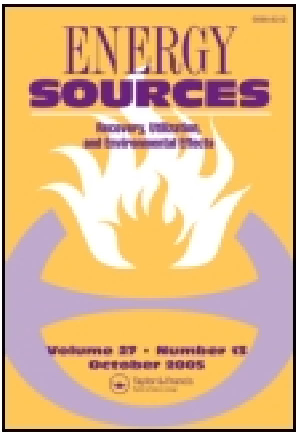

Energy Sources, Part A: Recovery, Utilization, and Environmental Effects

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/ueso20

Analytical and Numerical Modeling of CO_2 Sequestration in Deep Saline Aquifers

E. Ozgur [a] & F. Gümrah [a]

[a] Middle East Technical University, Petroleum and Natural Gas Engineering Department, İnönü Bulvar1, Ankara, Turkey

To cite this article: E. Ozgur & F. Gümrah (2010): Analytical and Numerical Modeling of CO_2 Sequestration in Deep Saline Aquifers, Energy Sources, Part A: Recovery, Utilization, and Environmental Effects, 32:7, 674-687

To link to this article: http://dx.doi.org/10.1080/15567030802606145

Energy Sources, Part A, 32:674–687, 2010

ISSN: 1556-7036 print/1556-7230 online
DOI: 10.1080/15567030802606145

Analytical and Numerical Modeling of CO_2 Sequestration in Deep Saline Aquifers

E. OZGUR[1] and F. GÜMRAH[1]

[1]Middle East Technical University, Petroleum and Natural Gas Engineering Department, İnönü Bulvarı, Ankara, Turkey

Abstract *The analytical and numerical modeling of CO_2 sequestration in deep saline aquifers having different rock and fluid properties was studied under diffusion and convection mechanisms. In a diffusion dominated system, an aquifer with 100 m thickness was saturated with CO_2 after 10,000,000 years. It was much earlier in a convective dominant system. In the diffusion process, the dissolution of CO_2 in aquifer increased with porosity increase; however, in a convection dominant process dissolution of CO_2 in aquifer decreased with porosity increase. The increase in permeability accelerated the dissolution of CO_2 in aquifer significantly, which was due to increasing velocity. The dissolution process in the aquifer was realized faster for the aquifers with lower dispersivity. The results of convective dominant mechanism in aquifers with 1 md and 10 md permeability values were close to that of the diffusion dominated system. For the aquifer having permeability higher than 10 md, the convection mechanism began to dominate gradually and it became a fully convection dominated system for 50 md and higher permeability values. These results were also verified with calculated Rayleigh numbers.*

Keywords CO_2 sequestration, convection, deep saline aquifer, diffusion, modeling, Rayleigh number

Introduction

Consuming fossil fuels, industrial activities, and deforestation of lands are increasing the atmospheric concentrations of carbon dioxide, methane, nitrous oxide, hydrofluorocarbons, perfluorocarbons, and sulfur hexafluoride day by day.

One way to protect the climate of our world is to prevent the release of CO_2 to the atmosphere or decrease its amount in the atmosphere by storing it in geological reservoirs. There are many options to store CO_2 in geological reservoirs, such as, depleted oil and gas reservoirs, coal beds, and deep saline aquifers. Deep saline aquifers have the potential to provide very large storage capacity worldwide at relatively low cost. There are a number of locations where deep saline aquifers have been used for natural gas storage, giving confidence that CO_2 could be stored safely for thousands of years in carefully selected saline aquifers (IEA, 2006).

There are three main trapping mechanisms for the immobilization of CO_2 in deep saline aquifers: gaseous phase storage under caprock, which is called hydrodynamic trapping; trapping of CO_2 as dissolved solute in the aqueous phase, which is called

Address correspondence to E. Ozgur, Middle East Technical University, Petroleum and Natural Gas Engineering Department, İnönü Bulvarı, Ankara 06531, Turkey. E-mail: eozgur@metu.edu.tr

solubility trapping; and trapping of CO_2 in stable minerals due to the reactions in the aquifer, which is called mineral trapping (Noh et al., 2004).

In this study, the transport of CO_2 dissolved in brine is examined by molecular diffusion and mechanical dispersion mechanisms. In the solubility trapping part, the effect of aquifer properties on the transportation of injected CO_2 is analyzed with analytical and numerical modeling approaches.

Transport Mechanisms

Solutes dissolved in groundwater are transported by the mechanisms: molecular diffusion, mechanical dispersion, and convection. The sum of the molecular diffusion and mechanical dispersion are called as hydrodynamic dispersion. All mechanisms may operate simultaneously or individually in flowing groundwater (Gorelick et al., 1993).

Molecular Diffusion

Molecular diffusion is caused by random molecular motions due to thermal kinetic energy of the solute (Domenico and Schwartz, 1998).

Fick's Second Law is used in non-steady diffusion as written in Eq. (1). In non-steady diffusion process, the concentration within the diffusion volume changes with respect to time:

$$D_e \frac{\partial^2 c}{\partial z^2} = \frac{\partial c}{\partial t}. \qquad (1)$$

The diffusion coefficient of a solute in water in a porous medium is smaller than in pure liquids. As the porosity of the medium decreases, the diffusion coefficent of a solute in water in a porous medium decreases. This is primarily due to the collision of solutes with the solids of the medium, which makes diffusion difficult in porous medium (Anderson, 1984). The effects of porosity and longer pores are often lumped together in the definition of an effective molecular diffusion coefficient (D_e) in Eq. (2) (Cussler, 1997), as shown below:

$$D_e = \frac{D_o \phi}{\tau}, \qquad (2)$$

where D_e is the effective diffusion coefficient within pores, D_o is the molecular diffusion coefficient within pores, ϕ is porosity, and τ is the tortuosity.

Unver and Himmelblau (1964) developed the quadratic molecular diffusion coefficient (D_o) equation for the temperature range 6 to 65°C at atmospheric pressure. Although results are valid at an atmospheric pressure, the trend is similar with temperature change at different pressures.

According to the work of Hirai et al. (1997), the diffusion coefficient between the gaseous CO_2 and liquid water changes with pressure very little. The measured values of Shimizu et al. (1995) are 40% larger than that of the Wilke-Chang equation, whereas Hirai et al.'s measured diffusion coefficients agree with the Wilke-Chang equation fairly well (Wilke and Chang, 1955). Although there are some differences between the results, it could be said that the diffusion coefficient of CO_2-H_2O system changes with pressure insignificantly. The trend is also similar for different temperatures based on Wilke-Chang equation. So the effect of pressure to diffusion coefficient of CO_2 is neglected in this study.

Convection

Convection is the movement of dissolved solutes with flowing stream in porous media (Bedient et al., 1994). When only convection process is considered, solutes move at the same rate with flowing stream without dispersing. But this is not possible in porous media due to the velocity profile of water in pores and heterogeneities in the medium; therefore, dispersion occurs when convection takes place in porous media. Sometimes, the term "advection" could be encountered in the literature when dealing with groundwater systems. The term advection is generally used for the horizontal movement of groundwater in porous media and the term convection is used for the vertical movement of groundwater in porous media.

In the aquifer, molecular diffusion normally arises due to the concentration difference in brine. But for the occurence of convection, concentration difference or density difference in the brine is not enough due to other parameters of the reservoir, such as permeability, porosity, aquifer height, and fluid properties like viscosity. The height of the aquifer has an important effect on the velocity of the brine column during natural convection and the velocity of the brine column could be determined from Eq. (3):

$$u = \frac{k.g.\Delta\rho}{\mu}. \tag{3}$$

The occurrence of convection could be determined by the dimensionless solutal Rayleigh number in Eq. (4). The equation consists of parameters that form the velocity term. Solutal Rayleigh number (Ra) determines if convection will begin or not. After a critical solutal Rayleigh number, convection starts to take place. The critical solutal Rayleigh number depends on the shape of the fluid system and the boundary conditions. For a fluid layer between two boundaries, constant concentration top boundary and impermeable bottom boundary, the critical solutal Rayleigh number has been computed theoretically to be $4\pi^2$ (approximately 39.48) for the occurence of convection process (Weatherill et al., 2004).

$$Ra = \frac{kg\Delta\rho H}{D_o\mu\phi} \tag{4}$$

Dispersion

There are three basic causes of pore-scale longitudinal dispersion (Fetter, 1994): (i) As groundwater moves through pores, it will move faster through the center of the pore than along the edges. (ii) Fluid that travels through larger pores will travel faster than fluid moving in smaller pores. (iii) Some of the fluid will travel in longer pathways than other fluid. The longer pathways are caused due to the tortuousity of an aquifer and in more tortuous aquifer dispersion increases.

The degree of the dispersion is expressed with a parameter "dispersivity" (α). Dispersivity is a property of an aquifer and scale dependent. There are many definitions about dispersivity term in the literature. Lake defined the dispersivity as "a measure of the local heterogeneity scale" (Lake, 1989). The dispersivity in the flow direction is called longitudinal dispersivity (α_L) and its value is generally 10% of flow length (Gelhar et al., 1992). Dispersion could take place in all directions or in one direction according to the aquifer and boundary conditions. However, when the flowing groundwater column enters over a broad front, the effects of transverse dispersion within the zone cancel each other due to the absence of concentration gradient, and only longitudinal dispersion needs to be considered as if one dimensional flow is occurring (Bouwer, 1978). Increasing anisotropy and heterogeneity increases the magnitude of dispersion but even in homogeneous medium dispersion occurs due to velocity profile.

Physical Properties of Water

The dissolved CO_2 has the effect of increasing water density, by up to 2–3% in the temperature range of 5–300°C (Enick and Klara, 1990). Garcia found a relationship for the apparent molar volume of CO_2 for the temperatures lower than 300°C on the basis of 53 data points where the effect of pressure is negligible (Garcia, 2001). The dissolved CO_2 in brine causes 1% change in brine density at aquifer conditions. Bachu and Adams (2003) used the mass conservation principle for determining the effect of solute on brine density.

There is no empirical equation in the literature for the effect of dissolved CO_2 on water viscosity. Tumasjan et al. (1969) published their experimental results for the water viscosity change with CO_2 and it changes insignificantly with CO_2 saturation. The viscosity change of brine with CO_2 saturation is neglected in the study.

Analytical Modeling

The transport of CO_2 in an aquifer is analyzed with diffusion-convection as shown in Eq. (5). The reasonable assumptions are done for the calculation of CO_2 distribution in the aquifer to simplify the problem. By considering the CO_2 cap as a boundary condition, the flow is assumed to be one-dimensional vertical flow in the aquifer. The pressure of CO_2 cap is also assumed as constant throughout the transport to develop an analytical solution for the diffusive and convective mixing process. The temperature along the aquifer is taken as constant. Besides, the velocity of brine column that arose from density difference is assumed as constant to develop an analytical solution for convective mixing process in analytical modeling part. Chemical reactions that could occur between brine-CO_2-rock are neglected in the study, because these processes take place generally in a very long period and the assumption is also made for the simplicity to enable the comparison between analytical and numerical modeling in the study.

$$D_e \frac{\partial^2 c}{\partial z^2} - \frac{u}{\phi}\frac{\partial c}{\partial z} = \frac{\partial c}{\partial t} \tag{5}$$

The hypothetical model is shown in Figure 1. There is a gas cap formed of CO_2 above the brine in the aquifer. The CO_2 diffuses into brine by time and the density of brine increases due to saturation by CO_2. The density increase in the upper layer of brine causes convection effect by the movement of layers. Beside this, it is assumed that CO_2 is injected periodically into gas cap to keep the pressure of the gas cap constant. The following assumptions are considered for the development of an analytical model:

- Isotropic homogenous medium.
- One dimensional diffusion in vertical direction.
- Gas cap is formed due to CO_2 injection.
- Initial CO_2 concentration is zero in the aquifer.
- Possible chemical reactions in the aquifer are neglected.
- Gravity tonguing and viscous fingering effects are neglected.

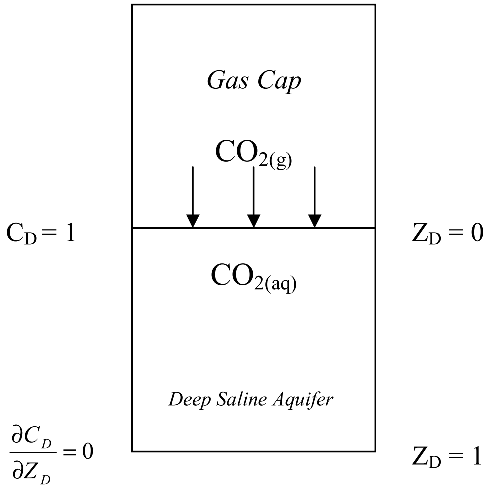

Figure 1. Geometry and boundary conditions of the model.

- Upper boundary's CO_2 concentration and pressure are taken as constant assuming the gas cap is filled with CO_2 periodically.
- Temperature is constant in the model of environment.
- The water in the medium and CO_2 in the gas cap cannot escape through the boundaries of the aquifer.
- The velocities are in terms of average values and 1% brine density difference for convection is used in the calculation of maximum velocity.

Analytical Solutions

The initial and boundary conditions are also defined in the hypothetical model for solving the problem for diffusion and convection dominated systems.

Initial Condition:

$$C_D = 0 \text{ for } t_D = 0 \text{ and for all } Z_D \tag{6}$$

Boundary Conditions:

$$\text{At } Z_D = 0\text{: } C_D = 1 \text{ for } t_D > 0 \tag{7}$$

$$\text{At } Z_D = 1\text{: } \frac{\partial C_D}{\partial Z_D} = 0 \tag{8}$$

where the dimensionless groups are

$$C_D = \frac{C_{CO_2}}{C_{CO_2,sat}} \tag{9}$$

$$Z_D = \frac{z}{H} \tag{10}$$

$$t_D = \frac{u.t}{\phi.H} \tag{11}$$

Diffusion-Dominated Mechanism

For only diffusion dominant process in the aquifer, the behavior of molecular diffusion can be expressed with Eq. (1) and its analytical solution is given in Eq. (12) (Cussler, 1997), as follows:

$$\frac{C(z,t)}{C_o} = erfc\left[\frac{z}{2\sqrt{D_e.t}}\right]. \tag{12}$$

Convection-Dominated Mechanism

If there is a vertical convection, Eq. (5) is used as a diffusion-convection equation. Equation (5) could be arranged in dimensionless form to make the equation unique with given boundary conditions as in Eq. (13) (Lake, 1989):

$$\frac{1}{N_{Pe}}\frac{\partial^2 C_D^2}{\partial Z_D^2} - \frac{\partial C_D}{\partial Z_D} = \frac{\partial C_D}{\partial t_D}, \tag{13}$$

where the Peclet number is given as

$$N_{Pe} = \frac{u.H}{\phi.D_e}, \tag{14}$$

where the effective diffusion coefficient for convection dominated systems is

$$D_e = \frac{D_o.\phi}{\tau} + \alpha.v. \tag{15}$$

By using the given boundary conditions, the final dimensionless CO_2 concentration becomes Eq. (16), which is an exact analytic solution for Eq. (5) (Lake, 1989):

$$C_D = \frac{1}{2}erfc\left(\frac{z_D - t_D}{2\sqrt{\frac{t_D}{N_{Pe}}}}\right) + \frac{e^{z_D N_{Pe}}}{2}erfc\left(\frac{z_D + t_D}{2\sqrt{\frac{t_D}{N_{Pe}}}}\right) \tag{16}$$

Numerical Modeling

Numerical reservoir simulations are used to combine the geological and engineering data to make estimations about the field performance by using any numerical methods. The solutions of problematic cases are easily made with these numerical reservoir simulations. The numerical solutions of the cases are realized with the computer program SEAWAT. SEAWAT is used for the simulation of transient three-dimensional flow of variable-density groundwater in porous media. SEAWAT-2000 was designed by combining a modified version of MODFLOW-2000 and MT3DMS into a single computer program. SEAWAT-2000 models all of the flow and variable-density transport processes.

Results and Discussion

The common data to be used in the analytical and numerical models are given in Table 1. The other conditions for analytical and numerical runs are given in Tables 2 and 3.

Table 1
Common data to all runs given in Tables 2 and 3

Data	Value
Aquifer thickness, m	100
Viscosity of water, cp	0.7
Temperature, °C	50
Pressure, atm	75
Aquifer top, m	850
Aquifer bottom, m	950
Molecular diffusion coefficient of CO_2 in water, cm^2/s	3.10^{-5}

Table 2
Run conditions for analytical and numerical modeling with only molecular diffusion

Run cases	Time, y	Porosity, fraction
1a	5,000	0.2
1b	10,000	0.2
1c	20,000	0.2
1d	100,000	0.2
1e	10,000,000	0.2
2a	20,000	0.1
2b	20,000	0.3

Table 3
Run conditions for analytical and numerical modeling with dispersion

Run cases	Dispersivity, m	Permeability, md	Porosity, fraction	Time, y
3a	1	100	0.2	200
3b	10	100	0.2	200
3c	20	100	0.2	200
4a	1	100	0.2	6,000
4b	10	100	0.2	6,000
4c	20	100	0.2	6,000
5a	10	1	0.2	1,000
5b	10	10	0.2	1,000
5c	10	100	0.2	1,000
5d	10	1,000	0.2	1,000
6a	10	100	0.1	200
6b	10	100	0.3	200

Diffusion-Dominated Mechanism

In the diffusion dominated part, the effect of duration and porosity are investigated using Eq. (12). Because dispersivity and permeability have an effect in convection mechanism, results related with them are given in the convection-dominated part.

Effect of Duration on CO_2 Saturation

In Figure 2, it could be seen that the results of analytical and numerical models match very well for diffusion-dominated system. However, after many years such as in Run 1d and Run 1e, there are some deviations. The dissolution of CO_2 in aquifer increases with time. But it takes about 10^7 years to saturate whole aquifer with CO_2 under only a diffusion-dominated system.

Effect of Porosity on CO_2 Saturation

In Figure 3, the results of analytical and numerical models match very well for Runs 2a, 1c, and 2b. With porosity increase in diffusion dominated system, dissolution of CO_2 increases, because of increase in contacted water volume with CO_2.

Convection-Dominated Mechanism

In the convection dominant process, Eq. (16) is used for the solution of the run cases. The only different parameter in this equation between analytical and numerical approach is the velocity parameter. In the numerical part, the velocity is calculated according to the varying concentration difference. On the other hand, for analytical part this velocity is taken as a constant value. The constant velocity is the average value of the varying velocity in the aquifer. It is calculated based on the geometric mean. The geometric

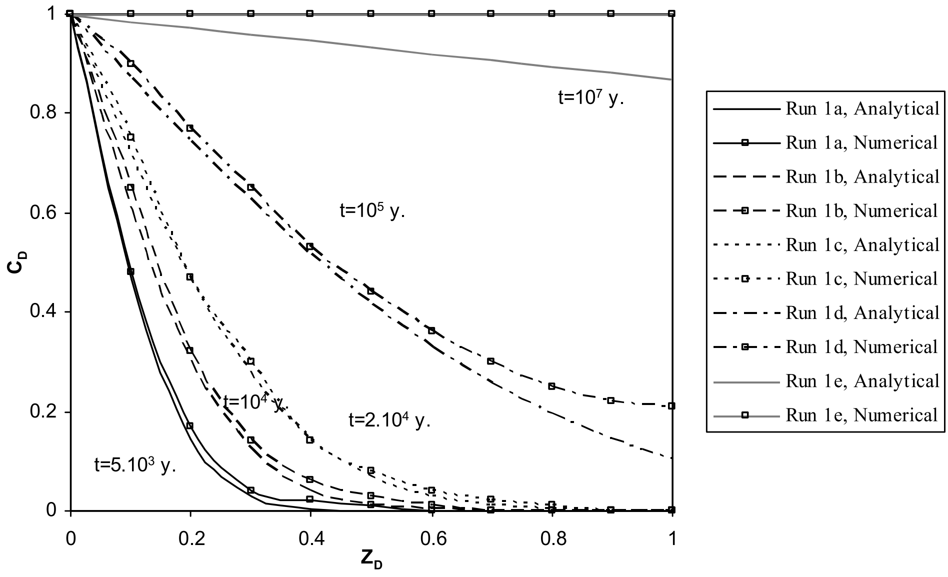

Figure 2. Effect of duration ($\phi = 0.2$).

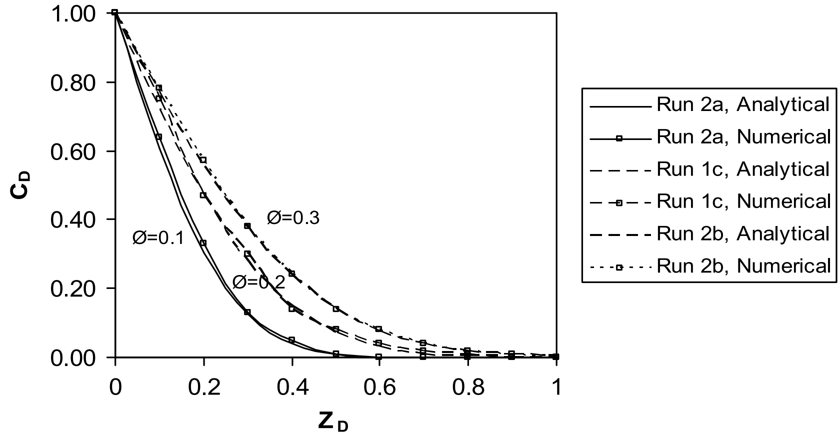

Figure 3. Effect of porosity (20,000 years).

mean is a measure of central tendency. To take the effect of $V_{\min}(V = 0)$ into account in geometric series, minimum velocity (zero velocity) is set to a very small value, 10^{-18} cm/s shown in Table 4. The maximum velocity values are in the order 10^{-5} cm/s and 10^{-8} cm/s in run cases calculated from Eq. (3). So, the minimum value is taken as the 10^{10} times smaller of the maximum velocity. The average velocity is found to be the 1% of the maximum velocity based on geometric average for the usage in analytical part. However, for best matching between analytical and numerical results, average velocities are taken between 0.5%–2% of the maximum velocity in the run cases.

Effect of Dispersivity on CO_2 Saturation

In Figures 4 and 5, the comparison is presented between the results of analytical and numerical models of the dispersivity effect. The results of both models match very

Table 4
Mean velocity calculation for analytical modeling

V	ΔC_D	
$V_{\max}$	1	$V_{avg} = 0.01\ V_{\max}$ from geometric mean
$0.9\ V_{\max}$	0.9	
$0.8\ V_{\max}$	0.8	
$0.7\ V_{\max}$	0.7	
$0.6\ V_{\max}$	0.6	
$0.5\ V_{\max}$	0.5	
$0.4\ V_{\max}$	0.4	
$0.3\ V_{\max}$	0.3	
$0.2\ V_{\max}$	0.2	
$0.1\ V_{\max}$	0.1	
$V_{\min} = 10^{-18}$ cm/s ≈ 0	0	

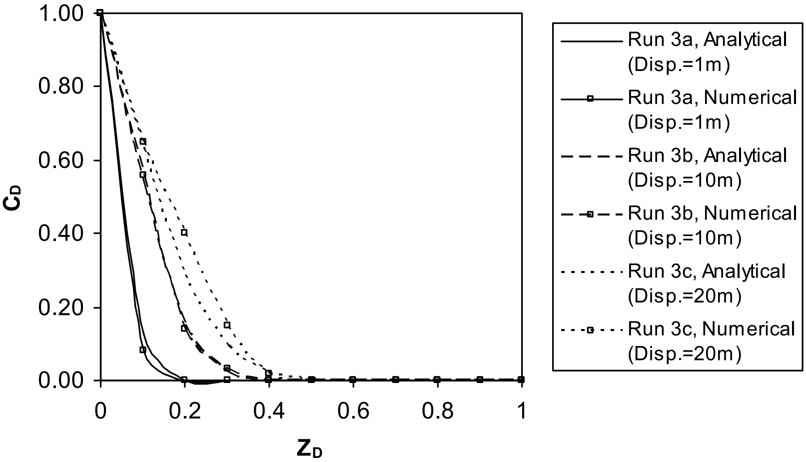

Figure 4. Effect of dispersivity (200 years).

well, generally for early (200 years) and late time (6,000 years) regions. In early time, dispersivity increases the convection rate; however, the total dissolution of aquifer by CO_2 convection takes place quicker in aquifers having low dispersivity. This may be due to the fact that concentration gradient becomes generally higher between saturated and unsaturated water layers in the low dispersivity system, and this leads to higher convection rates.

Effect of Permeability on CO_2 Saturation

The comparison of analytical and numerical modeling is made for permeability effect in Figure 6 for Run 5a, Run 5b, Run 5c, and Run 5d. The results match very well. The higher permeability increases the convective transport of CO_2 into the aquifer; as a result more volume of water becomes saturated with CO_2.

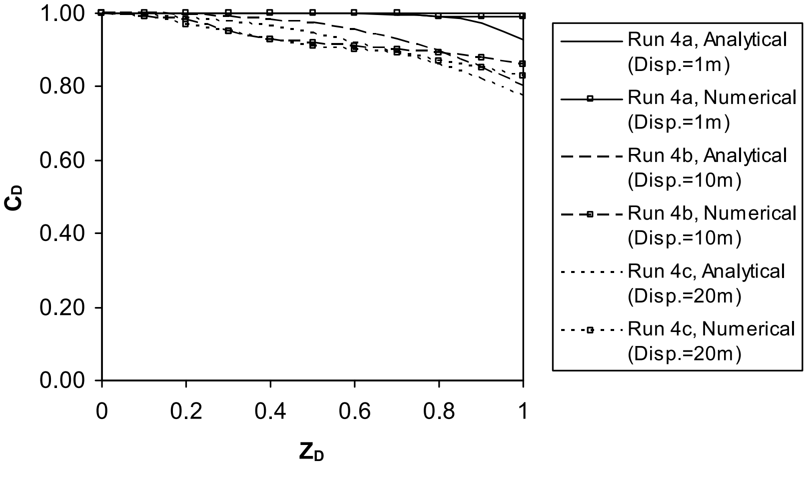

Figure 5. Effect of dispersivity (6,000 years).

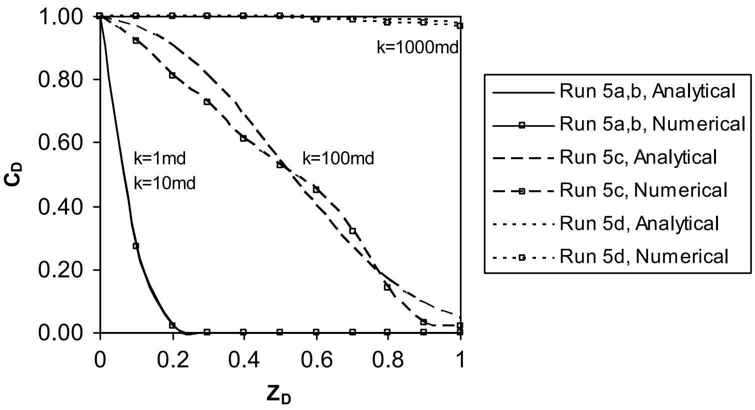

Figure 6. Effect of permeability (1,000 years).

Effect of Porosity on CO_2 Saturation

The comparison of analytical and numerical modeling is made for porosity effect in Figure 7 for Run 6a, Run 3b, and Run 6b. The results are in good agreement. For convection-dominated systems, the decrease in porosity increases the convection rate due to increased velocity.

Rayleigh Numbers

Rayleigh numbers for each run are calculated with Eq. (4) and are presented in Table 5. Rayleigh number gives an idea about the occurrence of convection. Since the velocity changes in the system as a function of space and time, the average velocities are used for the calculation of Rayleigh numbers. As seen in Table 5, Rayleigh numbers of Runs 6a and 6b are below the critical Rayleigh number which is about 39.5.

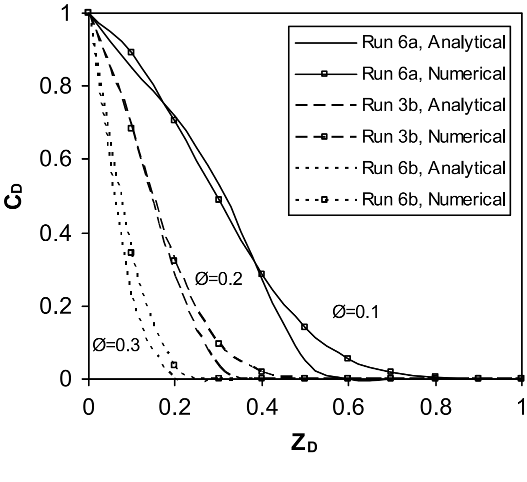

Figure 7. Effect of porosity (200 years).

Table 5
Rayleigh numbers

Run cases	Rayleigh number
3a	116
3b	233
3c	233
4a	116
4b	116
4c	116
5a	6
5b	8
5c	233
5d	1,164
6a	582
6b	77

Conclusions

A comparison is made between analytical and numerical modeling of CO_2 solute transport in a hypothetical deep saline aquifer in the study. The effects of aquifer properties on transport mechanisms are evaluated in a one-dimensional vertical system. The following remarks are concluded after having the results of analytical and numerical models:

- The complete dissolution of CO_2 in the aquifer by only diffusion takes thousands, even millions, of years. In a diffusion-dominated system, an aquifer with 100 m thickness becomes just about saturated after 10,000,000 years, whereas, this time is much smaller in the convective dominant systems.
- In a diffusion dominant process, porosity increase accelerates the dissolution of CO_2 in aquifer; however, in a convection dominant process, dissolution rate of CO_2 in aquifer becomes less with porosity increase due to the decrease in the velocity of brine column.
- The increase in permeability enhances the dissolution rate of CO_2 in aquifer remarkably due to increasing velocity of brine column.
- At the end of the dissolution process in the aquifer, the dissolved CO_2 amount in the aquifer is quicker with lower dispersivity values counter to the observations in the beginning of the dissolution process.
- The results of modeling in aquifers with 1 md and 10 md permeability values are so near in that diffusion-dominated system is governing. After 10 md, the convection mechanism begins to dominate gradually and it becomes totally convection dominated for 50 md and higher permeability values. These results are also verified by the Rayleigh number.
- Rayleigh number gives an idea about the occurrence of convection. The runs having Rayleigh numbers that are above the critical Rayleigh number of 39.5 are considered as convection-dominated systems.

References

Anderson, M. A. 1984. Movement of contaminants in groundwater: groundwater transport, advection and dispersion. In: *Groundwater Contamination*. Washington, D.C.: National Academy Press, pp. 37–45.

Bachu, S., and Adams, J. J. 2003. Sequestration of CO_2 in geological media in response to climate change: Capacity of deep saline aquifers to sequester CO_2 in solution. *Energy Convers. Mgmt.* 44:3151–3175.

Bedient, P. B., Rifai, H. S., and Newell, C. J. 1994. *Groundwater Contamination: Transport and Remediation.* Upper Saddle River, NJ: Prentice Hall.

Bouwer, H. 1978. *Groundwater Hydrology.* New York: McGraw-Hill.

Cussler, E. L. 1997. *Diffusion: Mass Transfer in Fluid Systems*, 2nd Edition. New York: Cambridge University Press.

Domenico, P. A., and Schwartz, F. W. 1998. *Physical and Chemical Hydrogeology*, 2nd Edition. New York: John Wiley & Sons.

Enick, R. M., and Klara, S. M. 1990. CO_2 solubility in water and brine under reservoir conditions. *Chem. Eng. Comm.* 90:23–33.

Fetter, C. W. 1994. *Applied Hydrogeology*, 3rd Edition. New York: Macmillan College Publishing Company.

Garcia, J. E. 2001. *Density of aqueous solutions of* CO_2. Report LBNL-49023, Berkeley, CA: Lawrence Berkeley National Laboratory.

Gelhar, L. W., Welty, C., and Rehfeldt, K. R. 1992. A critical review of data on field-scale dispersion in aquifers. *Water Res. Research* 28:1955–1974.

Gorelick, S. M., Freeze, R. A., Donohue, D., and Keely, J. F. 1993. *Groundwater Contamination: Optimal Capture and Containment.* Boca Raton: CRC Press LLC.

Hirai, S., Okazaki, K., Yazawa, H., Ito, H., Tabe, Y., and Hijikata, K. 1997. Measurement of CO_2 diffusion coefficient and application of lif in pressurized water. *Energy* 22:363–367.

IEA Greenhouse Gas R&D Programme. 2006. Capture and storage of CO_2. Available at http://www.ieagreen.org.uk (accessed February 2, 2006).

Lake, L. W. 1989. *Enhanced Oil Recovery.* Englewood Cliffs, NJ: Prentice-Hall.

Noh, M., Lake, L. W., Bryant, S. L., and Araque-Martinez, A. 2004. Implications of coupling fractional flow and geochemistry for CO_2 injection in aquifers. SPE Paper 89341. *SPE/DOE 14th Symposium on Improved Oil Recovery*, Tulsa, Oklahoma, April 17–21.

Shimizu, K., Kikkawa, N., and Nagashima, A. 1995. Diffusion coefficients. *Proc. 4th Asian Thermophys. Proper. Conf.* 3:771.

Tumasjan, A. B., Panteleev, V. G., and Mejncer, G. P. 1969. Influence of carbon dioxide on the physical properties of oil and water. *Nefteprom. delo*. 2:20–23.

Unver, A., and Himmelblau, D. M. 1964. Diffusion coefficients of CO_2, C2H4, C3H6, and C4H8 in water from 6°C to 65°C. *J. Chem. Engrg. Data* 9:428–431.

Weatherill, D., Simmons, C. T., Voss, C. I., and Robinson, N. I. 2004. Testing density-dependent groundwater models: Two-dimensional steady state unstable convection in infinite, finite and inclined porous layers. *Adv. Water Resources*. 27:548–563.

Wilke, C. R., and Chang, P. 1955. *Am. Inst. Chem. Eng. J.* 1:264–270.

Nomenclature

D_e	effective diffusivity coefficient (cm^2/s)
C_{CO_2}	concentration of CO_2 in aquifer (mol/cm^3)
$C_{CO_2,sat}$	concentration of CO_2 in saturated aquifer at aquifer conditions (mol/cm^3)
z	depth below the interface (cm)
t	time (second)
D_o	molecular diffusion coefficient (cm^2/s)
$\oslash$	porosity of reservoir, fraction

τ	tortuosity
u	superficial velocity (Darcy velocity) (cm/s)
k	permeability (cm^2)
g	gravitational acceleration (cm/s^2)
$\Delta\rho$	density difference (g/cm^3)
μ	viscosity (g/cm^2.second)
Ra	Rayleigh number
H	thickness (cm)
C_D	dimensionless concentration
t_D	dimensionless time
Z_D	dimensionless length
N_{Pe}	Peclet number
α	dispersivity (cm)
v_o	interstitial velocity (cm/s, $u/\emptyset$)

Conversions

1 md $= 10^{-11}$ cm^2
1 cp $= 0.01$ g/cm.second
1 year $= 31{,}536{,}000$ seconds