Modelling CO2 sequestration in deep saline aquifers

Modelling CO_2 Sequestration in Deep Saline Aquifers

Kamal Khudaida, & Dr D.B Das
Chemical Engineering department, Loughborough University, Loughborough

Geological CO_2 sequestration as one CCS techniques occurs in four mechanisms; *hydrodynamic trapping* is storage of free CO_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_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_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_2 underground.

To determine the optimum conditions for the sequestration process which leads to minimize the risk of CO_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_2, this project focuses on determining capillary pressures of CO_2 as a function of water saturation and CO_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_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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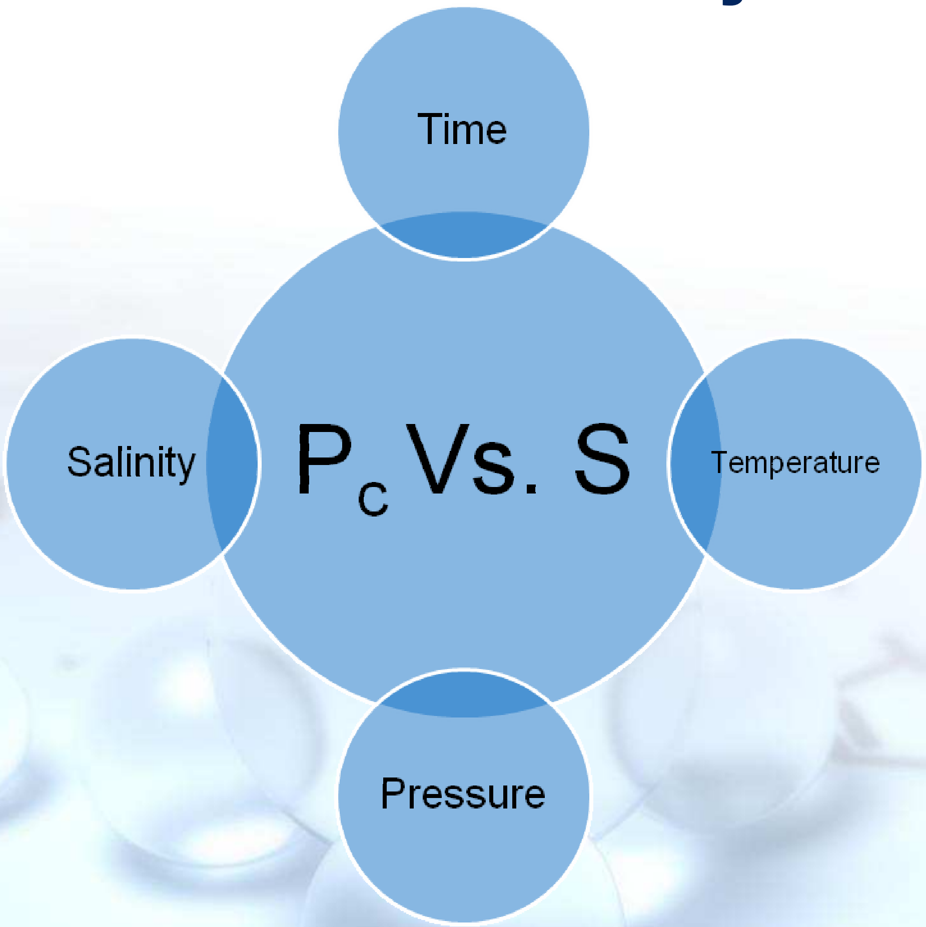
Kamal J. Khudaida
Chemical Engineering Department – January 2013

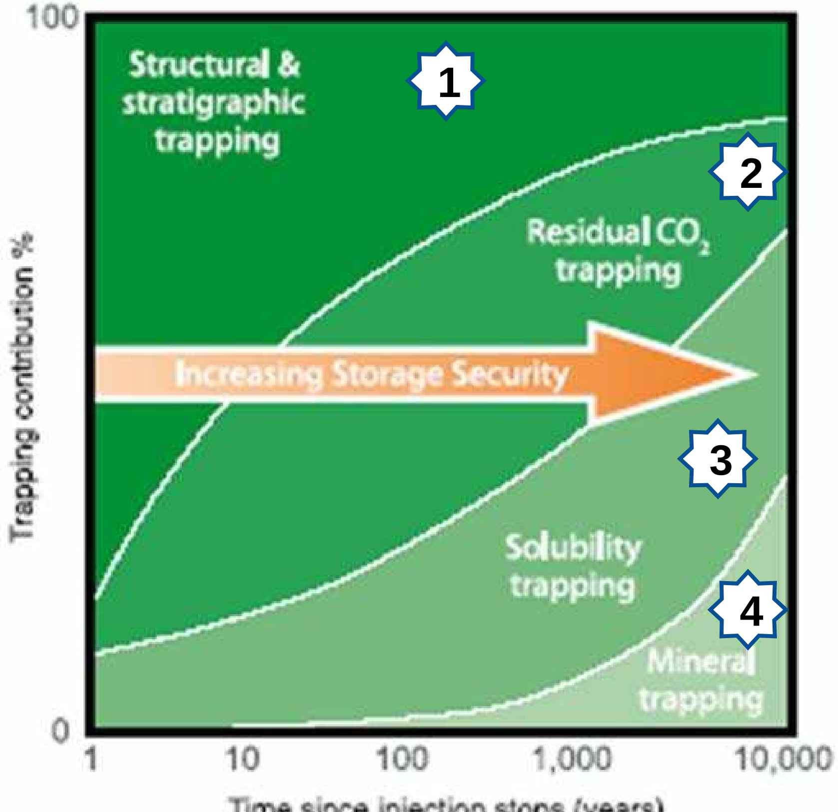
Project Aims



Develop a framework model to determine static and dynamic capillary pressure for water-co_2 system as a function of saturation at various times, temperatures, pressures and salinity.

CO_2 Sequestration in Saline Aquifers

Mechanisms of Storage



(www.Bellona.org)

1. Physical trapping below an impermeable layer
2. CO_2 adhered to the solid surface of the formation.
3. CO_2 dissolved in the existing fluids and increases it's density or react with information.
4. Carbonation reaction with the minerals contained in the formation aqueous.

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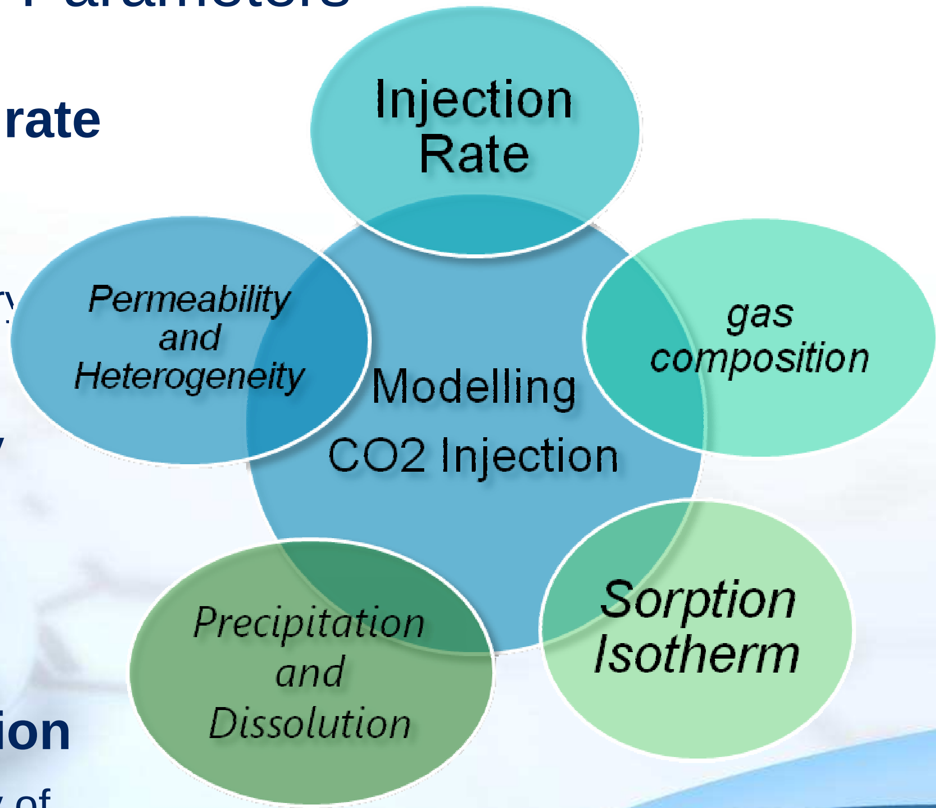
Modelling CO_2 Injection

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.



STOMP Simulator

Subsurface and Transport Over Multiple Phases

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.

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STOMP Code Governing Equations

Equations of Mass and Momentum

1. The conservation of motion is governed by Darcy's equation

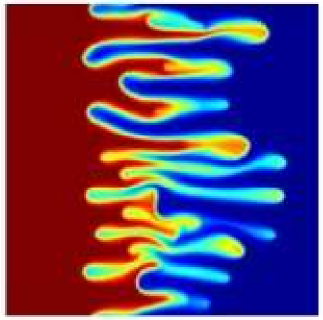
$$\frac{\partial (S_\alpha \phi \rho_\alpha)}{\partial t} + \nabla.(\rho_\alpha v_\alpha) - \rho_\alpha q_\alpha = 0$$

2. From the generalized Darcy's law, velocity vector v_α can be calculated

$$v_\alpha = -\frac{k_{r\alpha}}{\mu_\alpha} \mathrm{K}\left(\nabla p_\alpha - \rho_\alpha \mathrm{g}\right)$$

3. Solving the 2 equations gives;

$$\frac{\partial (S_\alpha \phi \rho_\alpha)}{\partial t} - \nabla.\left(\rho_\alpha \frac{k_{r\alpha}}{\mu_\alpha} \mathrm{K}\left(\nabla p_\alpha - \rho_\alpha \mathrm{g}\right)\right) - \rho_\alpha q_\alpha = 0$$



www.maths.ox.ac.uk

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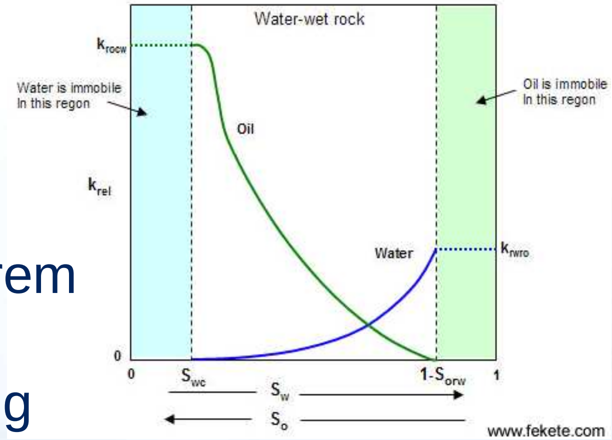
STOMP Constitutive relationships

capillary pressure-saturation and *relative permeability-saturation*

1. Brooks and Corey relationship defines the *effective saturation* as

$$S_e(p_c) = \frac{Sw - Swr}{1 - Swr} = \left(\frac{p_d}{p_c}\right)^{\lambda} \qquad \text{for } p_c \geq p_d$$



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

$$k_{rw} = S_e^{\frac{2+3\lambda}{\lambda}}$$

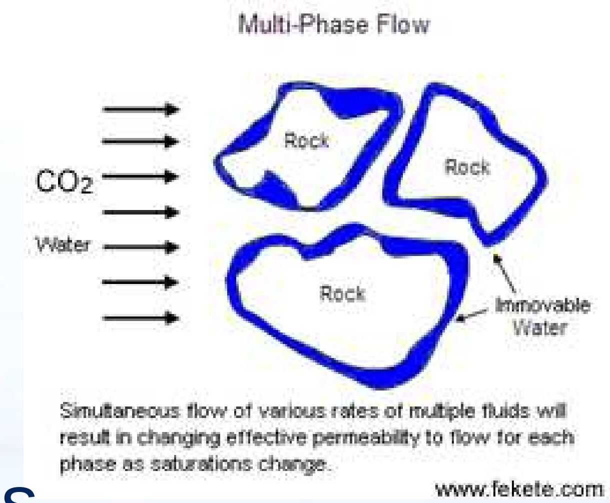
$$k_{rnw} = (1 - S_g)^2 (1 - S_e^{\frac{2+\lambda}{\lambda}})$$

λ : 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

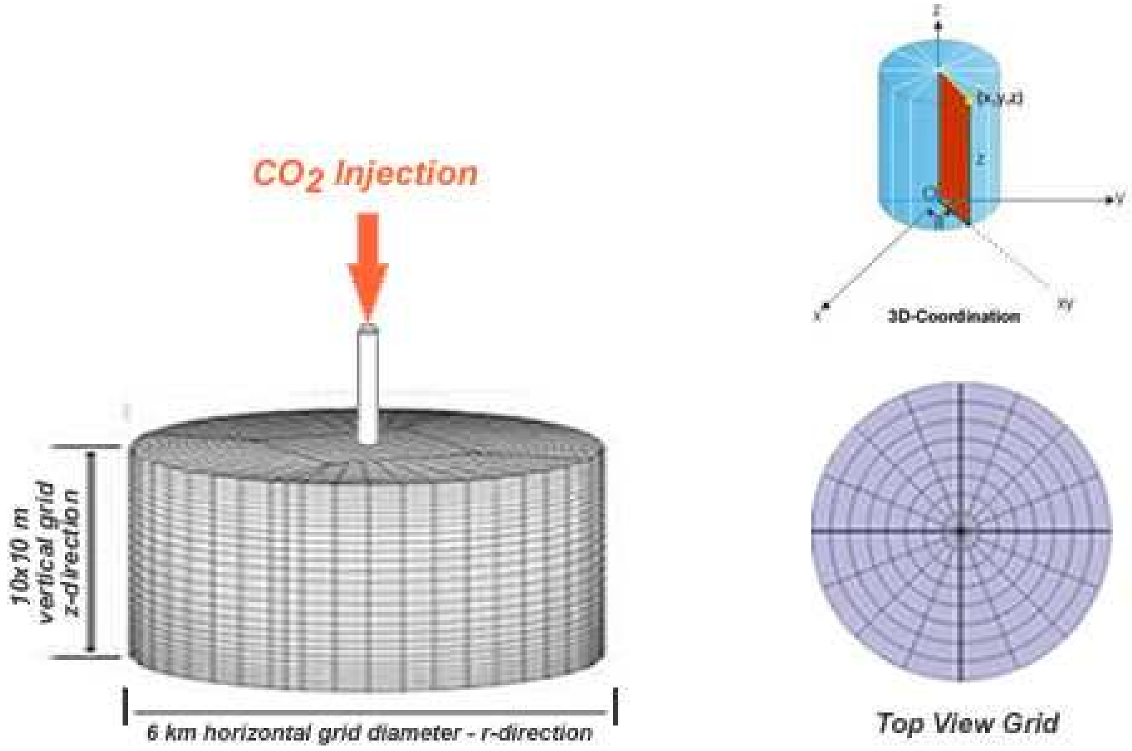


Fig. 3.3, 2-D cylinderical domain coordination system

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

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Simulation Methodology

Simulation Approach

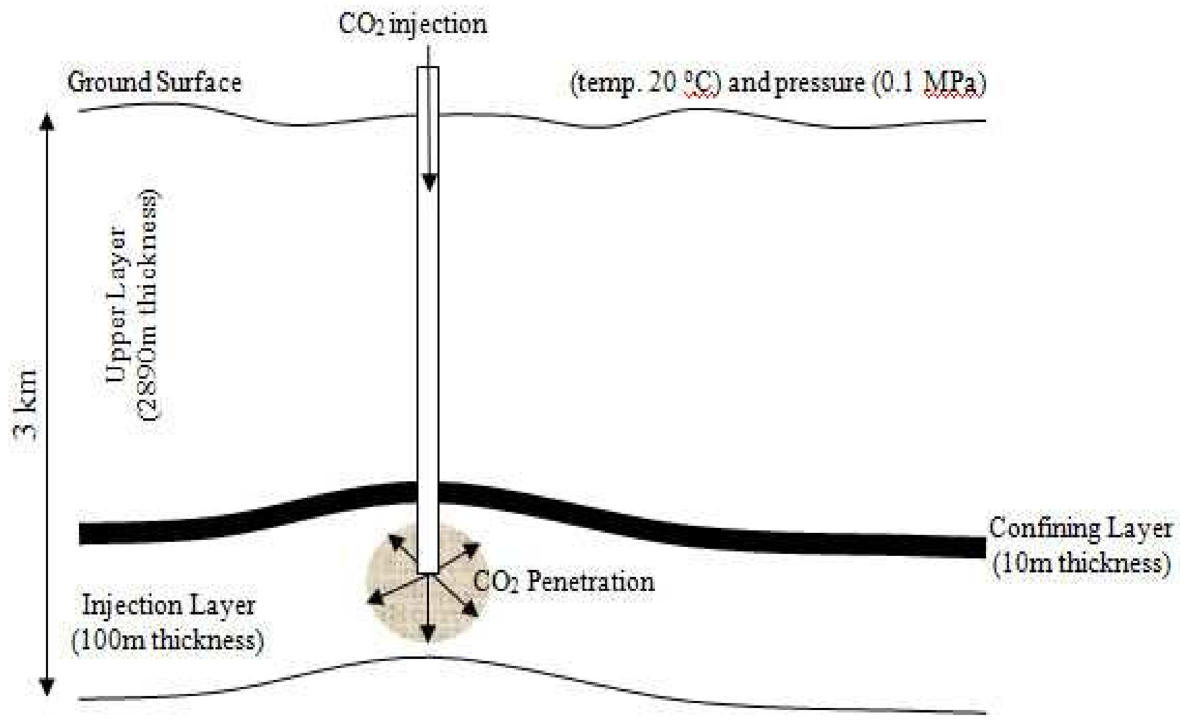
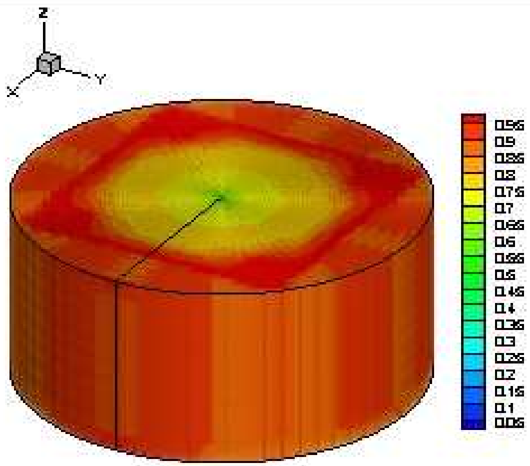


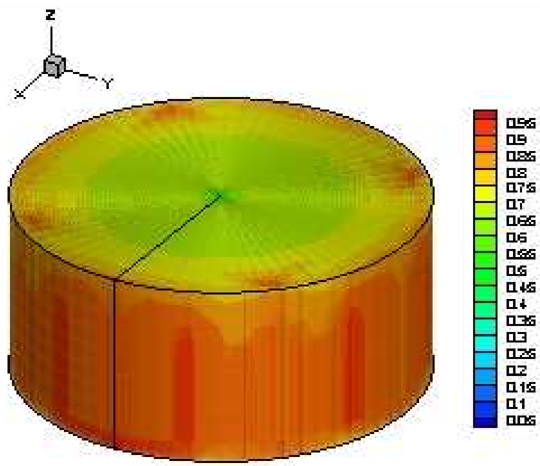
Fig. 3.4 Schematic illustration of CO_2 sequestration in deep saline aquifer.

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 calculted
6. Hydros. cond. 50 C & 100 Bar

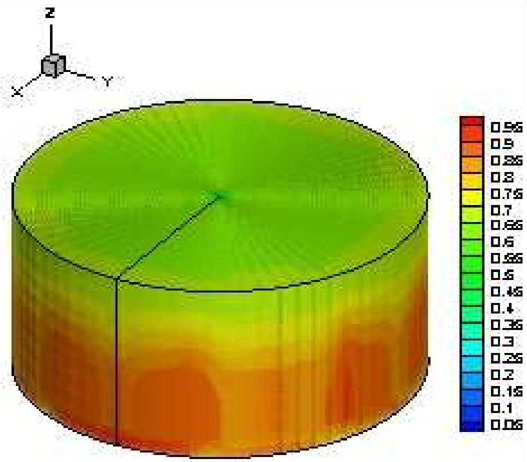
Simulation Results



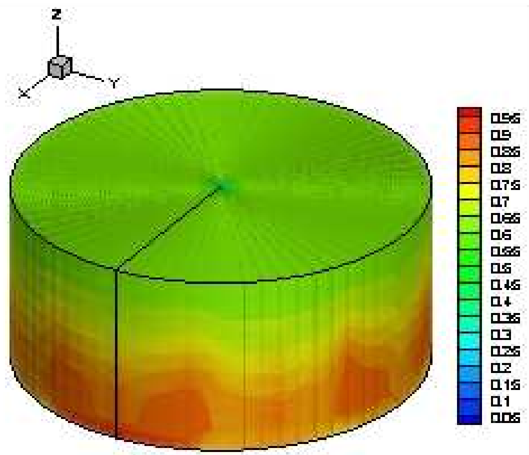
Aquous Saturation after 2 years simulation



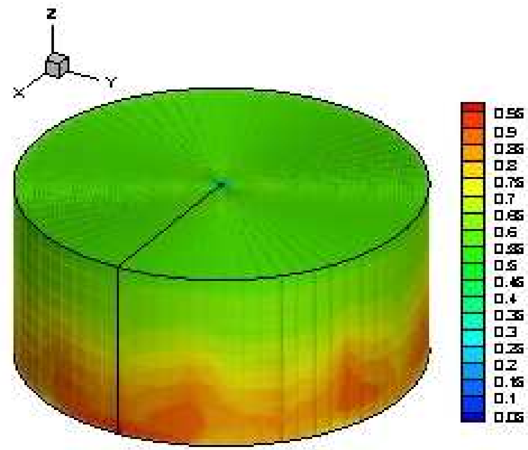
Aquous Saturation after 4 years simulation



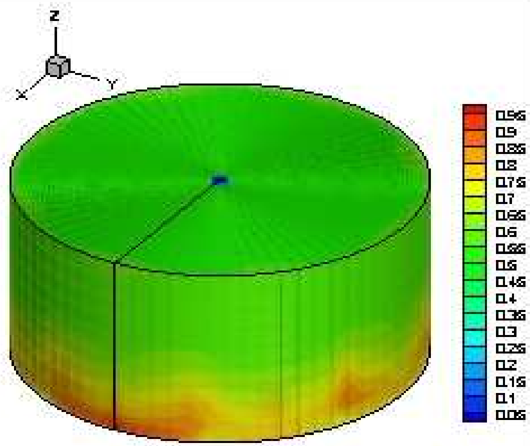
Aquous Saturation after 6 years simulation



Aquous Saturation after 8 years simulation



Aquous Saturation after 10 years simulation



Aquous Saturation after 20 years simulation

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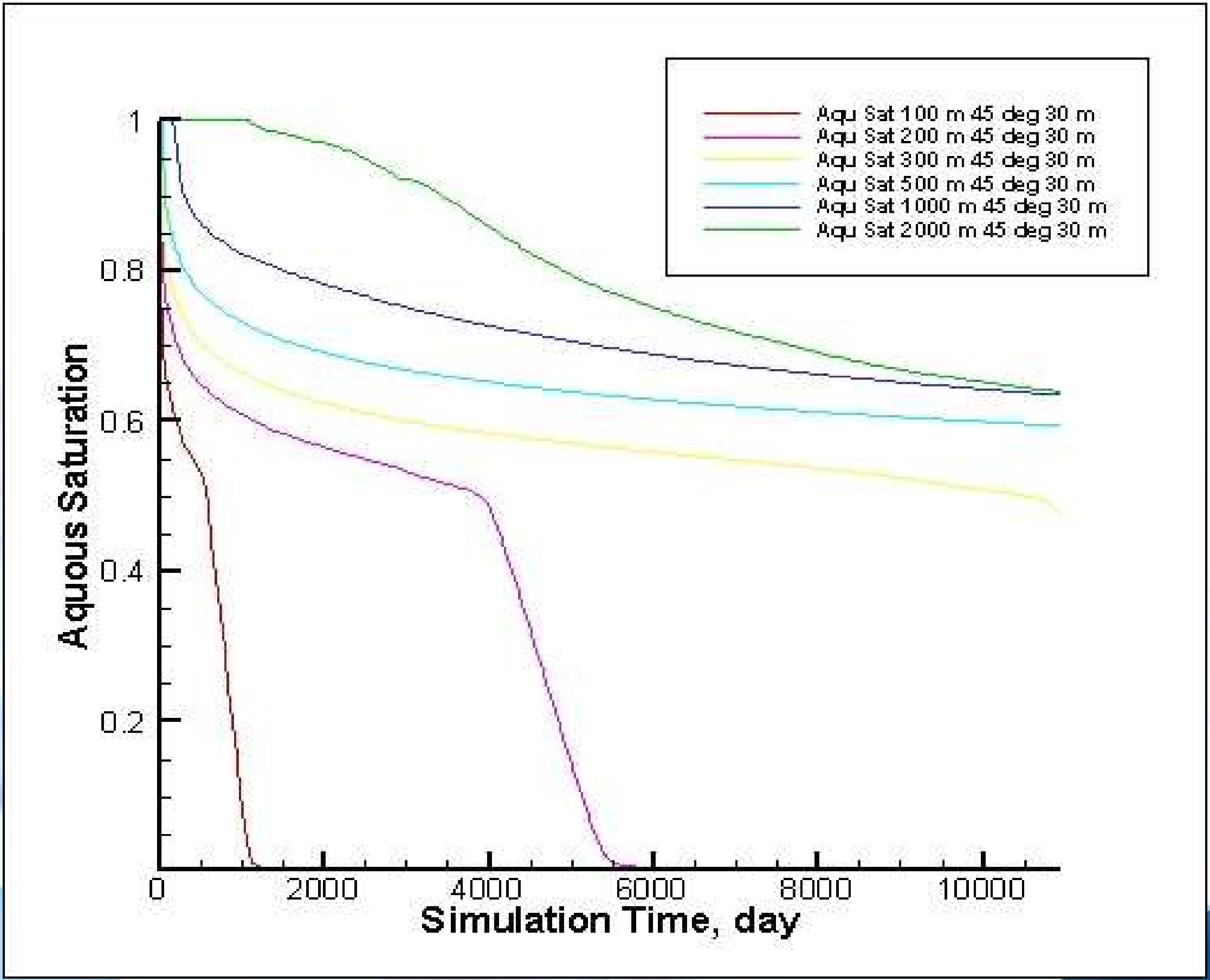
Simulation Results



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

Conclusions

1. Deep saline aquifers have a huge feasibility and potential for CO_2 sequestration
2. CO_2 storage occurs by structural, residual, solubility and mineral trapping mechanisms
3. Buoyancy and capillary forces enhance CO_2 immobilization
4. STOMP simulator is utilized to model CO_2 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.

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2nd Year Report – PhD Project

Chemical Engineering Department – January 2013

Thank You

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