Simulation of Carbon Sequestration in a Coal-Bed With a Variable Saturation Model

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Abstract

One of the pressing problems of CO2 sequestration is to guarantee a long-term storage of carbon dioxide in a coal seam. It depends on many factors such as properties of coal basin, fracture state, phase-equilibrium, etc. In particular, the porosity, permeability and saturation of the coal seam play a major role. In this study, a computer simulation was conducted with a purpose of predicting carbon dioxide transport in a two phases, multi-layer environment of a typical unmineable coal seam. As an example, the Appalachian basin was considered as a prototype case for injection of carbon dioxide. In the simulations the variable porosity and relative permeability were tracked as they were changing between the existing water-saturated in coal seams and subjected to the injection of CO2. The concentration of carbon dioxide and methane, which is in an absorbed state on the coal surface was analyzed by using Langmuir equation with the variable pressure and time.

The results indicate that the transport of carbon dioxide was affected by the properties of the coal seam. With carbon dioxide injection, the porosity and relative permeability of the gaseous CO2 phase were shown to increase, which contributes to the storage capacity of the coal seam, which is also increased due to the decrease of the residual water in the coal matrix. Thus increasing the CO2 injection pressure and the consequent reduction the amount of residual water contributes to the increase in the CO2 storage capacity of the reservoir. As history data match has shown, these results are in agreement with the Langmuir analysis. The study can provide projections for the CO2 sequestration operations in known coal seams.

1 Introduction

The most abundant greenhouse gas, CO_2 has risen from preindustrial levels of 280 parts per million (ppm) to present levels of over 365 ppm [1] with an accumulation rate of about 1.5 ppmv per year [2, 3]. Just this injection of enormous CO_2 amounts into the environment results in a series of global problems as warming of the climate and deforestation, caused by acid rain etc. For example, global average surface temperature of the earth has increased by approximately $0.6 \pm 30\,^{\circ}$C over the last century. Long-term storage of CO_2 in coal-bed, as a method may help to slow down the accumulation of CO_2 in the atmosphere and avoid further pollution of the natural environment. The injection of CO_2 into gassy coalbeds allows the production of a residual coal bed methane (CMB) thereby adding value to the sequestration operation [4].

The success of these operations depends on our understanding of gas-coal interactions and how they affect the properties of CO_2 transport in coal seams. Predictions concerning the long-term stability of the sequestered gas require knowledge of gas absorption and retainment inside a reservoir, and of the factors which might induce its release, including water contained in the coalbed. Reliable estimates of the gas-retention capacity of coal-beds are needed for economic assessments of the viability of candidate seams. Water and CH_4 production from coalbeds has led to extensive investigations into factors that affect its adsorption capacity, both to determine the gas-in-place accurately and because of safety issues in coal mining [5, 6, 7]. However, studies of the CO_2 capacity of coals under in-seam conditions have been rather limited. A recent proposal that the injection of CO_2 into coal seams can be a viable option to mitigate the increasing worldwide CO_2 emissions has stimulated interest in developing a better understanding of the coal-CO_2 interactions and the adsorption capacity of a candidate coal seam for CO_2 sequestration [8]. In order to ensure the optimal relationship between sequestration costs for a particular coal reservoirs and its storage efficiency, detailed simulations of gas-coal interaction needs to be performed. Such simulations should take into account the geological properties such as density and rank of coal, porosity and permeability of geology, physical and chemical processes, including fluid flow and thermodynamics.

Injection of CO_2 changes partial pressure of water which effectively expells water and thereby enhances CH4 desorption from coal surfaces and saturates the reservoir with the absorbed CH_4. CO_2 adsorbs mored strongly to coal surfaces than CH4, which results in more rapid complete displacement of CH_4 from coal [9]. From this perspective this study focused on the activity of CO2 and water in a moist coalbed. Some of the typical parameters were used to simulate CO2 sequestration with the purpose of analyzing long term containment characteristics of the reservoirs.

2 Method

In this study, the COMSOL package (www.comsol.com) based on the finite-element method [13, 14] was adopted to predict CO2 transport in the coal-bed, porous media. The geophysical module of COMSOL is widely used to solve some earth science and porous media problems such as flow and solid deformation, solute transport related problems etc. [10, 11, 12].

2.1 Governing Equations

The complete equation system consists of the following set of equations (more details can be found in [15] and [16, 17, 18, 19]).

2.1.1 Momentum equations

Darcy's velocity equation

$$\frac{\phi_\beta \partial p_\beta}{\partial t} + \nabla \cdot \{ \frac{K_\beta}{\mu_\beta} \nabla (p_\beta + \rho_\beta g D) \} = S_\beta \tag{1}$$

Where, β is the phase, ϕ_β is porosity, K_β - permeability, μ_β - viscosity, and S_β represent source terms. In this representation, the two components and phases are considered: CO2 as non-wetting, methane as a wetting phase, and water. The Darcy's velocity equation for non-wetting and wetting are represented as follows:

- Gas phase:

$$\frac{\phi_g \partial Se_g}{\partial t} + \nabla \cdot \{ \frac{-k_{abs} k_{r,g}}{\mu_g} \nabla (p_g + \rho_g g D) \} = S_g \tag{2}$$

- Water phase:

$$\frac{\phi_w \partial Se_w}{\partial t} + \nabla \cdot \{ \frac{-k_{abs} k_{r,w}}{\mu_w} \nabla (p_w + \rho_w g D) \} = S_w \tag{3}$$

Where ϕ_β is the initial porosity, S_e is the effective saturation, k_{abs} is the absolute permeability of the porous medium (in m^2), $k_{r,\alpha}$ is the relative permeability, μ is dynamic viscosity ($kgm^{-1}s^{-1}$), S is the source term, p is the pressure ($kgm^{-1}s^{-2}$), rho is fluid density (kgm^-3), g is the acceleration of gravity, and D is the vertical elevation (m). The auxilliary equations are defined as follows:

$$p_c = p_g - p_w \tag{4}$$

where p_c is the capillary pressure.

$$Se_g + Se_w = 1 \tag{5}$$

The change between the effective saturation and capillary pressure is shown as:

$$C_{p,w} = -C_{p,g} = \frac{\phi_\alpha \partial Se_w}{\partial p_c} \tag{6}$$

Combining the capillary pressure and effective expression to governing equations, yieds:

$$\frac{C_{p,w} \partial (p_g - p_w)}{\partial t} + \nabla \cdot \{ \frac{-k_{abs} k_{r,w}}{\mu_w} \nabla (p_w + \rho_w g D) \} = S_w \tag{7}$$

$$\frac{-C_{p,w} \partial (p_g - p_w)}{\partial t} + \nabla \cdot \{ \frac{-k_{abs} k_{r,g}}{\mu_g} \nabla (p_g + \rho_g g D) \} = S_g \tag{8}$$

For these two phases, the relationships among of capillary pressure, porosity, effective saturation and relative permeability are discussed as above. Capillary pressure head is defined as $H_c = p_c/(\rho_{water} g)$.

- For the wetting phase:

1. If $H_c > 0$:

$$\phi_w = \phi_{r,w} + Se_w(\phi_{s,w} - \phi_{r,w}) \tag{9}$$

$$Se_w = \frac{1}{[1 + |\alpha H_c|^n]^m} \tag{10}$$

$$C_w = \frac{\alpha m}{1-m}(\phi_{s,w} - \phi_{r,w}) Se_w{}^{\frac{1}{m}}(1 - Se_w{}^{\frac{1}{m}})^m \tag{11}$$

$$k_{r,w} = Se_w{}^L(1 - (1 - Se_w{}^{\frac{1}{m}})^m)^2 \tag{12}$$

2. If $H_c <= 0$:

$$\phi_w = \phi_{s,w} \tag{13}$$

$$Se_w = 1 \tag{14}$$

$$C_w = 0 \tag{15}$$

$$k_{r,w} = 1 \tag{16}$$

For $C_{p,w}$, the specific moisture capacity is the slope of the curve of q and H_c, which can be calculated by formula of $C_{p,w}(p_w) = C_w \rho_w^{-1} g^{-1}$.

- For non-wetting phase:

$$\phi_g = \phi_{s,w} - \phi_w \tag{17}$$

$$Se_g = 1 - Se_w \tag{18}$$

$$C_g = -C_w \tag{19}$$

$$k_{r,g} = 1 - Se_w{}^L(1 - Se_w{}^{\frac{1}{m}})^{m2} \tag{20}$$

The boundary condition for above Darcy's equations for wetting phase is at the inlet is:

$$n \cdot [-\frac{k}{\mu}\nabla(p_w + \rho_w g D) = 0 \quad (21)$$

and for the outlet:

$$p_w = p_{w0}(t) \quad (22)$$

For all other sides:

$$n \cdot [-\frac{k}{\mu}\nabla(p_w + \rho_w g D) = 0 \quad (23)$$

For non-wetting phase at the surface:

$$n \cdot [-\frac{k}{\mu}\nabla(p_g + \rho_g g D) = 0 \quad (24)$$

and at the inlet:

$$p_g = p_{g0}(t) \quad (25)$$

and at all other sides:

$$n \cdot [-\frac{k}{\mu}\nabla(p_g + \rho_g g D) = 0 \quad (26)$$

2.1.2 Concentration equation

Considering the case of CO_2 sequestration, the transport equation used here was that of [20, 21]:

$$\frac{\partial(\phi_\beta c_\beta)}{\partial t} + \frac{\partial(\rho_b c_p)}{\partial t} + \nabla\cdot[-\phi_\beta D_L \nabla c_\beta + u_\beta c_\beta] = \sum R_L + \sum R_p + S_c \quad (27)$$

Where c_β is dissolved concentration (kg/m), c_P is mass of adsorbed contaminant (mg/kg), ϕ_β is the porosity, ρ_b is the bulk density (kg/m^3), $\rho_b c_P$ is the solute mass attached to the soil, u_β is Darcy‘s velocity, D_L is hydrodynamic dispersion tensor (m^2/d), R_L is reaction in water (m^2/d), R_p is reactions involving solutes attached to soil particles $(kgm^{-3}d^{-1})$, S_c is solute added per unit volume of soil per unit time $(kgm^{-3}d^{-1})$. Expanding the left hand side, yields:

$$\frac{\partial(\phi_\beta c_\beta)}{\partial t} + \frac{\partial(\rho_b c_p)}{\partial t} = \phi\frac{\partial c_\beta}{\partial t} + c_\beta\frac{\partial \phi_\beta}{\partial t} + \rho_b\frac{\partial c_p}{\partial c_\beta}\frac{\partial c}{\partial t} \quad (28)$$

Also, because $k_p = \frac{\partial c_p}{\partial c_\beta}$, $c_p = k_p \cdot c_\beta$, the solution transport equation becomes:

$$[\phi_\beta + \rho_b k_p]\frac{\partial(c_\beta)}{\partial t} + c\frac{\partial(\phi_\beta)}{\partial t} + \nabla\cdot[-\phi_\beta D_L \nabla c_\beta + u_\beta c_\beta] = \phi_\beta \phi_L + \rho_b k_p \phi_p c_\beta + S_c \tag{29}$$

Where ϕ_L, ϕ_p denote the decay rates for the dissolved and sorbed solution concentrations, respectively.

The boundary condition at the inlet is:

$$c_\beta = c_0 \tag{30}$$

and at the surface:

$$n \cdot [-\phi D_L \nabla c_\beta] = 0 \tag{31}$$

2.1.3 Temperature equation

The convection and conduction equation used is as follows:

$$\frac{\partial T}{\partial t} + \nabla \cdot (-K_{eq} + \nabla T + C_L u T) = 0 \tag{32}$$

Where T is temperature, K_{eq} is effective thermal conductivity of the fluid and solid mixture, C_L is fluid's volumetric heat capacity.

2.1.4 Langmuir equation and Extended Langmuir equation

Langmuir equation is:

$$V = \frac{vpb}{1 + bp} \tag{33}$$

which is used to express the capacity of single adsorption and desorption. For a multi-component system, an extended Langmuir equation was used as:

$$V = \frac{v_j p y_j b_j}{1 + p\sum_{j=1}^{n} b_j y_j} \tag{34}$$

Where V is the adsorbed gas volume for component j, v_j, b_j: Langmuir parameter of component j, p: Sum pressure, which is $\sum p_j$, and y_j: Ratio of the partial pressure for component j, that is $\frac{p_j}{p}$.

As stated, Darcy's velocity, the momentum equation and mass equation are coupled together with the temperature. The simulations based on this model were performed with a set of parameters of a typical coal-bed obtained from the literature data. The results are presented in the following sections.

Table 1: Parameters of Coal-bed

Parameter	Value
Coal-bed size, ft	7500X7500
Coal-bed depth, ft	30
Reservoir temperature, ^0F	60^0F
Coal bulk density,kg/m^3	1360
Initial coal-bed Pressure, psia	800
Permeability, md	5
Porosity, %	6.9%
Initial Water Saturation, %	99%
Initial CO_2 Saturation, %	1%

3 Results

The properties of the typical coal-bed were taken from the literature sources [22, 23, 24, 25, 26]. Also, the parameters for extended Langmuir computing were referenced from [27, 28, 26].

The validation simulation was done on the set of data [26], with the injection point located in the middle of the geometry. The rate of the pressure driven injection was 1.15 psi/hour, to provide the flux of CO2 into the coal-bed. The results of transient simulations executed with COMSOL simulator are shown in the figures.

Figure 1 shows capillary pressure comparison with the literature data. 2 is the match between water phase relative permeability and history. 3 shows the validation of CO2 adsorption. 4 is the results of water and CO2 relative permeability variabe with water saturation. 5 shows the density changing with increasing pressure. 6 shows the porosity variable vs pressure increasing. 7 is the total CO2 adsorption in coal-bed at some known pressure.

4 Conclusions and Future Work

Simulation of CO2 sequestration in geological formations can suggest valuable long-term forecasts of capacity, durability and containment characteristics of reservoirs with different properties and operation condition such as pressure, saturation etc. Especially, with the lack of accurate data on CO2

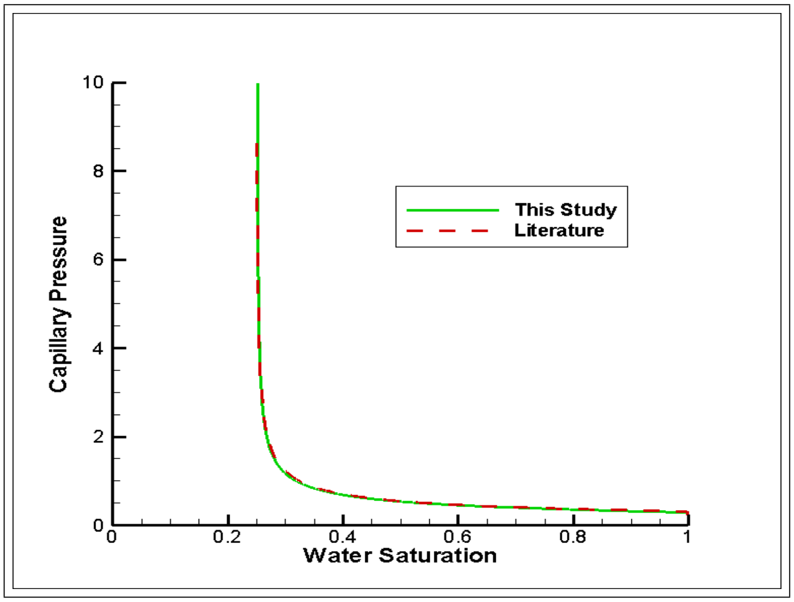

Figure 1: Capillary pressure vs Water saturation

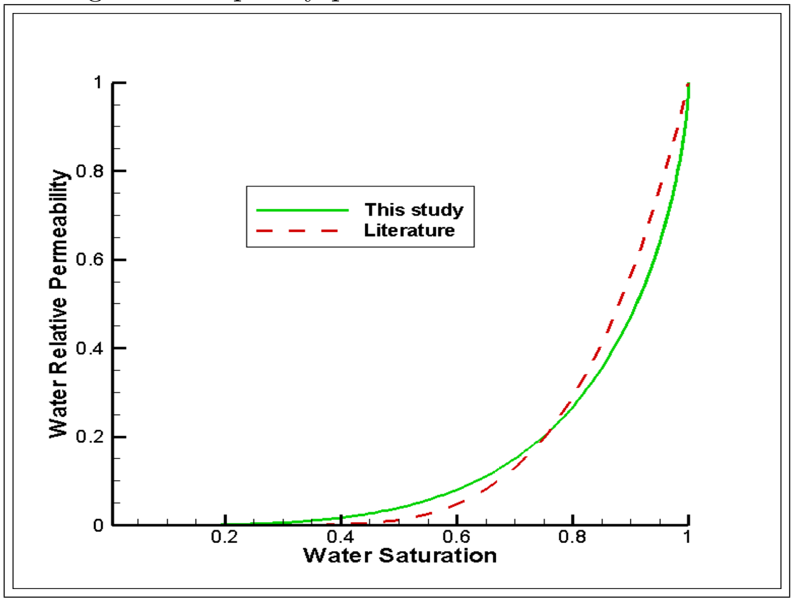

Figure 2: Relative permeability vs Water saturation

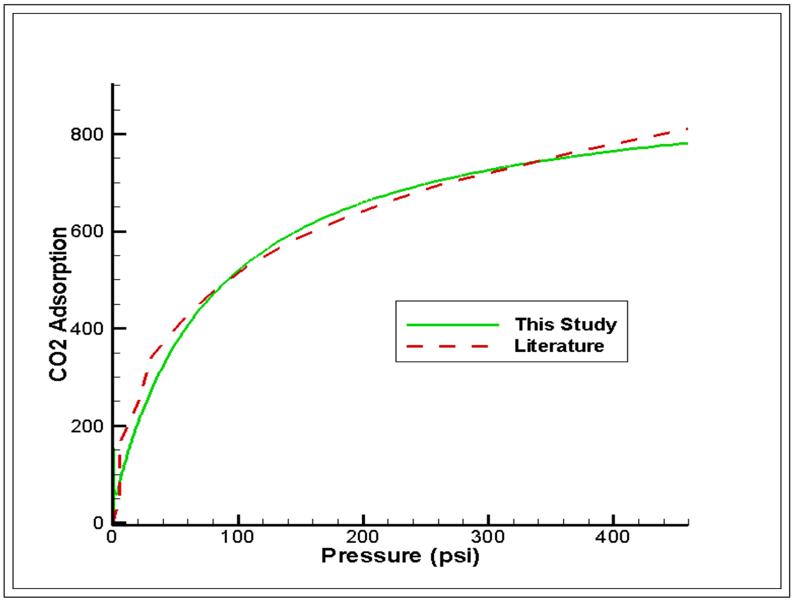

Figure 3: Adsorption between literature and this study vs Variale pressure

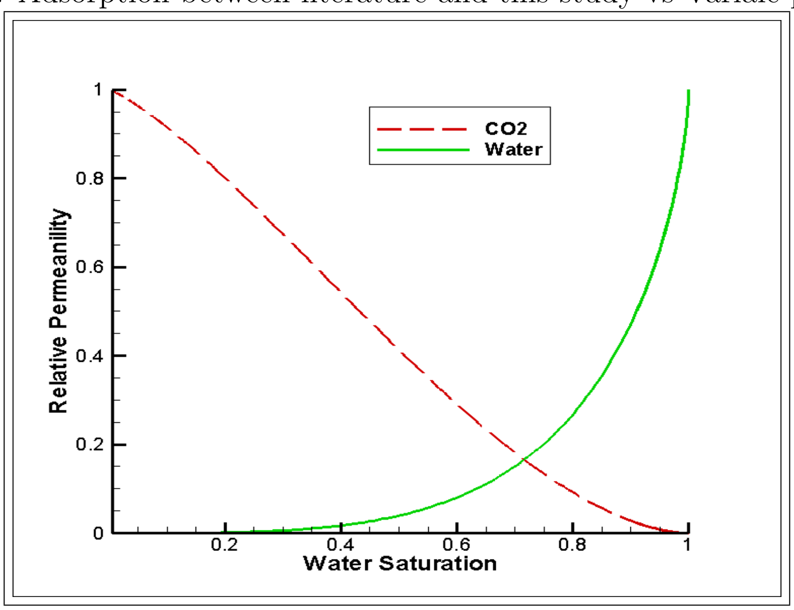

Figure 4: CO2 and water relative permeability variable vs Water saturation

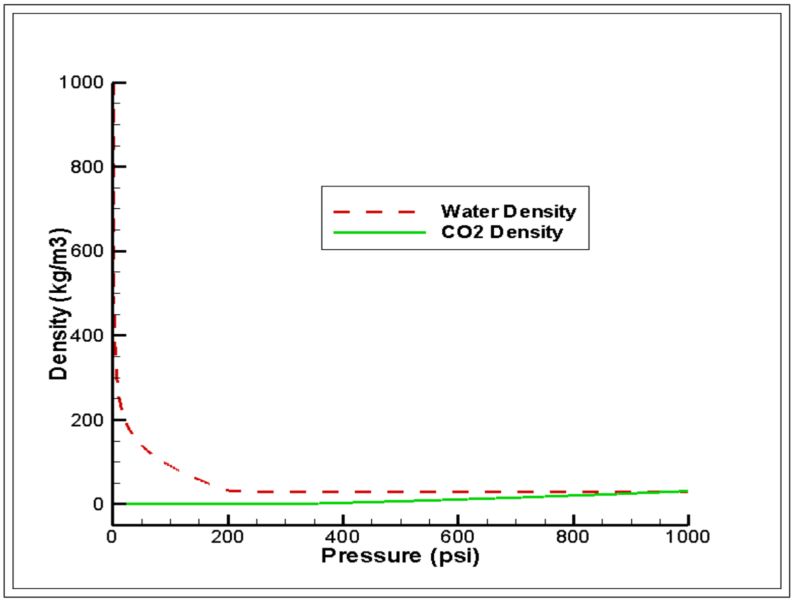

Figure 5: CO2 and water density variable vs Pressure

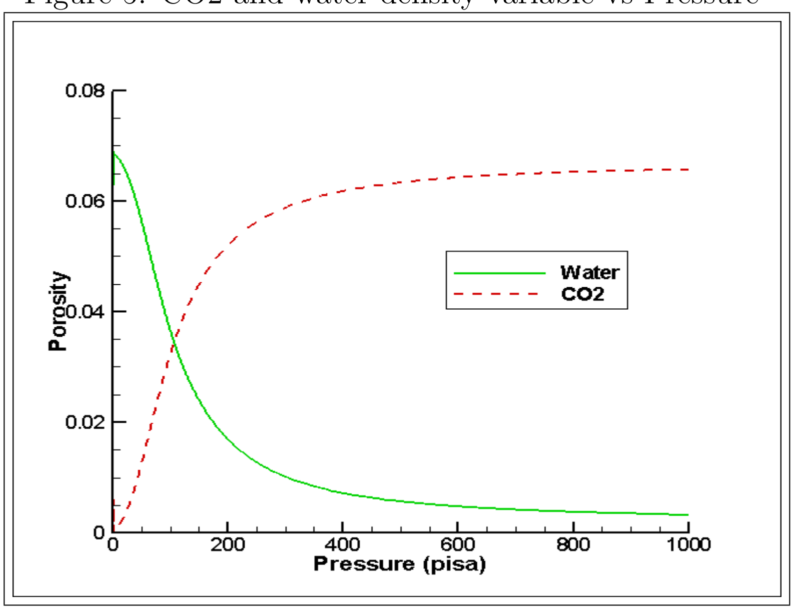

Figure 6: CO2 and water porosity variable vs Pressure

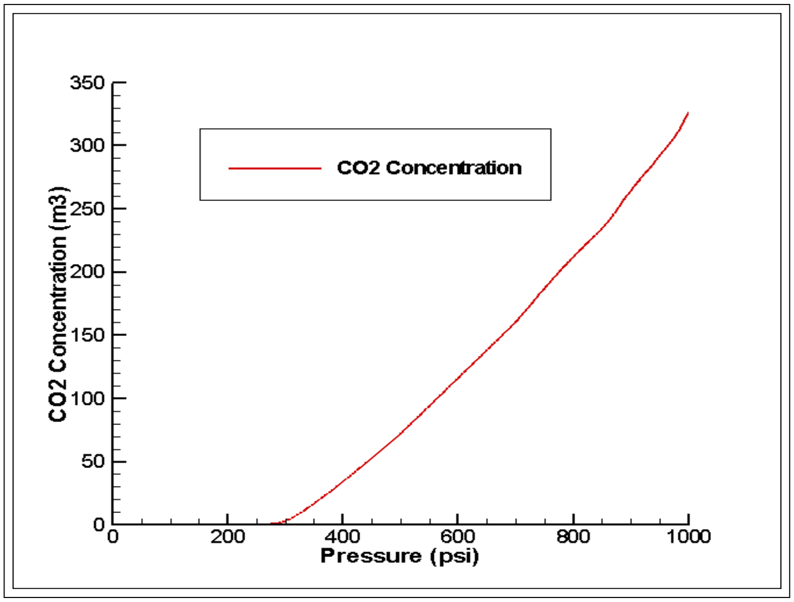

Figure 7: Amount CO2 concentration in coalbed vs Variable pressure

injection, the simulation can help to investigate the feasibility of sequestration of CO2 in a reservoir by designing and trying different scenarios as well as accounting of statistical uncertainties, and extreme and hight risk cases based on the suitable error estimates and efficient modelling techniques.

In this study, a variable saturation model was used because the saturation can change with the CO2 injection in a coal-bed. With the varying saturation, the porosity and permeability can also increse or decrease due to the variations of CO2 pressure. At the same time, the water or adsorbed methane can be recovered as a useful by-product. In this enhanced coal-bed metane recovery procedure by CO2 injecton, the porosity, permeability and saturation were traced with the varying partial pressures of water and CO2. The surface of the CO2 and water, in the two phases were computed using the variable saturation model. The concentration of the CO2 in pore of coal-bed was calculated as well as the capacity prediction of coal adsorbed was computed via extended Langmuir model.

Based on the published data in literature of the [26], the variable saturation model was valided in two aspects. One is the fluid flow model which was matched in the saturation, porosity and permeability of both water and

CO_2. The other is the sorption validation of coal for CO_2 under varying pressure. The results show that the data agree with the literature data.

Since methane exists in a coal-bed as a non-liquid phase, further work should be done with the improved modeling capabilities and validation to forecast the production of methane with mixture gaseous injection.

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