Modelling CO₂ sequestration in deep saline aquifers

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Metadata Record: https://dspace.lboro.ac.uk/2134/14563

Version: Accepted for publication

Publisher: UK Carbon Capture and Storage Research Centre (UKCCSRC)

Please cite the published version.
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Modelling CO\textsubscript{2} Sequestration in Deep Saline Aquifers

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Geological CO\textsubscript{2} sequestration as one of CCS techniques occurs in four mechanisms; hydrodynamic trapping is storage of free CO\textsubscript{2} in pore spaces of sedimentary layers, residual trapping occurs as a result of a hysteresis effect in the permeability of the supercritical phase of carbon dioxide which can happen when the saturation direction is reversed, solubility trapping occurs via CO\textsubscript{2} dissolution in the brine, mineral trapping is a result of carbon dioxide gas dissolves into fluid in the aquifer and reacts with water to form carbonic acid which reacts with dissolved ions within the brine aquifer and minerals forming the host.

This research project aims to carry out a series of modelling to investigate the injection and transport behaviour of CO\textsubscript{2} in deep saline aquifers as a multiphase flow in porous media in addition to studying the influence of different parameters such as time scale, temperature, pressure, permeability and geochemical condition on the stability of CO\textsubscript{2} underground.

To determine the optimum conditions for the sequestration process which leads to minimize the risk of CO\textsubscript{2} leakage back to the atmosphere. A simulation code named STOMP (Subsurface Transport Over Multiple Phases) is utilized to numerically predict thermal and geological flow and transport phenomena in variably saturated subsurface environments by numerically solving the governing partial differential equations of mass, momentum and thermal energy that describe the subsurface environment simultaneously using Newton-Raphson iterations to resolve the nonlinearities in them. In contrast to most other works which are focussed on determining mass fraction of CO\textsubscript{2}, this project focuses on determining capillary pressures of CO\textsubscript{2} as a function of water saturation and CO\textsubscript{2} dissolution rate in groundwater at different time scales, temperature and pressure conditions. A series of figures were produced to illustrate how saturation, capillary pressure and dissolved CO\textsubscript{2} changes with the change of injection process, hydrostatic pressure and geothermal gradient.
Modelling CO$_2$ Sequestration
In Deep Saline Aquifers

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Chemical Engineering Department – January 2013
Project Aims

Develop a framework model to determine static and dynamic capillary pressure for water-$\text{co}_2$ system as a function of saturation at various times, temperatures, pressures and salinity.
**CO₂ Sequestration in Saline Aquifers**

Mechanisms of Storage

1. Physical trapping below an impermeable layer

2. CO₂ adhered to the solid surface of the formation.

3. CO₂ dissolved in the existing fluids and increases its density or react with information.

4. Carbonation reaction with the minerals contained in the formation aqueous.
Modelling CO$_2$ Injection

Effective Parameters

- **Gas composition and injection rate**
  - SO$_2$ contaminant CO$_2$ reduces mineral precipitation and dissolution
  - Increasing injection rate increases capillary residual trapping

- **Permeability and heterogeneity**
  - High permeability increases CO$_2$ mobility
  - Increased heterogeneity enhances lateral migration and CO$_2$ dissolution

- **Mineral precipitation and sorption**
  - Related to the porosity and permeability of the porous media.
1. Capable of analyzing multiple phase subsurface flow and transport
2. Competent at analyzing all mechanisms of CO$_2$ sequestration
3. Needs a FORTRAN compiler to generate executable code from source files
4. Produces numerical predictions of thermal and hydrogeologic flow and transport phenomena in variably saturated subsurface environments.
1. The conservation of motion is governed by Darcy’s equation

\[ \frac{\partial (S_\alpha \phi \rho_\alpha)}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{v}_\alpha) - \rho_\alpha q_\alpha = 0 \]

2. From the generalized Darcy’s law, velocity vector \( \mathbf{v}_\alpha \) can be calculated

\[ \mathbf{v}_\alpha = -\frac{k_{r\alpha}}{\mu_\alpha} K (\nabla p_\alpha - \rho_\alpha \mathbf{g}) \]

3. Solving the 2 equations gives;

\[ \frac{\partial (S_\alpha \phi \rho_\alpha)}{\partial t} - \nabla \cdot \left( \rho_\alpha \frac{k_{r\alpha}}{\mu_\alpha} K (\nabla p_\alpha - \rho_\alpha \mathbf{g}) \right) - \rho_\alpha q_\alpha = 0 \]
1. Brooks and Corey relationship defines the **effective saturation** as

\[ S_e(p_c) = \frac{S_W - S_{wr}}{1 - S_{wr}} = \left(\frac{p_d}{p_c}\right)^\lambda \quad \text{for} \quad p_c \geq p_d \]

2. Brooks-Corey relationships with the Burdine theorem are used to define the **relative permeability-saturation** relationships for wetting and non-wetting phases

\[ k_{rw} = S_e \left(\frac{2 + 3\lambda}{\lambda}\right) \]

\[ k_{rnw} = (1 - S_e)^2 \left(1 - S_e \frac{2 + \lambda}{\lambda}\right) \]

\[ \lambda \text{ : form parameter - describes the uniformity of the material} \]

- usually between 0.2 - 0.3
STOMP Simulation
Assumptions to Simplify Coupled Equations Solution

1. Rigid rock (No permeability)
2. Both fluids are incompressible
3. Constant dynamic viscosity
4. Formation is homogeneous
5. Isotropic under isothermal conditions
6. Thermodynamic equilibrium
7. No NAPL phase and no dissolved oil
Simulation Methodology

Computational Domain

1. Depth 2900 m
2. Radius 3000 m
3. Grid Nodes 50-1-10
4. Injection Well 0.4 m
5. Injection Rate 10 kg/s
6. Inj. Temperature 40-70°C
7. Inj. Pressure 16-25 MPa

Fig. 3.3, 2-D cylindrical domain coordination system
1. Quasi-static and dynamic experiments at diff. Time steps.

2. Equilibrium reached when no saturation change in all nodes

3. Water replacement occur when $P^c = P^d$

4. Injection into lower 3 layers

5. Av. $P^c$ and $S^w$ calculated

6. Hydros. cond. 50 C & 100 Bar

Fig. 3.4 Schematic illustration of CO$_2$ sequestration in deep saline aquifer.
Simulation Results

Aquous Saturation after 2 years simulation

Aquous Saturation after 4 years simulation

Aquous Saturation after 6 years simulation

Aquous Saturation after 8 years simulation

Aquous Saturation after 10 years simulation

Aquous Saturation after 20 years simulation
Simulation Results

1. Gas Pressure Distribution
2. 10 yrs Injection
3. 20 yrs Lockup
4. Injection into lower 3 layers
5. Locally Measured variables

![Graph showing aquous saturation over simulation time](graph.png)
Conclusions

1. Deep saline aquifers have a huge feasibility and potential for CO₂ sequestration

2. CO₂ storage occurs by structural, residual, solubility and mineral trapping mechanisms

3. Buoyancy and capillary forces enhance CO₂ immobilization

4. STOMP simulator is utilized to model CO₂ sequestration in saline aquifers for the wide capabilities of analyzing multiple phase flow and all trapping mechanisms

5. STOMP post processing data includes using perl script files to convert stomp files to data structured files to be used in Tecplot to plot output files variables.
Thank You