

Numerical Simulations For CO2 Storage in Saline Aquifer

Keni Zhang

Beijing Normal University



Long-Term Fate of Stored CO₂



Different Storage Modes

- 1. free gas
- 2. trapped gas
- 3. dissolved in brine

4. sequestered as solid minerals

1, 2, and 3 can be simulated with multiphase flow simulator; 4 can be simulated by reactive transport model.

Source: 2005 IPCC Special Report on Carbon Dioxide Capture and Storage; http://www.ipcc.ch/activity/srccs/index.htm



The simulation technology needed to solve these problems(1)

- ✓ How do the relative proportions of CO_2 in these different storage modes change over time?
- ✓ How does the evolution of CO_2 leaks depend on coupling of chemical, mechanical, and thermal effects? What is the fate of leaking?
- ✓ What fraction of subsurface volume can be accessed by CO_2 ?
- ✓How is the utilization of subsurface space affected by viscous instability, gravity override and formation heterogeneities?



The simulation technology needed to solve these problems(2)

 \checkmark Can CO₂ leaks self-seal or self-enhance?

✓ What is the role of relative permeability and capillary pressure effects in CO_2 containment and leakage?

✓ What is the role of different phase compositions and phase changes in CO_2 leakage?(supercritical, liquid ,gaseous CO_2 , dissolved in water)?

✓What is the pressure build up and CO2 plume distribution after CO2 injection?

 \checkmark Help for design and analysis of tests.



Simulators for CO₂ Storage in Saline Aquifers

ECLIPSE **≻FEHM ≻GEM** ≻GPRS ≻TOUGH2 **≻**STOMP >Other simulators :COORES, DuMu, IPARS-CO2, MUETE, RockFlow, RTAFF2

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TOUGH Family Code For CO₂ Sequestration

Fluid dynamics: TOUGH2/ECO2N

- •Multiphase flows of water/CO₂/NaCl mixtures
- •Applications to studies of reservoir dynamics, storage capacity, CO₂ leakage

Geochemistry: TOUGHREACT/ECO2N

- •Reactions between gas-aqueous-solid phases
- •Study mineral trapping, caprock integrity, natural CO₂ reservoirs

Geomechanics: TOUGH-FLAC

- •TOUGH2 coupled to commercial FLAC3D geomechanics code
- •Stress-strain: analyze leakage through caprock and faults
- Large Scale Simulations: TOUGH2-MP/ECO2N



Computation Challenging

- ✓ Site characterization needs basin-scale model
- ✓ Refined grids are needed for catching CO2 convection
- ✓ Multi-Scale, multiphase flow
- ✓Complex geochemical reaction and mechanical processes
- ✓Leakage of CO2 through boreholes, faults, and other high permeability paths (may be non-Darcy flow)
- ✓THMC coupling simulations



Phase Diagram of CO2 for Numerical Simulations



Examples for permeability influences on CO2 storage



Simulation results for a storage site in Western China

Simulation results for a storage site in Eastern China



Example 1: Tokyo Bay Model (from Hajime, Zhang et al. 2008)

Large-scale injection (several MtCO₂/yr) into virgin aquifers would:

- Push large volume of water out of the aquifers.
- Potentially affect subsurface groundwater environment (Pressure, Water Quality)







Hydrogeological Model(1)

Continuous Layer Model

Assume perfect lateral continuity



Hydrogeological Model(2)

Discontinuous Layer Model

Represents lateral lithofacies changes



Geostatistical Unconditional Simulation(10 realizations)

- Lateral lithofacies changes
- Continuity of layers
 - 5km (horizontal)
 - 20m (vertical)

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Figure 1. 3D grid system (about 10 million gridblocks, only connections are shown)



Hypothetical CO₂ Injection

- Target aquifer:
 - Middle Kazusa Group
 - Depth = 800 to 1000m
- Supercritical CO₂
 - e.g.,Density ~ 0.56 t/m³
 - (at P=10MPa, T=40 °C)
- Injection rate:
 - 1Mt/year/hole × 10 holes
 - = 10 Mt/year
- Assume CO₂ injection over a period of 100 years.
- Simulation is performed until 1000 years



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Results –**CO**₂ migration-





Results –Head Build-up (1)-Change in head with time at urban inlands



Base Case (Continuous Layer Model)

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Results – Surface Discharge –

How much water pushed out is discharged at the surface



Base Case

Discharge occurs in the sea floor and under the boundary of Shimosa/Kazusa G.

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Example 2: Dissolution-Diffusion-Convection Process(Zhang and Pruess 2007)

 ✓ Role of irregular features (geometry, heterogeneity) and 3-Deffects in "real" systems?
 ✓ Growth of dissolved CO₂ inventory.
 ✓ How can the multi-scale nature of the dissolution-

diffusion-convection process be captured in fieldscale simulations?



3D Model



3-D domain for
simulating brine
convection induced by
CO2 dissolution and
associated increase in
aqueous phase density.
(Xco2=0.0493 at top
boundary)



Random Heterogeneity Field for Triggering Brine Convection



Characterizing DDC Processes

✓ Constant dissolved concentration at the interface
 ✓ The rate of CO2 entering the system equals to its dissolution rate at the top boundary.

✓The growth of total dissolved CO2 inventory over time

Comparison with the case without convection
 Investigating different random seeds



Dissolved CO2 concentrations at different times



3D Model results



Random permeability influence on CO2 flux at top boundary





