Identify key physical & chemical phenomena ➔ Predict core- and field-scale processes ➔ Quantify behavior and uncertainties for each subsystem ➔ Calculate risks using integrated assessment models

Model Complexities

Rajesh Pawar, Los Alamos National Laboratory
Presenting efforts of multiple NRAP collaborators
Modeling Goals

• Predict CO₂ injection and migration as well as reservoir response in support of:
  – Permit Application
  – Site Operations (short-term)
  – Risk assessment & management (short & long-term)
• Help design & deploy monitoring techniques and approaches
• Identify impact of uncertainties on project goals
Models

- Models and modeling approaches are dependent on questions to be answered as well as type and amount of available data
  - Can range from simple to complex
  - Analytical/semi-analytical/numerical
  - Deterministic or probabilistic

- CO₂ Sequestration applications require multi-scale, multi-physics models
  - Type of questions to be answered
  - Hydrologic, thermal, chemical (reactions), mechanical processes
  - Focused on specific parts of a sequestration site or entire system
Models and Data

• Pre-characterization Phase:
  – Limited data: site specific or analog
  – More analytical and/or simplistic (homogeneous) reservoir simulations
  – Simulations with single/multiple wells
  – Area of review, Plume boundary, preliminary assessment of storage capacity, injectivity
  – Risk screening (FEPs analysis)
  – Higher uncertainty
Models and Data

• Characterization Phase:
  – Increased data availability
  – Site-specific data
  – Complex models including reservoir simulations
  – Define operational parameters
  – Risk assessment and management
  – Inform effective monitoring deployment

• Operational Phase:
  – Site-specific observations for model validation/update
  – Improved monitoring design
  – Improve predictions for post-injection monitoring deployment and long-term risk management
Key aspects of geologic CO$_2$ storage sites

atmosphere; anthropogenic systems

terrestrial ecosystems; subaqueous systems (offshore)

groundwater
wells
CO$_2$ storage reservoir

mineral resources
faults
Schematics of processes: example to assess potential impacts of CO\(_2\) and brine leakage

Groundwater Aquifer

CO\(_2\)/Brine Migration

Intermediate Zones

CO\(_2\)/Brine Migration

Sequestration Reservoir

CO\(_2\) Plume

Pressure Front

CO\(_2\)/Brine migration through leakage pathways
Selecting modeling approach: Challenges

- Complexities:
  - 3-dimensional
  - Complex Geology: Heterogeneity, uncertainty
  - Complex processes for different parts (reservoir, wells, faults, intermediate zones, shallow aquifer): different time-scales
- System parts are inter-dependent: Do we simulate the entire system together?
  - Do we have computational abilities to do that?
- How can we perform calculations in a probabilistic way? to account for effects of uncertainties?
One way to simulate entire site is using an integrated assessment modeling approach

A. Divide system into discrete components

B. Develop detailed component models that are validated against lab/field data

C. Develop reduced-order models (ROMs) that rapidly reproduce component model predictions

D. Link ROMs via integrated assessment models (IAMs) to predict system performance & risk; calibrate using lab/field data from NRAP and other sources

E. Develop strategic monitoring protocols that allow verification of predicted system performance

Large number of calculations need computationally efficient models for predicting behavior of individual parts
ROMs are developed and tested through a comparison to validated simulators.

**Detailed simulations**
Multiple simulations of detailed component models (reservoir, wellbores, faults, aquifer)

**Sensitivity analysis**
Identify key variables that control component behavior

**Develop ROMs**
- Look-up tables (LUTs)
- Response surfaces (e.g. via PSUADE)
- Artificial intelligence approaches
- Simplified relationships (e.g., PCE)

Validate ROMs against simulations

ROMs are not simple models but models that capture complex processes and are computationally efficient
ROM example: leakage through cemented wellbore

- **Purpose:** Predict time-dependent leak rate of CO$_2$ and brine through a cemented wellbore
  - Function of CO$_2$ saturation and pressure at reservoir/wellbore intersection
  - Multi-phase flow, phase-change, buoyancy-driven flow, capillary and residual effects
  - Allow variability in wellbore completions, wellbore effective cement permeability, wellbore depth
  - Predict leakage into intermediate zones, shallow aquifer and atmosphere
Wellbore ROM development: Approach

- Complex reservoir simulations of CO$_2$ injection and leakage through wellbore: 20 years injection, 30 years relaxation
- Monte-Carlo simulations: vary multiple uncertain parameters, ~1500 runs
- Simulated leak rates used to develop ROM using MARS (Multi-variate Adaptive Regression Splines)
Wellbore ROM development
Wellbore ROM Development

Leak rates used to develop a ROM(s) using MARS. ROM predicts leak rate as function of multiple parameters (pressure, saturation, wellbore perm, wellbore length, thief zone location, etc.)
ROMs: Reservoir

- **Purpose:** Predict pressure, saturations at reservoir/seal interface at different times/locations
  - During & Post-injection for long term (up to 1,000 years)
  - Allow variability in reservoir and seal properties, geologic complexity
  - Multi-phase flow, CO\textsubscript{2} dissolution, residual saturations
  - Different types of reservoirs: Brine reservoirs, Gas fields, Oil fields
  - LUTs, Surrogate Reservoir Models based on artificial intelligence, Polynomial Chaos Expansion, Gaussian Regression Analysis

Kimberlina, San Joaquin Basin, CA

Otway, Australia

SACROC, TX
• **Purpose:** Predict impact of CO$_2$ and brine leakage in shallow aquifers
  - Changes in pH, TDS, trace metal and organics concentrations
  - Multi-phase flow, CO$_2$ dissolution, reactive transport
  - Unconfined carbonate aquifer (Edwards), Confined sandstone aquifer (High Plains)

• Site-specific geologic & geochemical data
• Multiple uncertain hydrologic & transport parameters
• ROM: Multivariate Adaptive Regression Splines (MARS), linking functions
Risk calculations using the integrated system model

**Multiple Realizations**

Each Realization: Dynamic simulation over 100s-1000s yr, run linked models simultaneously

Each Realization

Sample uncertain parameters (reservoir, wells, faults, seals, shallow/intermediate aquifers)

Utilize reservoir abstractions to estimate time-dependent saturation and pressure in sequestration reservoir given the chosen set of reservoir and injection parameters

Utilize leakage abstractions to estimate CO\(_2\) and brine leak rate given chosen set of parameters and estimated time/space-dependent pressure and CO\(_2\) saturation in sequestration reservoir

Utilize aquifer abstraction to estimate change in pH and TDS given chosen set of aquifer parameters and estimated CO\(_2\)/brine leak rates
Example results: Change in pH of shallow aquifer due to leakage through cemented wellbore

Means of calculated volume of shallow aquifer with pH < 6.5 over 200 years as a function of wellbore spatial density (10,000 realizations)
Tying it all to monitoring

- Developments in progress
- Aquifer ROMs predict size of affected aquifer volumes (volumes as well as x, y dimensions)
- Spatial information of leakage points coupled with plume dimensions will be used to identify location of affected aquifer volume
- CO$_2$ plume and pressure change due to leakage in intermediate aquifer
- Pressure, saturation and geochemical changes (magnitude & locations) in shallow & intermediate aquifers will be used to identify type of monitoring technologies and their deployment
Conclusions

• Risk assessment and management (including monitoring & mitigation) requires predictions of CO₂ leakage & impacts
• Need to do it probabilistically to account for uncertainties
• Complex, coupled models for entire system are computationally challenging
• Computational efficiency can be achieved by reduced order models coupled together to represent the system: need to ensure important processes and parameters are captured
• Probabilistic simulations help to optimize monitoring technologies deployment