## cags

# Numerical Simulations For CO2 Storage in Saline Aquifer 

Keni Zhang

Beijing Normal University

## Long－Term Fate of Stored $\mathrm{CO}_{2}$



## 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)

$\checkmark$ How do the relative proportions of $\mathrm{CO}_{2}$ in these different storage modes change over time?
$\checkmark$ How does the evolution of $\mathrm{CO}_{2}$ leaks depend on coupling of chemical, mechanical, and thermal effects? What is the fate of leaking?
$\checkmark$ What fraction of subsurface volume can be accessed by $\mathrm{CO}_{2}$ ?
$\checkmark$ 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 $\mathrm{CO}_{2}$ leaks self－seal or self－enhance？
$\checkmark$ What is the role of relative permeability and capillary pressure effects in $\mathrm{CO}_{2}$ containment and leakage？
$\checkmark$ What is the role of different phase compositions and phase changes in $\mathrm{CO}_{2}$ leakage？（supercritical，liquid，gaseous $\mathrm{CO}_{2}$ ， dissolved in water）？
$\checkmark$ What is the pressure build up and CO2 plume distribution after CO2 injection？
$\checkmark$ Help for design and analysis of tests．


## Simulators for $\mathrm{CO}_{2}$ Storage in Saline Aquifers

＞ECLIPSE
$\Rightarrow$ FEHM
$\rightarrow$ GEM
$\Rightarrow$ GPRS
＞TOUGH2
＞STOMP
$>$ Other simulators ：COORES，DuMu， IPARS－CO2，MUETE，RockFlow，RTAFF2
ca
China Australia Geological Storage of $\mathrm{CO}_{2}$
中澳 二氧化碳地质封存
$(0 y)$

## TOUGH Family Code For $\mathrm{CO}_{2}$ Sequestration

## Fluid dynamics：TOUGH2／ECO2N

－Multiphase flows of water／ $\mathrm{CO}_{2} / \mathrm{NaCl}$ mixtures
－Applications to studies of reservoir dynamics，storage capacity， $\mathrm{CO}_{2}$ leakage
Geochemistry：TOUGHREACT／ECO2N
－Reactions between gas－aqueous－solid phases
－Study mineral trapping，caprock integrity，natural $\mathrm{CO}_{2}$ 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


China Australia Geological Storage of $\mathbf{C O}_{2}$中澳 二氧化碳地质封存

## Computation Challenging

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

## Phase Diagram of CO2 for Numerical Simulations



China Australia Geological Storage of $\mathbf{C O}_{2}$
中澳二氧化碳地质封存

## 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 $\mathrm{MtCO}_{2} / \mathrm{yr}$ ）into virgin aquifers would：
－Push large volume of water out of the aquifers．
－Potentially affect subsurface groundwater environment （Pressure，Water Quality）


Lithofacies Analysis


Model


China Australia Geological Storage of $\mathrm{CO}_{2}$中澳二氧化碳地质封存

## Hydrogeological Model（1）

## Continuous Layer Model

Assume perfect lateral continuity


Sensitivity cases
1．Rock compressibility $\quad 10^{-9} \rightarrow 10^{-8} 1 / \mathrm{Pa}$
2．Permeability of mud layers $1 \rightarrow 10 \mathrm{md}$


China－Australia Geological Storage of $\mathrm{CO}_{2}$
中澳二氧化碳地质封存

## Hydrogeological Model（2）

## Discontinuous Layer Model

## Represents lateral lithofacies changes

Shimosa G．（mud）：kh＝1md

$>$ Geostatistical Unconditional Simulation（10 realizations）
－Lateral lithofacies changes
－Continuity of layers
5km（horizontal）
20m（vertical）


China－Australia Geological－Storage of $\mathrm{CO}_{2}$中澳二氧化碳地质封存


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

## Hypothetical $\mathrm{CO}_{2}$ Injection

- Target aquifer:
- Middle Kazusa Group
- Depth $=800$ to 1000 m
- Supercritical $\mathrm{CO}_{2}$

$$
\begin{aligned}
& \text { e.g.,Density } \sim 0.56 \mathrm{t} / \mathrm{m}^{3} \\
& \text { (at } \mathrm{P}=10 \mathrm{MPa}, \mathrm{~T}=40^{\circ} \mathrm{C} \text { ) }
\end{aligned}
$$

- Injection rate:
$1 \mathrm{Mt} /$ year/hole $\times 10$ holes

$$
\text { = } 10 \text { Mt/year }
$$

- Assume $\mathrm{CO}_{2}$ injection over a period of 100 years.
- Simulation is performed until 1000 years



## Results $-\mathrm{CO}_{2}$ migration－



## Results－Head Build－up（1）－ <br> Change in head with time at urban inlands



Base Case（Continuous Layer Model）

China Australia Geological Storage of $\mathrm{CO}_{2}$中澳二氧化碳地质封存

## 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.


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

$\checkmark$ Role of irregular features（geometry， heterogeneity）and 3－Deffects in＂real＂systems？
$\checkmark$ Growth of dissolved $\mathrm{CO}_{2}$ inventory．
$\checkmark$ How can the multi－scale nature of the dissolution－ diffusion－convection process be captured in field－ scale simulations？
ca

## 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

$\checkmark$ Constant dissolved concentration at the interface $\checkmark$ The rate of CO2 entering the system equals to its dissolution rate at the top boundary．
$\checkmark$ The growth of total dissolved CO2 inventory over time
$\checkmark$ Comparison with the case without convection
$\checkmark$ Investigating different random seeds
ca

## Dissolved CO 2 concentrations at different times





cags
China－Australia Geological Storage of $\mathrm{CO}_{2}$中澳二氧化碳地质封存

## 3D Model results





## Random permeability influence on CO2 flux at top boundary




## Thank you

China Australia Geological Storage of $\mathrm{CO}_{2}$
中澳 二氧化碳地质封存

