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A NUMERICAL ANALYSIS OF SUPERCRITICAL CO₂ INJECTION INTO GEOLOGICAL FORMATIONS

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KEYWORDS

Modelling Carbon Sequestration, CO₂ Storage Capacity, CO₂ Storage Efficiency, Simulation of CO₂ Sequestration, Injecting CO₂ into Saline Aquifers.

ABSTRACT

One of the most promising means of reducing carbon contents in the ambience and tackling the global warming threat is injecting carbon dioxide into deep saline aquifers (DSAs). Selecting a site to store CO₂ depends on many controlling parameters including permeability, heterogeneity, hydrostatic conditions, injection scenarios and domain grid resolution. In this research study, we aim to investigate the influence of different injection scenarios and flow conditions on the storage capacity and efficiency of CO₂ in geological formations. This is carried out through a series of numerical simulations employed on 3-D hypothetical homogeneous and heterogeneous aquifers utilizing STOMP-CO₂ simulation code. The results of this work are expected to play a key role in providing insight knowledge for assessing the feasibility of various geological formations for CO₂ storage.

1. INTRODUCTION

Injecting CO₂ into deep saline aquifers (DSAs) is one of the most viable means of tackling the global warming arising concern, which has become a critical warning to the universe. This is owing to that these aquifers offer more extensive storage potential than other geological formations and that technology is immediately applicable due to the experience gained from oil and gas exploration and waste disposal methodologies (IPCC, 2005). Consequently, many research studies have been conducted to assess their storage capacity and efficiency to inject and sequester CO₂ safely. In spite of the high uncertainty because of the lack of geological data, these assessments propose considerable value to understand the deployment of CO₂ sequestration in saline aquifers across the globe.

The suitability of any potential storage site CO₂ is assessed based on its geological characteristics including; capacity and injectivity, hydrostatic conditions, the integrity of the cap rock, porosity and permeability.

Theoretically, the storage capacity of an aquifer is the substantial limit of CO₂ that can be admitted into it. However this limit is not practically achievable due to

various geological factors and engineering barriers, therefore a new term called effective storage capacity has been a subject of many researches using different calculation methods. A detailed comparison study by (Goodman et al. 2013) has been conducted to evaluate the impact of a variety of approaches and methodologies on estimating CO₂ sequestration in geological formations. They include; the method employed by Carbon Sequestration Leadership Forum (CSLF) (Bachu et al. 2007), an analytical methodology by (Zhou et al. 2008), and the widely used method by U. S. Department of Energy (US-DOE) which has been adopted in this research work. It assumes infinite-boundary conditions and determines the CO₂ mass storage capacity and efficiency for an aquifer by;

$$G_{CO_2} = A_t h_g \phi_t \rho_{CO_2} E_{aq} \quad (1)$$

Where A_t is the total cross-sectional area of the domain, h_g defines the gross thickness of the formation, ϕ_t is the total porosity of the rock, ρ_{CO_2} and E_{aq} represent CO₂ density and storage efficiency of the aquifer respectively.

A recent method developed by (Szulczewski et al. 2012) considers both residual and solubility trapping mechanisms in addition to the CO₂ migration capacity. Unlike the US-DOE methods, it counts the net thickness of the aquifer to calculate the pores volume.

For the open-boundary systems, the total mass of CO₂ (C_t) in an aquifer can be determined by;

$$C_t = \rho_g L_t W H \phi (1 - S_{wc}) \frac{z}{\epsilon_T} \quad (2)$$

where ρ_g is the density of CO₂, L_t is the migration length, W is the width of the well, H is the net thickness of the aquifer, ϕ is the porosity of the rock, S_{wc} defines the connate water saturation and $\frac{z}{\epsilon_T}$ represent the storage efficiency factor.

For the pressure-limited systems, the CO₂ mass is calculated by;

$$C_p = \rho_g H W \sqrt{\frac{k_{aq} c T}{\mu_w} \frac{P_{frac} - (p_o + \bar{\rho}_w g D)}{4 \tilde{p}_{max}}} \quad (3)$$

Where k_{aq} is the permeability of the aquifer, c is the compressibility, T is the temperature, μ_w is the brine viscosity, P_{frac} is the fracture pressure of the rock.

p_o is the hydrostatic pressure, $\bar{\rho}_w$ is the average density of brine, g is the gravitational acceleration, D is the depth to the top of the aquifer and \tilde{p}_{max} represents the maximum

dimensionless pressure, which can be determined by numerically solving the partial differential equation (PDE) for the pressure-limited flow system.

2. MODEL SETUP

To assess the storage capacity and efficiency in open storage aquifers, a cylindrical computational domain extending from 0.3 m to 6000 m laterally and 96 m vertically, was stipulated with two types of grid resolution namely, coarse and fine grids. For the coarse-grid the domain was discretized with 88 and 24 nodes in the horizontal and vertical directions respectively elements. For the fine resolution, the grid spacing was increased by 100% in both directions. Supercritical CO₂ (ScrCO₂) to be injected into the centre of the domain at a constant rate of 32.0 Kg/s (about 1 MMT/year) which represents a typical benchmark value, via number of cells at the lower section of the reservoir.

The simulation parameters used for this work are based on the geological settings for Sleipner Vest Field which is located in Norwegian part of the North Sea at an approximate depth of 110 m. All petrophysical parameters are listed in Table 1.

Table 1, Lithostratigraphic Division and Petrophysical Parameters from Sleipner Vest Field, after (White et al. 2013).

Parameter	Units	Sands	Shales
Thickness	(m)	30	3
Porosity	-	0.35	0.1025
Horizontal permeability	(m ²)	3.0e ⁻¹³	0.1e ⁻¹³
Vertical permeability	(m ²)	3.0e ⁻¹³	0.1e ⁻¹³
Density	(kg/m ³)	2650	
Pore Compressibility	(Pa ⁻¹)	4.5e ⁻¹⁰	
Aquifer pressure	(MPa)	11.2	
Pressure gradient	(KPa/m)	10.012	
Aquifer temperature	(°C)	37	
Salinity	Wt%	0.032	
Aquifer depth	(m)	800-1100	
Water depth	(m)	110	

The CO₂ properties adopted in our simulation code have been arranged in a data table developed from the equation of state by (Span and Wagner 1996). The phase equilibria calculations in STOMP-CO₂ code are conducted via a couple of formulations by (Spycher et al. 2003) and (Spycher and Pruess 2010) that are based on Redlich-Kwong equation of state with fitted experimental data for water-CO₂ flow systems. Details of these equations can be found in the STOMP-CO₂ guide by (White et al. 2013).

Aqueous saturation (S_w) is calculated by (Van Genuchten 1980) formulation that correlates the capillary pressure (P_c) to the effective saturation (S_e);

$$S_e = \frac{S_w - S_{wr}}{1 - S_{wr}} = [1 + (\alpha \cdot P_c)^n]^m \quad \text{for } P_c > 0 \quad (4)$$

Where S_{wr} is the water residual saturation and α , n and m are the Van Genuchten parameters that describe the characteristics of the porous media. Formulations factors used in the equations above are listed in Table.2.

Table 2, Functions Parameters of the simulated aquifer, after (White et al. 2013*, Holtz 2002**).

Description	Symbol	Value	Units
Irreducible aqueous saturation*	S_{lr}	0.2	-
Irreducible gas saturation*	S_{gr}	0.05	-
Van Genuchten parameter for (Sand)*	α	2.735	m ⁻¹
Van Genuchten parameter for (Shale)*	α	0.158	m ⁻¹
Saturation function parameters*	m	0.4	-
	n	1.667	-
Pore index parameter	λ	0.667	-
Max. residual gas sat. for aquifer**	S_{grm}	0.208	-
Max. residual gas sat. for aquitard**	S_{grm}	0.448	-

During the injection period (drainage process), there is no gas entrapment therefore the injected CO₂ can be either existed as free or trapped gas. STOMP-CO₂ code deploys a model developed by (Kaluarachchi and Parker 1992) to compute the potential effective trapped gas by;

$$\hat{S}_{gt}^{potential} = \left[\frac{1 - \hat{S}_l^{min}}{1 - R(\hat{S}_l^{min})} \right] \quad (5)$$

Where \hat{S}_l^{min} is the minimum aqueous saturation and R is the Land's parameter (Land 1968) which relates to the maximum trapped gas saturation;

$$R = \frac{1}{\hat{S}_{gt}^{max}} - 1 \quad (6)$$

The aqueous and gas relative permeabilities are computed by (Mualem 1976) correlation in combination with (Van Genuchten 1980) formulation according to the following Equations (7) and (8) respectively;

$$k_{rl} = (\bar{S}_l)^{1/2} \left[1 - \left(1 - \left(1 - (\bar{S}_l)^{1/m} \right)^m \right) \right]^2 \quad (7)$$

$$k_{rg} = (1 - \bar{S}_l)^{1/2} \left[1 - \left(1 - \left(1 - (\bar{S}_l)^{1/m} \right)^m \right) \right]^2 \quad (8)$$

Where m is the pore distribution index, \bar{S}_l is the effective aqueous saturation which is calculated from Eq.(4) and \bar{S}_l represents the apparent aqueous saturation which is defined as the sum of the effective aqueous and entrapped CO₂ saturations (White and Oostrom et al. 2004).

3. INITIAL AND BOUNDARY CONDITIONS

The simulated domains adopted in this study are assumed to be isotropic and isothermal under hydrostatic pressure gradient of 10.012 KPa/m with an open boundary condition. The domains are symmetrical with no heterogeneity in the azimuthal direction. The aquifer is considered to be fully saturated with brine prior to injecting ScrCO₂ with initial conditions illustrated in Table 1. No flux boundary condition is considered for the aqueous wetting phase (brine) at the injection well border as a West boundary whilst the East boundary was set to be infinite with zero flux for CO₂. Zero flux is also considered at the top and bottom confining layers with the ignorance of gravity and inertial effects.

The injection rate for our system was set according the fracture pressure (P_{frac}) using the simplified model

adopted by (Szulczewski, MacMinn et al. 2011) which calculates the pressure-limited storage capacity by;

$$M_p = 2\rho_{CO_2}HW\sqrt{\frac{kC}{\mu_b T}}\frac{P_{frac}}{\hat{p}_{max}} \quad (9)$$

Where all variable defined in Eq.(3) above.

For infinite aquifer, the value of the maximum dimensionless pressure (\hat{p}_{max}) in Eq.(9) is about 0.87 (Szulczewski, MacMinn et al. 2011). All parameters in Eq.(9) are known except the fracture pressure of the rock which can be defined as the effective vertical stress for deep aquifers and determined by Eq.(10) (Szulczewski 2009);

$$\sigma'_v = (\rho_b - \rho_w)Z \quad (10)$$

Where ρ_b , ρ_w represent bulk and brine densities respectively and Z is the depth of the aquifer.

From equations (9-10) we set the value of the injection rate for our model at 32 Kg/s. According to Eq. (9), this rate results pressure build-up values less than 1.5 magnitudes of the hydrostatic pressure that are far away from the average default values of the sustainable pressure.

4. METHODOLOGY

Generally CO₂ sequestration efficiency in saline aquifers can be assessed by using the equation developed by USDOE (Wang et al. 2013);

$$E_{aq} = \frac{G_{CO_2}}{A_t h_g \phi_{tot} \rho} \quad (11)$$

Where G_{CO_2} is the mass of CO₂, A_t , h_g and ϕ_{tot} represent the area, thickness and average porosity of the aquifer respectively. ρ , is the density of CO₂.

In this study case we used an archetype of actual field heterogeneity in a domain that consists of three stratum of sands intermingled with two layers of low permeability shales. Six simulation cases (presented in Table 3.) were setup to demonstrate different models of the computational domain.

Table 3. Simulation Cases and Conditions

Case No.	Domain	Heterogeneity	Grid	Nodes (r,θ,z)	Injection scheme
1	Homogeneous	N/A	coarse	88,1,24	30 yrs continuous
2	Heterogeneous	uniform	coarse	88,1,24	30 yrs continuous
3	Heterogeneous	non-uniform	coarse	88,1,24	30 yrs continuous
4	Heterogeneous	non-uniform	coarse	88,1,24	batch* 10-5-10-5-10
5	Homogeneous	N/A	coarse	88,1,24	batch* 10-5-10-5-10
6	Homogeneous	N/A	Fine +100%	176,1,48	30 yrs continuous

* Batch injection schemes refer to the years of (injection – stop – injection – stop – injection).

The first injection scheme involved 30 years of continuous injection and in the second scenario the injection period was divided into three stages of 10 years separated by two

stopping periods of 5 years in between. In all cases, the total simulation time was 5000 years including injection and stopping times.

Because of the density difference driving forces between the injected CO₂ and the existing brine, initially the former percolates upward to be trapped under the upper impermeable layer. During this time, part of the gas dissolves in the brine forming an aqueous phase rich of CO₂ which is heavier than the ambient liquid and hence sinks down to settle at the bottom of the aquifer. As soon as the injection stops the replaced water (brine) invades the domain to reinstate the CO₂ leaving some traces of it behind in some small-sized pores in a process called residual or capillary trapping. These amounts of CO₂ are determined by the simulation code for different cases and utilized to calculate the capacity and efficiency factor of the simulated aquifer;

$$\text{Total integrated CO}_2 = \text{Integrated aqueous CO}_2 (CO_2^{aq}) + \text{Integrated gas CO}_2 (CO_2^g) \quad (12)$$

$$CO_2^g = \text{Trapped gas } (CO_2^{gt}) + \text{Free gas } (CO_2^{gf}) \quad (13)$$

$$E_{aq}^{perm} = \frac{CO_2^{aq} + (CO_2^{gt})}{A_t h_g \phi_{tot} \rho} \quad (14)$$

Where all parameters were explained in Eqs.11.

In our work the focus is on the storage efficiency of the aquifer in terms of the permanent sequestration of the injected CO₂ which in our case of study, occurs mainly through solubility and residual trapping due to the insignificant influence of the mineral trapping mechanism before few thousands of years (De Silva and Ranjith 2012).

5. RESULTS AND DISCUSSIONS

To assess our numerical simulation validity we plotted the results versus the similarity variable (r^2/t) that relates the variable dependence on both lateral distance and simulation time for four time steps at a radial distance of 500 m, (O'Sullivan 1981, Doughty, Pruess 1992). Fig. 1 presents changes in the average capillary pressure values with the similarity variable. The plot shows excellent agreement for all time steps, which reflects the high accuracy of our simulation results.

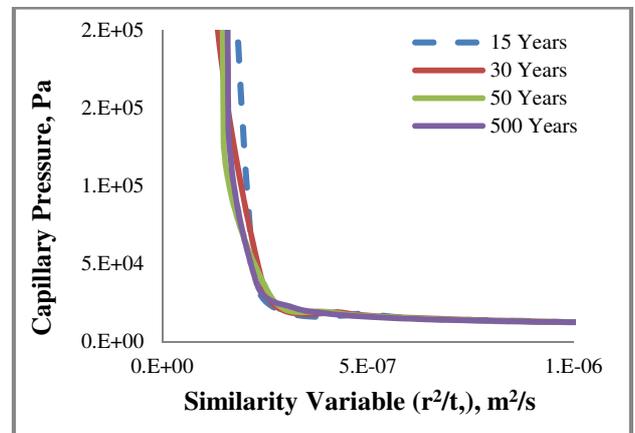


Figure1. Capillary Pressure Development as a function of the Similarity Variable at 500 m radial distance.

5.1. Impact of Heterogeneity

To investigate the impact of heterogeneity on the propagation of CO₂ profiles, saturation-capillary pressure relationships and storage efficiency, three numerical cases (1, 2 and 3) with their employed conditions illustrated in Table 3. have been developed in this study.

Permeability of geological formations is strongly related to their porosity any heterogeneity, which is a key role in controlling water-CO₂, flow in sequestration sites. Heterogeneity is found to have significant impact on capillary pressure-saturation relationships as illustrated in Fig.2, which demonstrates significantly higher values of capillary pressure for both heterogeneous domains.

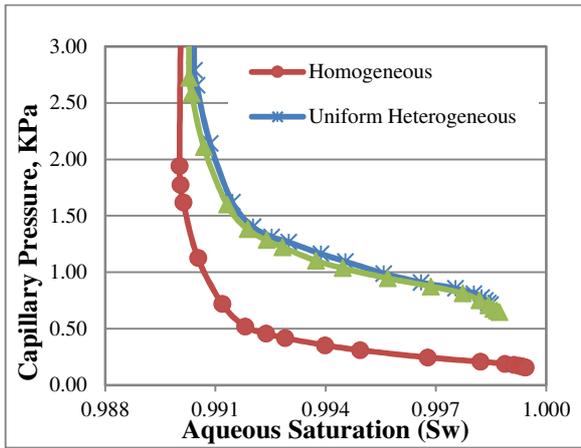


Figure 2. Effect of Heterogeneity on Saturation-Capillary Pressure relationships.

This influence is evidently reflected on the amount of trapped CO₂ because higher values were achieved in heterogeneous formations. This is owing to the existence of intermingled layers of shale that restrict the injected gas from moving between layers of the domain which results in less contact with brine and consequently less subjectivity of gas entrapment in more small-sized pores.

Fig.3 demonstrates no effect of heterogeneity on CO₂ solubility before 800 years of simulation. After this time, it is observed that more CO₂ dissolved in the homogeneous domain compared to both types of heterogeneous ones by about 15% at 2000 years of simulation.

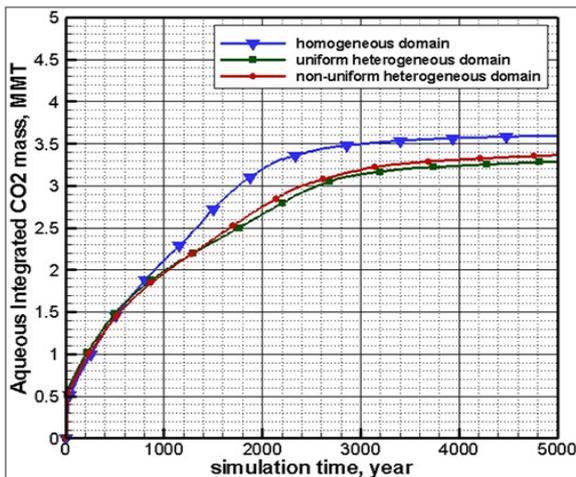


Figure 3. Effect of Heterogeneity on CO₂ Solubility.

5.2. Impact of Cyclic Injection

To inspect the effect of cyclic injection of CO₂ on the characteristics of sequestration in saline aquifers, four schemes of injection were employed in cases 1, 3, 4 and 5 (shown in Table 3) using continuous and cyclic injection scenarios in different porous domains. Injected CO₂ distribution contours after 100 years of simulation in Fig.4 display almost equal maps of carbon dioxide distribution in the homogeneous domain for both continuous and cyclic injection of 30 years. However, the impact of injection scenario is more obvious in the heterogeneous domain map in Fig.5(c-d) where more gas is exposed to be dissolved or trapped in the lower and middle segments of the domain for cyclic injection.

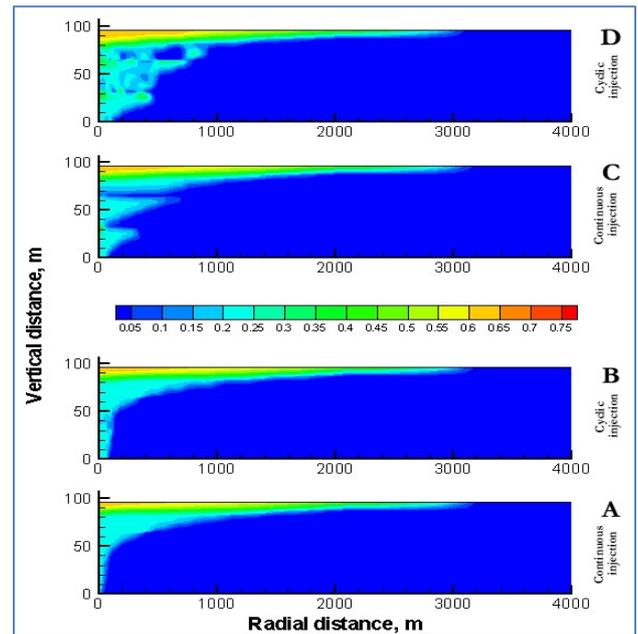


Figure 4. CO₂ plume evolution in Cyclic and Continuous schemes of injection.

Additionally, results reveal no effect on the amount of CO₂ dissolution in homogeneous domain as demonstrated in Fig.5 however less dissolved CO₂ was achieved in the case of cyclic injection into heterogeneous domain after 2000 years.

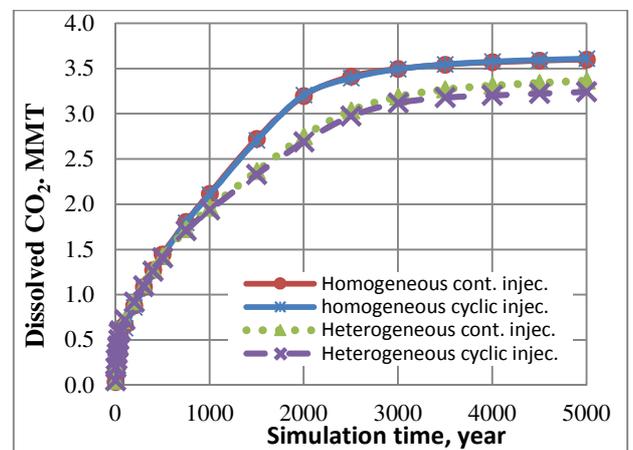


Figure 5. Effect of Injection scheme on CO₂ Solubility.

Similarly, for trapped CO₂, no sensitive impact of cyclic injection was observed for homogeneous media in spite of a slight difference shown in Fig.6 after 3500 years of simulation. Residual trapping of CO₂ in heterogeneous media was found to be more sensitive to injection method because simulation results revealed that more CO₂ was trapped in cyclic injection case compared to continuous one specifically after 300 years as illustrated in Fig.6.

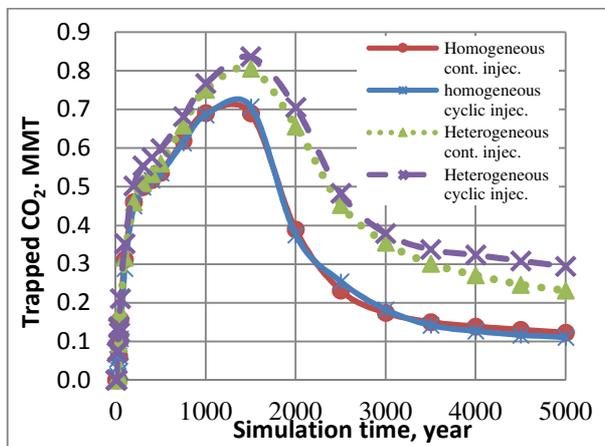


Figure 6. Effect of Injection scheme on Residual Trapping of CO₂.

According to the attained results, injection scheme appears to have no influence on the storage efficiency of CO₂ in geological formations. However, more research work is required to investigate the optimization of the cyclic injection in terms of injection and stopping intervals in long-term sequestration projects.

6. CONCLUSIONS

A set of numerical simulation cases were developed and conducted using STOMP-CO₂ simulation code to investigate the influence of various types of heterogeneity, injection schemes and grid resolution on CO₂-water flow system behaviour and storage efficiency in saline aquifers. The conclusions of the results can be summarized as follows;

- 1- Heterogeneity has significant impact on saturation-capillary pressure relationships because results demonstrated greater values of capillary pressure at any specific saturations in heterogeneous domains compared to homogeneous ones. Consequently, this amplifies the residual trapping of the injected gas in heterogeneous geological formations.
- 2- The presence of intermingled layers of shales in sand rocks increases the storage efficiency to a limited extent because it promotes more CO₂ dissolution in the existed brine by restricting the vertical migration of the injected gas and maintaining more contact with the hosted brine.
- 3- Using cyclic injection scheme appeared to have no sensitive influence on the storage efficiency of CO₂ in geological formations in medium terms of sequestration however; this finding requires more research work to investigate the impact of CO₂ injection methodology in closed aquifers for longer terms of sequestration.

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REFERENCES

- Bachu, S., Bonijoly, D., Bradshaw, J., Burruss, R., Holloway, S., Christensen, N.P. and Mathiassen, O.M., 2007. *CO₂ storage capacity estimation: Methodology and gaps*. International Journal of Greenhouse Gas Control, 1(4), pp. 430-443.
- De Silva, P.N.K. and Ranjith, P.G., 2012. *A study of methodologies for CO₂ storage capacity estimation of saline aquifers*. Fuel, 93(0), pp. 13-27.
- Doughty, C. and Pruess, K., 1992. *A similarity solution for two-phase water, air and heat flow near a linear heat source in porous medium*. Journal of Geophysical Research, 97(B2), pp. 1821-1838.
- Goodman, A., Bromhal, G., Strazisar, B., Rodosta, T., Guthrie, W.F., Allen, D. and Guthrie, G., 2013. *Comparison of methods for geologic storage of carbon dioxide in saline formations*. International Journal of Greenhouse Gas Control, 18, pp. 329-342.
- IPCC, 2005. *Carbon dioxide capture and storage*. IPCC Special Report. Cambridge University Press: Prepared by Working Group III of the Intergovernmental Panel on Climate Change.
- Kaluvarachchi, J.J. and Parker, J.C., 1992. *Multiphase flow with a simplified model for oil entrapment*. Transport in Porous Media, 7, pp. 1-14.
- Land, C.S., 1968. *Calculation of imbibition relative permeability for two- and three-phase flow from rock properties*. Trans. Am. Inst. Min. Metall. Pet. Eng, 243, pp. 149-156.
- Mualem, Y., 1976. *A new model for predicting the hydraulic conductivity of unsaturated porous media*. Water Resources Research, 12(3), pp. 513-522.
- O'sullivan, M.J., 1981. *A similarity method for geothermal well test analysis*. Water Resour. Res., doi:10.1029/WR017i002p00390, 17(2), pp. 390-398.
- Span, R. and Wagner, W., 1996. *A new equation of state for carbon dioxide covering the fluid region from the triple-point temperature to 1100 K at pressures up to 800 MPa*. Journal of physical and chemical reference data, 25(6), pp. 1509-1596.
- Spycher, N. and Pruess, K., 2010. *A Phase-Partitioning Model for CO₂-Brine Mixtures at Elevated Temperatures and Pressures: Application to CO₂-Enhanced Geothermal Systems*. Transport in Porous Media, doi:10.1007/s11242-009-9425-y, 82, pp. 173-196.

Spycher, N., Pruess, K. and Ennis-King, J., 2003. CO₂ - H₂O mixtures in the geological sequestration of CO₂. I. *Assessment and calculation of mutual solubilities from 12 to 100°C and up to 600 bar*. *Geochimica et Cosmochimica Acta*, **67**(16), pp. 3015-3031.

Szulczewski, M.L., 2009. *Storage capacity and injection rate estimates for CO₂ sequestration in deep saline aquifers in the conterminous United States*. Diss. Massachusetts Institute of Technology.

Szulczewski, M.L., Macminn, C.W. and Juanes, R., 2011. *How pressure buildup and CO₂ migration can both constrain storage capacity in deep saline aquifers*. *Energy Procedia*, **4**, pp. 4889–4896.

Szulczewski, M.L., Macminn, C.W., Herzog, H.J. and Juanes, R., 2012. *Lifetime of carbon capture and storage as a climate-change mitigation technology*. *Proceedings of the National Academy of Sciences of the United States of America*, **109**(14), pp. 5185-5189.

Van Genuchten, M.T., 1980. *A closed-form equation for predicting the hydraulic conductivity of unsaturated soils*. *Soil Science Society of America Journal*, **44**(5), pp. 892-898.

Wang, Y., Zhang, K. and Wu, N., 2013. *Numerical Investigation of the Storage Efficiency Factor for CO₂ Geological Sequestration in Saline Formations*. *Energy Procedia*, **37**(0), pp. 5267-5274.

White, M.D., Oostrom, M. and Lenhard, R.J., 2004. *A Practical Model for Mobile, Residual, and Entrapped NAPL in Water-Wet Porous Media*. *Ground Water*, **42**(5), pp. 734-746.

White, M.D., Watson, D.J., Bacon, D.H., White, S.K., Mcgrail, B.P. and Zhang, Z.F., 2013. *STOMP- Subsurface Transport Over Multiple Phases- STOMP- CO₂ and - CO₂ e Guide, Version 1.1*. Pacific Northwest National Laboratory, Prepared for the U.S. Department of Energy under Contract DE-AC05-76RL01830, .

Zhou, Q., Birkholzer, J.T., Tsang, C. and Rutqvist, J., 2008. *A method for quick assessment of CO₂ storage capacity in closed and semi-closed saline formations*. *International Journal of Greenhouse Gas Control*, **2**(4), pp. 626-639.