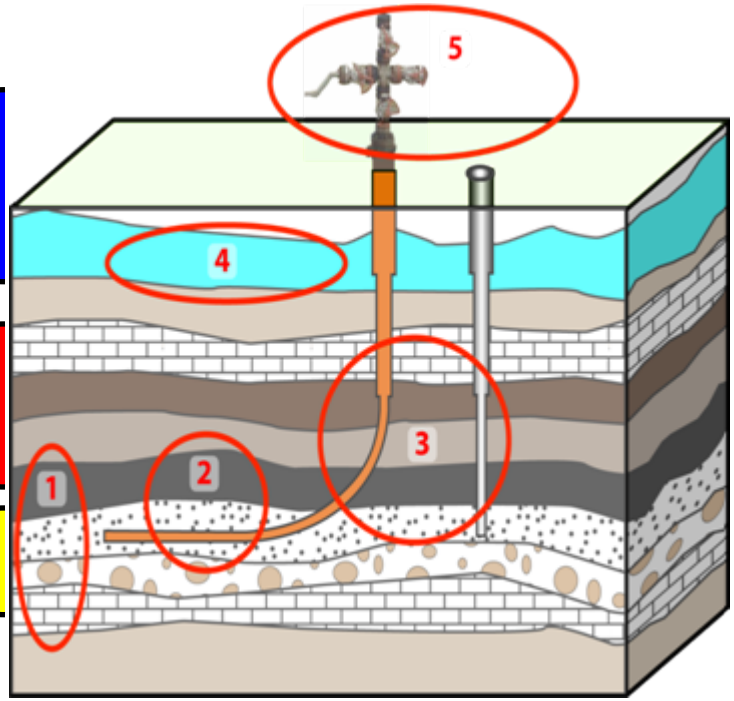
NRAP's approach to quantifying system performance relies on integrated assessment models (IAMs) to predict behavior of coupled systems (reservoir to receptor).



Potential Receptors or Impacted Media

Release and Transport

Storage Reservoir



① Fluid Flow in Reservoir
- fluid flow (porous flow & discrete fractures)
- trapping mechanisms
- heterogeneous and uncertain permeability

② Ground Motion Response
- geomechanical response to pressure changes (induced seismicity; hydraulic fracturing; etc.)

③ Wellbore/Seal Integrity
- flow in pipe/fracture (coupled to reservoir flow)
- wellbore/fracture locations & geometries
- effective permeabilities
- cement behavior (stemming/completion)
- geochemical and geomechanical effects

④ Groundwater Protection
- fluid flow and fluid–rock geochemistry
- contaminant transport

⑤ Atmospheric Emissions
- release(s) from subsurface
- emissions from surface activities

NRAP Focus

- **Quantification of risk profiles (change in risk over time)**
  - return of CO_2 to atmosphere
  - groundwater (TDS and pH; metals and organics)
  - induced ground motion
- **Quantification of key uncertainties**
- **Risk-based monitoring strategy**

NRAP Outputs

- **Field-confirmed (validated) methodology and platform**
- **Lessons learned for risk quantification to inform best practices; risk-based monitoring and mitigation strategies**
- **Scientific results that reduce the uncertainty in risk quantification**

Thoughts on "Virtualizing" Fossil Energy

Virtualizing Carbon Capture

- **Develop software tool set for reducing the cost and time of capture technology development (CCSI)**
- **Additional R&D needs**
  - Models for solvent and oxy-combustion systems
  - Extension to model pre-combustion systems (Gasification)

Virtualizing Carbon Storage

- **Generate long-term quantitative risk profiles for carbon storage to enable quantification of potential liabilities (NRAP)**
- **Additional R&D needs**
  - ROMs for uncertainty quantification
  - Field scale model validation
  - Extension to basin-scale model

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