

**SIMULATION OF CO₂ SEQUESTRATION IN DEEP
SALINE AQUIFERS
GORDON CREEK FIELD, UTAH.**

By

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ABSTRACT

CO₂ emissions during recent decades have been increasing due to the use of fossil fuels in the generation of electricity and other industrial processes like oil refineries, cement works, and iron and steel production.

Each power plant emits several millions of tons of carbon dioxide annually during this process. CO₂ sequestration has been proposed as one of the best ways to reduce these emissions from the atmosphere and keep them stored underground for long periods of time. Numerous methods of capturing CO₂ underground have been proposed (Greenhouse Gas R&D Programme IEA, 2008). The most viable due to their storage capacity, are depleted oil and gas fields, unminable coal seams, and deep saline Aquifers.

Deep saline aquifers are considered the best reservoirs to storage CO₂, because they exist in most regions of the world and they have a large capacity of storage. These types of reservoirs have not been studied deeply and for that reason more research is being performed to get a better idea of the geology of sand formations saturated with water, as well as, shale present above these formations which act as barriers to flow. Studies of the solubility and chemical reactions between the CO₂ and brine present in the formations also have been completed.

This project presents a simulation study for CO₂ sequestration in a saline aquifer below the Gordon Creek Field in Utah. The presented work is a pre-cursor to a pilot project to inject up to 2.94 million tons of CO₂ over a four year period. Simulations were used to characterize relative impacts of geologic structures, water characteristics, reservoir flow properties, seal formation characteristics and to identify reasonable injectivity goals for the Navajo and Entrada Sandstones.

A simulation model of the area of interest was constructed using the GRIDGENR module of Nexus and preliminary structural contour maps of the Navajo formation and well logs of the zones of interest. Petrophysical properties were determined using the LESA log analysis software and well logs from the Gordon Creek No. 1 well. CMG simulator was used to model the injection of CO₂ into the aquifer formations. CMG was used to model gas trapping due to residual gas saturation, solubility of CO₂ into brine and chemical reactions between minerals present in the water, rock and CO₂. Storage capacities of carbon dioxide for each trapping mechanism, flow direction into the reservoir and seal performance were analyzed over time. Injectivity goals for the pilot were also validated.

Sensitivity Analyses for the most important reservoir parameters were accomplished for brine salinity, temperature, residual gas saturation and initial pressure. The effects of each one of those parameters in the total amount of CO₂

trapped by solubility in water and residual gas saturation mechanisms were studied and quantified.

Keywords: CO₂ Sequestration, Structural Trapping, Residual Gas Trapping, Solubility Trapping, Mineralization Trapping, Gordon Creek Field, Reservoir Simulation, CMG Software, Sensitivity Analysis.

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Date

I release this document to the New Mexico Institute of Mining and Technology.

Student's Signature

Date

1. INTRODUCTION

The concentration of carbon dioxide in the atmosphere has been increasing dramatically since the onset of industrialization in the 19th Century. This incremental increase may have an impact on the world's climate, evident as a global temperature increase and local weather extremes. The highest emissions of carbon dioxide come mainly from the generation of electricity at power plants, oil refineries, cement works, iron and steel production and transportation. Figure 1 represents the main sources of CO₂ emissions in 2006.

In recent years, international legislations related to air quality have been set. The main objective of these legislations is to protect human health and the environment by defining air quality objectives, limit values, and monitoring emissions. One of the most prominent is the Kyoto Protocol, which is an agreement where the developed countries agreed to reduce their carbon dioxide emissions by 5.2% below 1990 levels. In order to accomplish these limits, significant amounts of greenhouse emissions have to be reduced from the atmosphere (Sengul, 2006).

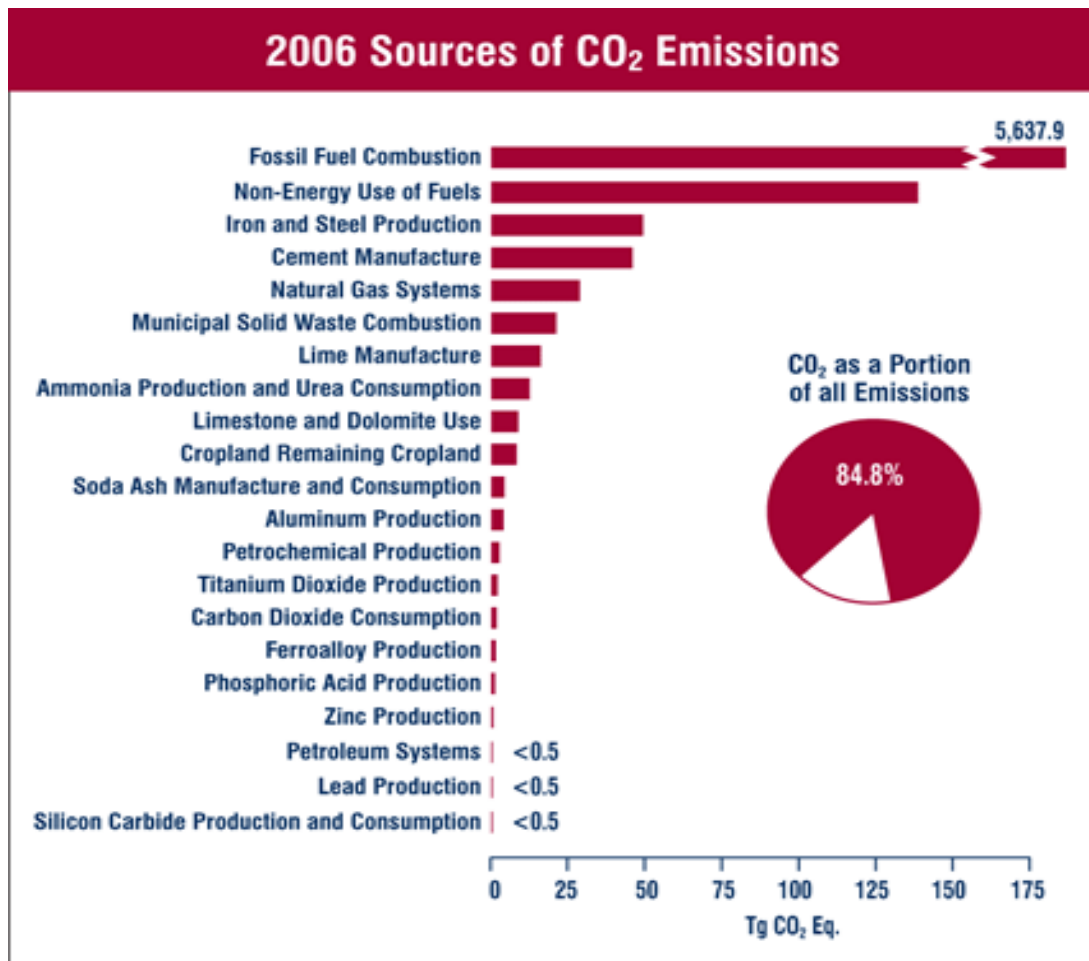


Figure 1. 2006 Sources of CO₂ Emissions.

Potential ways to reduce the carbon dioxide emissions from the atmosphere include reducing the need for fossil fuel combustion through more efficient energy use, substituting the transportation and electric power generation sources with biofuel or hydrogen, substituting natural gas for coal in electric power generation, and capturing and sequestering carbon dioxide.

Carbon Dioxide sequestration can mainly be achieved by the storage of this gas in depleted oil and gas reservoirs (EOR projects that have been developed and studied for many decades), unminable coal beds, deep ocean, and in deep saline aquifers. Figure 2 represents the main storage mechanisms of CO₂ that are currently being examined. Several studies have been proposed to study each of these options, their advantages, and possible problems (Greenhouse Gas R&D Programme IEA).

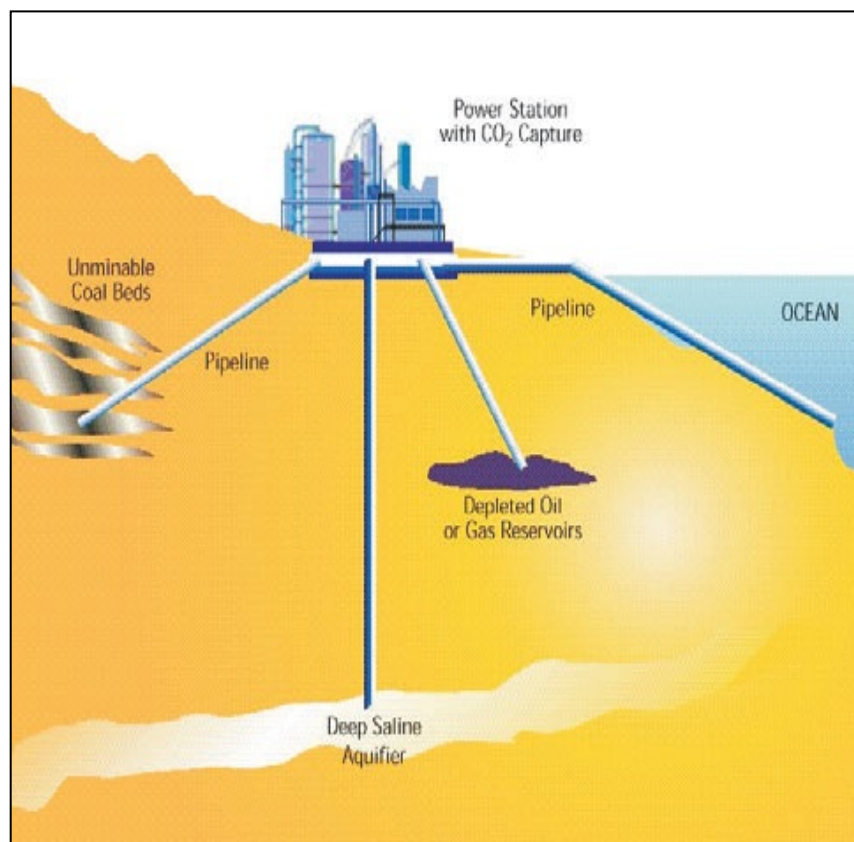


Figure 2 CO₂ Sequestration Methods

According to recent studies, oil and gas reservoirs as well as the deep saline aquifers present large storage capacities that could considerably help in the reduction of greenhouse gases from the atmosphere. However, aquifers represent the most important venue for CO₂ storage since they have the largest capacity and are more common than oil and gas reservoirs. Table 1 (DOE and NETL, Carbon and Sequestration Atlas for the United States and Canada, 2008) shows the dominance of saline aquifers for CO₂ storage.

TABLE 1 – STORAGE CAPACITY FOR CO ₂ STORAGE IN NORTH AMERICA		
<u>Formation Type</u>	<u>10⁹ metric tons</u>	<u>%</u>
Saline Aquifers	3297 – 12,618	91.8 – 97.5
Unmineable Coal Seams	157 – 178	4.4 – 1.4
Mature Oil & Gas Reservoirs	138	3.8 – 1.1
<i>Total Capacity</i>	<i>3,592 – 12,934</i>	<i>100.0</i>

Table 1. Storage Capacity for CO₂.

Due to the high storage capacity in the deep saline formations, it is important to study these type of formations and try to characterize them. These types of reservoirs represent the largest potential storage volume worldwide and they are spread broadly around the world. However, most of these formations have not been extensively explored, and the lack of information related with the Geological Structure and reservoir properties has led to uncertainty related with their storage capacity.

Storage in brine filled formations involves immiscible displacement by supercritical CO₂ (CO₂ critical point is at 1071 psi and 87.9°F, where the density of the carbon dioxide is 600 to 800 kg/m³ and is optimal for storage (Xie,2009)) with only 20 percent or less dissolving into the brine phase. Over time, CO₂ accumulates and spreads at the top of the formation because of the density differences, also called buoyancy force; this increases the surface area between the brine and the carbon dioxide, which means an increase in the amount of CO₂ dissolved in the brine (Kumar, 2004). The resulting CO₂ saturated brine will be slightly heavier than the unsaturated brine and will tend to sink to the bottom of the formation and stay there for a long periods of time in a very secure state.

Shale formations play a very important role in the carbon dioxide sequestration.

The integrity of the seals has to be analyzed through time. The integrity can be affected due to the interactions between these formations and the CO₂ during and after the injection of the gas. Changes in pore pressure, temperature, dissolution of CO₂ into the aqueous phase and chemical reaction between the CO₂ and the cap rock can lead to permeability changes, which can cause leaks that affect the effective storage of carbon dioxide underground.

The objective of this study is to build a Reservoir Simulation model that best represents the CO₂ injection in a saline aquifer. The flow direction and saturation

of the carbon dioxide in the reservoir over time is analyzed. The seal capacity and integrity of the shale formations surrounding the aquifer are also studied. Analysis of solubility of CO₂ into brine and possible chemical reactions that could affect the storage capacity is included.

2. LITERATURE REVIEW.

Many studies have been made related with simulation of CO₂ sequestration in deep Aquifers using a Reservoir Simulation Software. However, there are not any studies available in the area of interest of this study. For this reason, this is the first study of CO₂ sequestration in Gordon Creek Field in Utah.

Chang (1996) studied the CO₂ solubility in water. Correlations for computing the solubility of CO₂ in water as a function of temperature, pressure, and water salinity were presented. Water formation volume factor, water compressibility, and water viscosity correlations were also studied. The CO₂ trapping model must include these properties in order to correctly characterize the interaction between the CO₂ and the brine present in the aquifer.

A compositional reservoir simulation study of a prototypical CO₂ sequestration project in a deep saline aquifer was proposed. The study was done by Kumar et al (2004). The impact of some parameters in the sequestration of CO₂ was studied, including the ratio of vertical to horizontal permeability, residual gas saturation, salinity, temperature, aquifer inclination angle, and mineralization. The impact of these parameters in the mechanisms of sequestration was analyzed. The main mechanisms covered in this study are the pore-level trapping, dissolution and mineralization. Kumar used the Computer Modeling Group's GEM simulator in order to complete the project. On this study it was found that the residual gas

saturation has a large impact in the sequestration of CO₂ at the pore level. A small increase in the Sgr increases the amount of CO₂ trapped as residual gas by a large factor. Another conclusion of this study was that the aquifer dip and horizontal to vertical permeability ratio have a significant effect on gas migration, which in turn affects CO₂ dissolution in brine and mineralization. Tables and references related with CO₂ solubility in brine, mineral reactions and correlations to find the Sgr using the porosity values are also presented.

Ozah et al (2005) continued the work done by Kumar (2004) and expanded the study in important ways including results of behavior of mixtures of CO₂ and H₂S and the use of horizontal wells to maximize both trapping and dissolution and also avoid contact with the seal formations. Local Grid Refinement (LGR) was also applied to the grid to improve the accuracy of the gas saturation in the plume and around the well. Better focus on buoyancy driven fingering due to the unstable upward flow of the gas when it is injected low in the aquifer was also achieved with the local grid refinement.

A study of CO₂ sequestration in an aquifer was performed by Kartikasurja et al (2008). This project was designed to inject the CO₂ extracted from the gas produced in the offshore B Field in Malaysia (to meet the gas sales specification) into a formation and avoid the venting of this gas to the atmosphere. The main

tasks associated with the study are related with the geological evaluation of the aquifer formations and the reservoir engineering involved in the injection of CO₂ in formations with limited reservoir data. Some important elements to choose an aquifer as a storage formation are presented. A black oil simulator was used to model this process. However, since the option to model dissolved gas in the water phase is not included in the simulator, an indirect method was used. This indirect method consisted in assigning water properties to the oil phase and setting the “oil” as live oil, so that it could dissolve the gas phase during the simulation run. This method allowed the behavior of CO₂ to be modeled quite accurately.

Sensitivity studies were carried out in order to select the number of injection wells required to accomplish the objectives. The main properties of the reservoir were also analyzed, and the implications of each one in the injection of CO₂ were studied.

Two studies done by Ngheim et al (2004 and 2009) described the equations required to develop a fully-coupled Geochemical EOS compositional simulator (GEM-GHG). Validation runs were used to validate simulator results. Experimental data was also used to model CO₂ sequestration in aquifers. The study concluded that residual gas trapping and solubility trapping are competing mechanisms, the residual gas trapping is important in low-permeability aquifers and water injection can be used to accelerate and enhance residual gas trapping.

Geo-mechanical calculations coupled with the flow simulator to predict potential failures of the caprock were also presented.

3. METHODOLOGY

3.1 INTRODUCTION.

Sequestration in deep saline aquifers or in oil-gas reservoirs is mainly achieved by a combination of the following mechanisms.

- **Structural Trap.** The carbon dioxide can be trapped as a supercritical fluid under a seal formation, in the same way that gas is trapped in a gas-oil reservoir. This process is commonly referred to as hydrodynamic trapping and in the short term, is likely to be the most important mechanism for sequestration.
- **Solubility.** This mechanism involves the dissolution of CO₂ into the fluids present in the formations (oil or water). This mechanism depends upon brine salinity, temperature and pressure. This mechanism is not as fast as seal trapping, but large quantities of CO₂ can be trapped.
- **Chemical Reactions.** Involves the reaction of CO₂ dissolved in water with the minerals present in the formation to form stable, solid compounds like carbonates. The principal geochemical driver accompanying storage is the acidification of the brine resulting from

dissociation of dissolved CO₂. This process is very slow and can take from hundreds to thousands of years to reach equilibrium.

- **Residual Gas Trapping.** The CO₂ is captured as an immobile phase where the relative permeability to CO₂ is zero because of capillary forces. The principal petro-physical parameters influencing this type of storage are the relative permeability, including hysteresis, and the residual saturation of a non-wetting phase.

Sequestration of carbon dioxide in aquifers is dominated initially by the displacement of fluids, but dissolution and reaction becomes more important over time scales of decades and centuries. The residual trapping also plays an important role and can trap significant quantities of CO₂.

The goal of the CO₂ sequestration in aquifers is to keep the gas trapped underground over long periods of time (hundreds to thousands of years) and reduce the risk or leakage of CO₂ to the atmosphere. The mechanisms mentioned above represent a potential cause of leakage. The risk of leakage in the seal trapping mechanism is the highest because the carbon dioxide can migrate through the caprock if there are any micro fractures or if the rock fails due to geo-mechanical and/or geochemical effects. Solubility trapping is a safe storage

mechanism because the CO₂ is dissolved into the brine. The only way for CO₂ to come out is with a drastic decrease in pressure which is very unlikely in aquifers. Residual trapping is a safe storage mechanism due to the non-mobility of CO₂ present in the pores of the formation. Mineral trapping is the safest storage mechanism for CO₂ in aquifers, since the gas is converted into carbonate minerals which are very stable over geologic time scales. The only disadvantage of this type of mechanism is that the process is very slow and takes hundreds to thousands of years to yield a reasonable quantity of minerals. Figure 3 (From the IPPC report, 2005) shows qualitatively the increase in storage security with time.

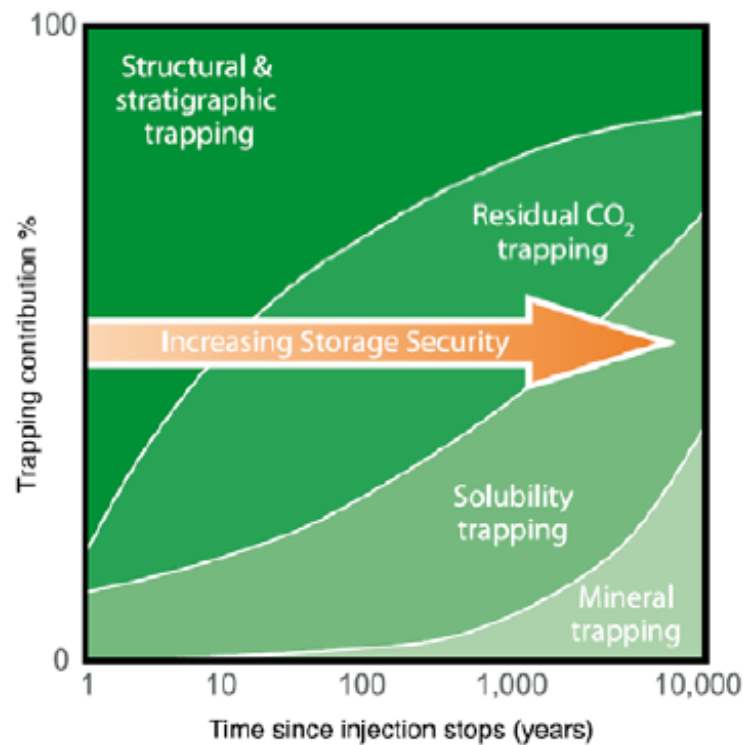


Figure 3 CO₂ storage security overtime for trapping mechanisms.

All the mechanisms present in the CO₂ sequestration process were analyzed in this project using a reservoir simulation model and best available information for the target injection zones.

3.2 GEOLOGY AND RESERVOIR DESCRIPTION

Gordon Creek field is located in the northeast part of Utah in the T 14.S and R8E quadrants. Figure 4 shows the location of the field and the area of interest. This field comprises 5953 gross acres (4879 net acres) in the Carbon County and is geologically situated in the Uinta Basin. The formations of interest for this project are of Jurassic age, and include the Summerville, Curtis, Entrada, Carmel and Navajo Formations. Figure 5 shows a stratigraphic column with the relationships of the formations of interest. This research is focused on the Navajo formation as the Injection formation and the Carmel as the seal.

The Carmel Formation is a marine deposit of fine clastics and gypsum that exhibits cyclic deposition in eastern Utah. The cycles are well developed and consist of three divisions: a lower reduced unit of shale, siltstones, and platy limestone, an oxidized middle member of silty shale, and a top member of irregular bedded gypsum. The probable cause of the cycles is a slow regression of the sea combined with minor periodic advances. Climate changes are proposed as

the mechanism for the cyclical retreat and advancement of the sea (Richards 1958).

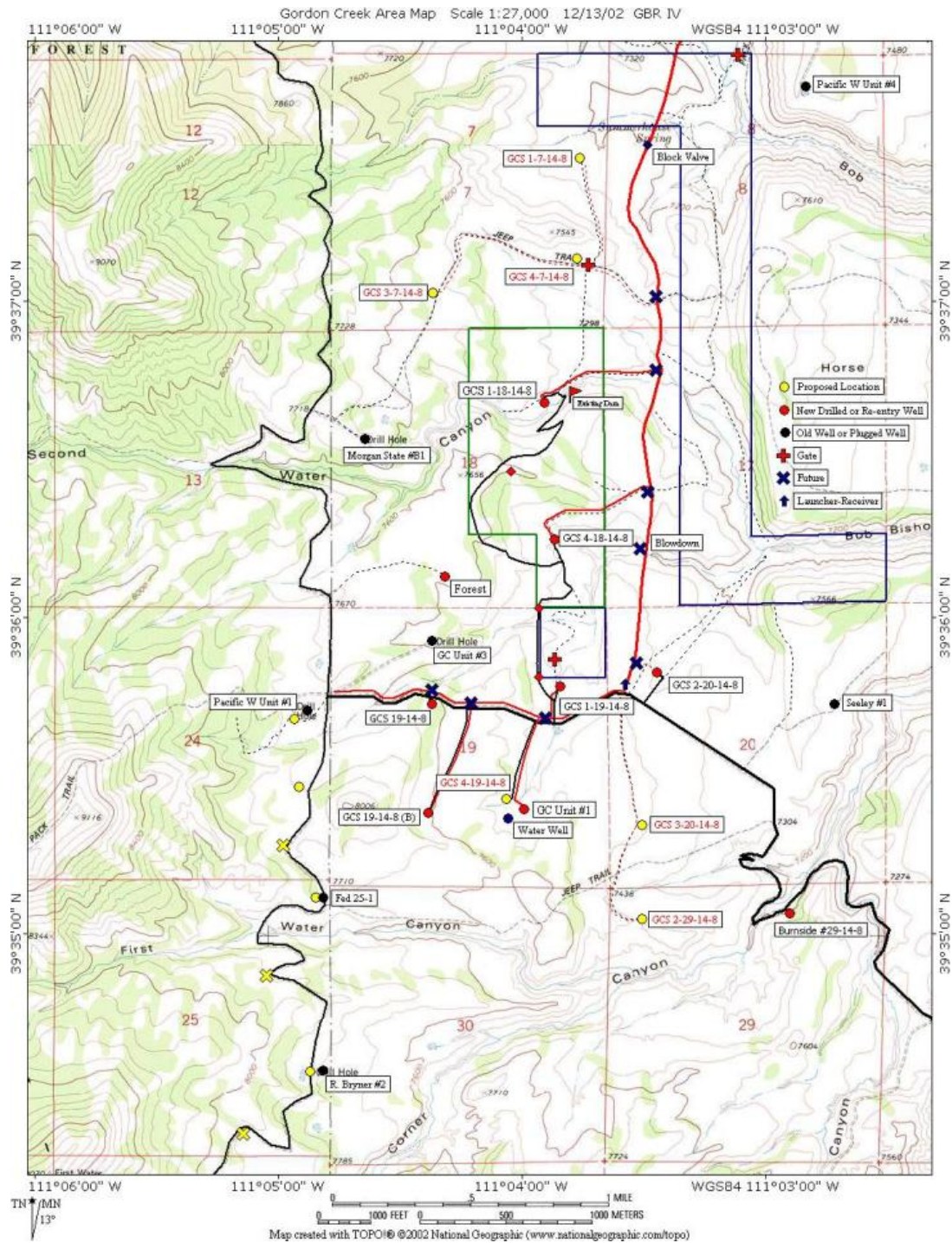


Figure 4 Gordon Creek Map

Period	Symb [†]	Formation / Member	Thickness (feet)	Depth (feet)*	Lith.
CRET	Km	Mancos Shale	Emery Ss Mbr	0	
			Blue Gate Sh Mbr	<250	3115
			Ferron Ss Mbr	10-110	3250
			Tununk Sh Mbr	200-300	4000
	Kd	Dakota Sandstone	0-30	4025	
	Kcm	Cedar Mtn Fm	Upper member	150-750	4120
			Buckhorn Cg Mbr	0-50	
JURASSIC	Jm	Morrison Formation	800±	4460	
	Js	Summerville Formation	120-180	5895	
	Jct	Curtis Formation	140-180	6275	
	Je	Entrada Formation	150-950	6585	
	Jc	Carmel Formation	300-700	7650	
	Jc	Page Sandstone	<70		
	Jgc	Navajo Sandstone	150-300	8400	
		Kayenta Formation	120-200	8750	
		Wingate Sandstone	300-400	8885	
TRIASSIC	Trc	Chinle Fm	Upper member	200-300	9225
			Moss Back Mbr	20-60	
	Trmt	Moenkopi Fm	Upper member	550-700	9520
	Trms		Sinbad Ls Mbr	50	10460
	Trmbd		Black Dragon Mbr	250-350	
PERM	Ppc	Kaibab / Park City Fm	170	10890	
	Pwr	White Rim Sandstone	500-700	11135	

CO₂ Source

CO₂ Sink

Methane Producer

Seal

† Geologic symbols for correlation to units in Morgan (2007)

Modified from Hintze (1992)

Figure 5 Stratigraphic Column Uinta Basin

The Navajo Formation is a homogeneous feldspathic quartz arenite with outcrops along the boundaries of the Colorado Plateau in southern Utah, southern Colorado, and northeastern Arizona. The Navajo Formation comprises the uppermost portion of the Glen Canyon Group and overlies the Kayenta Formation and is in turn overlain by the Carmel Formation. It has a desert-eolian origin, as demonstrated by large scale cross bedding, lack of shale in the

stratigraphic column, no fossil evidence, vast areal extent, well rounded, well sorted and frosted grains(Freeman 1975).

The area of interest is two miles by two miles. This area has been producing gas since the beginning of 1970 in the Ferron Formation and now underlying saline aquifers in the Navajo and Entrada are being considered for CO₂ sequestration.

Currently there is one deep well penetrating the Navajo in the area, the Gordon Creek #1. This is the injection well for the project. The well was drilled in 1979 and then abandoned. A re-entry program was completed in 2003; since then, the well has been producing gas from the Ferron formation and water has been injected into the Navajo Formation for disposal purposes. The well was drilled to a total depth of 11,680 feet, reaching the White Rim Sandstone. Well logs were taken when the well was drilled. These logs have been used to analyze the formations of interest and obtain the reservoir properties needed for the simulation.

3.3 GRID GENERATION.

Implied structure contours from a regional map of the Navajo Sandstone have been used to build the model of the area. Figure 6 presents the structural contours

of the Navajo Sandstone. These contours show faults in the north-south direction that are also included in the project since the regional model could be an anticline or a faulted anticline. A value of zero in the transmissibility of the fault was used in this study which means that the fault is acting as a barrier of flow.

The real structure of the area is not well defined. As it was mentioned before, the aquifers' reservoirs have not been studied deeply and more work has to be done in order to characterize the structure of the grid and to be able to include this information into the simulation model. Seismic data that will be acquired later in the project can help to obtain a better image of the aquifer of interest and identify the faults present in the zone that can play an important role in the carbon dioxide displacement and trapping.

The Landmark Grid Generator (GRIDGENR) was used to create the grid. GRIDGEN is a computer application that helps you describe the three-dimensional structure and properties of a reservoir, then compile the data into a format that can be used to drive reservoir simulation models. A simulation grid can also be created using GRIDGEN. For this model a Cartesian grid with 96 grid blocks in the X and Y direction was generated. The dimension of each cell in the X and Y directions is 110 feet which should correspond roughly with seismic bin spacing when that data is acquired.

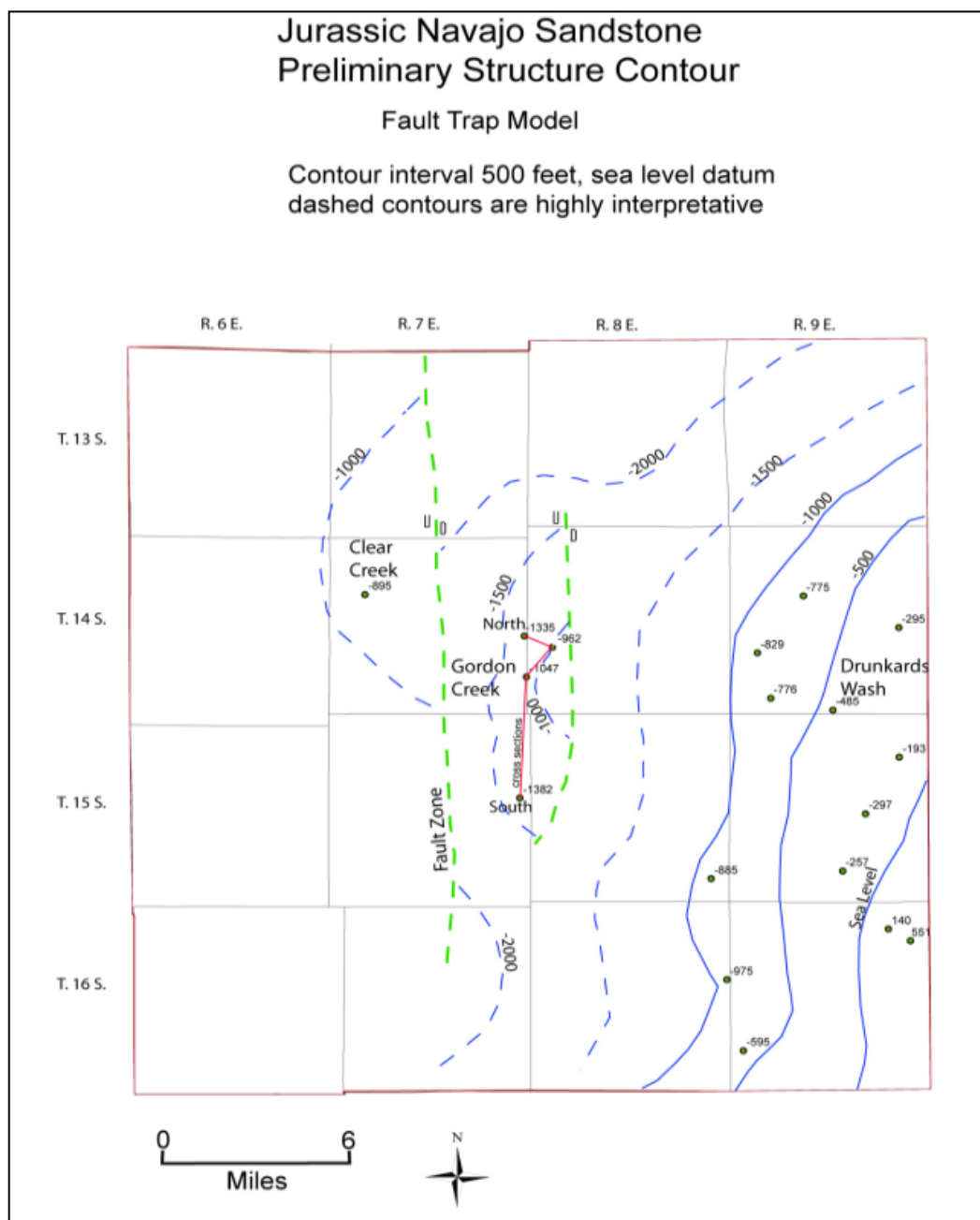


Figure 6. Structure Contour Navajo Sandstone.

Due to buoyancy forces, CO₂ will migrate upwards from the injection formation up to the seal formation. To simulate the direction of carbon dioxide displacement and possible leakage zones, 30 simulation layers of different thicknesses were created to include all the zones mentioned in this project (from the Summerville Formation to Navajo Sandstone). Thinner layers were created in the Sandstones where the CO₂ is injected and in the seal formations since these areas require the most detailed analysis possible for fluid flow.

As a result, a simulation grid with 96x96x30 grid blocks was created with a total of 276,480 grid blocks. Figure 7 shows the model and the location of Gordon Creek #1 well (GC1).

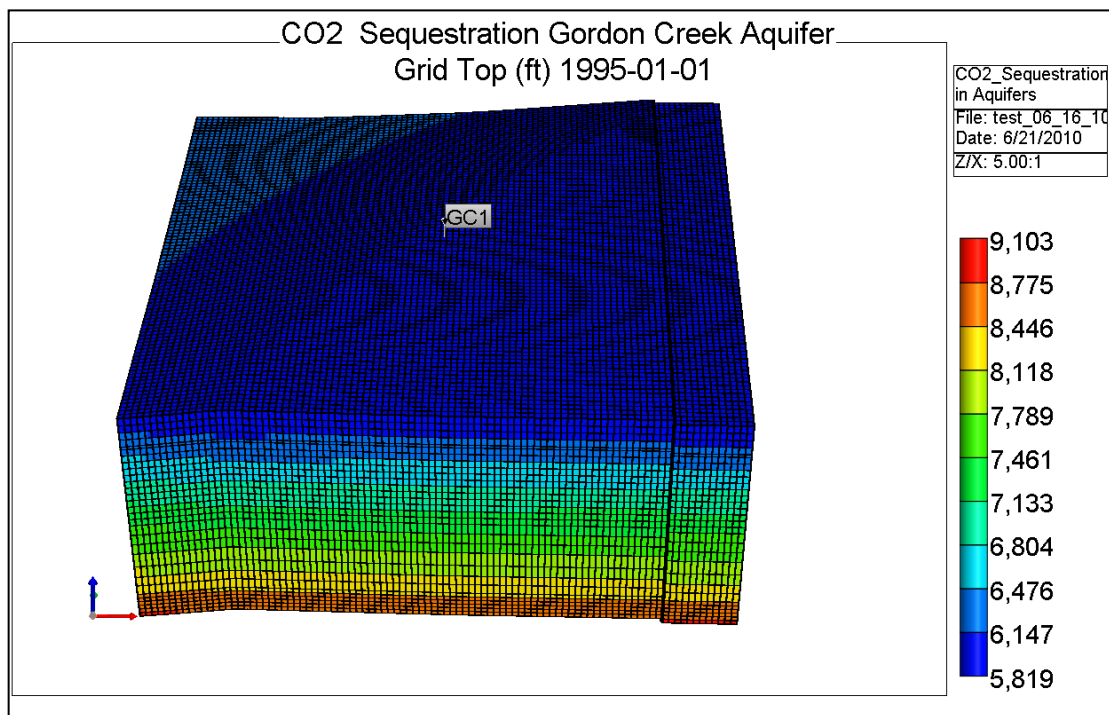


Figure 7. Grid Model. Gordon Creek Field.

After the grid was created using GRIDGENR, a model was built in NEXUS which is a Reservoir Simulator created by Landmark. A gas-water model was created in Nexus to simulate the CO₂ and water injection in the Navajo Formation. These initial results did not include the solubility and chemical reactions present in the CO₂ sequestration process. Due to the reactions between the CO₂ and the aqueous phase, equations for thermodynamic equilibrium have to be included, as well as, the chemical equilibrium equations. The best way to model this type of process is using a compositional model.

The compositional module in NEXUS was not designed to handle CO₂-water systems and while a compositional model was created the results were not as detailed as desired. Work has been done by Landmark in order to build a module for CO₂ sequestration, but was not available at the time of this study

It was decided to use another simulator due to the need of including the trapping mechanisms into the model. The grid created in GRIDGENR was exported into a RESCUE format (Reservoir characterization using Epicenters format). The RESCUE format is a common binary code that allows transferring information such as structural frameworks (faults and horizons), 3D grids, and wells with their

log data, between different simulators. Major simulators have the option to import or export geomodels as a RESCUE file.

The Computer Modeling Group's (CMG) simulator was selected to build the model. The Compositional simulator of Computers Modeling Group GEM was designed to handle injection of carbon dioxide in aquifers with the purpose of sequestering it. The GEM simulator has the ability to include the mechanisms of CO₂ sequestration and analyze them independently to see the contribution of each of them in the overall amount of carbon dioxide trapped.

3.4 RESERVOIR PROPERTIES.

Most of the information related with this model was obtained from the well logs and well reports available for Gordon Creek #1 well. This information was acquired at the Utah Oil and Gas-Department of Natural Resources website, where numerous reports and logs for the wells in the Gordon Creek field are available.

The porosity and permeability values were calculated using the well logs for the GC #1 well. NEURAL LOG Software was implemented to digitize the original logs. These digitized logs were introduced in a log analysis software (LESA) which

is a program used to do a complete shaley formation log analysis, either for single or multi-well studies. Values for permeability and porosity for each simulation layer in the model were calculated using LESA. Appendix A shows a table with the values of these properties for each layer.

Water properties have been calculated using different correlations (Dirik, I. et al, 2004); values for stock tank density, formation volume factor, viscosity and density were also calculated. The values calculated take into account the pressure, temperature of the reservoir and salinity of water, which was obtained after an analysis of a water sample of the zone taken when the well was drilled.

The temperature was assumed constant, with a value of 150°F, which is the temperature in the Navajo Sandstone according to the well report. A Reference pressure of 3700 psi in a reference depth of 8540 feet was used. Rock compressibility was also calculated using the Hall equation (Hall 1953). Table 2 presents the values calculated for these properties.

Reservoir Properties.	Value
Water Stock Tank Density.	64.3659 lb/ft ³
Water Formation Volume Factor.	1.00765 Rb/ Stb.
Water Viscosity.	0.5791 cp.
Water Compressibility.	2.63032 E-6 1/PSIA.
Water Salinity.	58004 ppm.
Rock Compressibility	4.9 E-6 1/PSIA.
Reservoir Temperature.	150° F.

Table 2. Reservoir properties.

Proper values for relative permeability were also needed. However, because CO₂ sequestration in aquifers in this area is an emerging research area, to date no relevant laboratory tests have been done in order to get these curves using real cores of the area of interest at the time of this study. To overcome this limitation, tables found in literature for CO₂-water systems were used (Bennion and Bachu, 2005). The tables used by this project correspond to the deep Basal Cambrian Sandstone aquifer in the Wabamun Lake area southwest of Edmonton in Alberta, western Canada. This sandstone has similar characteristics to the Navajo sandstone and was taken at a similar depth as the Navajo sandstone.

The simulator used for this project also requires the oil-water relative permeability curves, just in case the reservoir conditions reach a state where the gas may form

condensate. For this project the saturation of gas (hydrocarbons compounds) and oil is zero, so a “fake” table was entered to be able to run the model. Figure 8 presents the relative permeability curves for the CO₂-water system used in this model.

Capillary pressure in a CO₂-water system was not included in the study. More work has to be done in order to realize a better characterization of the CO₂ flow in a saline aquifer and get real values for relative permeability and capillary pressure.

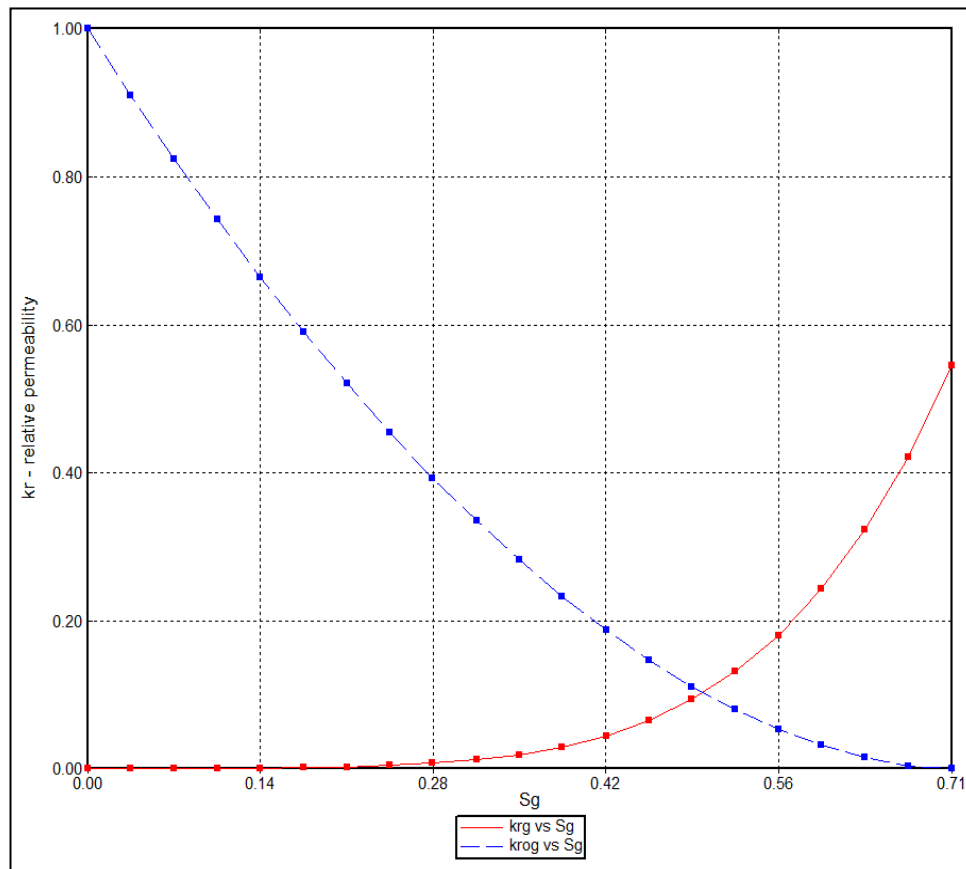


Figure 8. Relative Permeability Curve CO₂-Water System (Bennion and Bachu, 2005)

3.5 WELL DEFINITION AND CONSTRAINTS.

The Gordon Creek #1 well was defined as a water and CO₂ injection well. This well is located in the center of the grid (cell 48,48,1) and has been perforated in the layers 26 through 30 which are located in the Navajo Formation. The well was defined in 01/01/1995 for simulation purposes. The simulation time for this model is 25 years. The following constraints were applied:

1. Water was injected for a period of 25 years which is the total period of simulation:

From January 1995 to December 2010, 1000 BPD were injected.

From January 2010 to Dec 2020, 5000 BPD were injected.

2. CO₂ was injected for four years starting in January 2012. After this period of time the injection was stopped and the CO₂ displacement was analyzed. The following rates were used:

- 1st Year: 14383 MScfd (300000 tons of CO₂ per year)
- 2nd Year: 28766 MScfd (600000 tons of CO₂ per year)
- 3rd Year: 47945 MScfd (1 Million tons of CO₂ per year)
- 4th Year: 47945 MScfd (1 Million tons of CO₂ per year)

A total of 2.9 Million Tons of CO₂ are injected. The CO₂ for injection is produced from a CO₂ reservoir located in the South of the Gordon Creek field. A pipeline will be designed to transport the CO₂ from its source to Gordon Creek #1 well.

3.6 BOUNDARY CONDITIONS.

The model is considered to have closed Flow boundaries. Flow in the lateral barriers is not allowed. The formation of interest is limited at the top and bottom by shale formations with very low permeability. These shales are considered to be impermeable formations and for that reason no influx or efflux in the upper and lower boundaries is permitted. In order to reduce the effect of the lateral boundaries, volume modifiers of 1E+5 were used in the edge blocks.

3.7 GEM, RESERVOIR SIMULATION SOFTWARE.

Computer Modeling Group (CMG) has developed the GEM simulator. GEM is the advanced general equation of state compositional simulator which includes options such as equation of state, dual porosity, CO₂, miscible gases, volatile oil, gas condensate, horizontal wells, well management, complex phase

behavior and many more. The CO₂ module of this simulator was used in this study to model the injection and sequestration of CO₂ into an aquifer formation, as well as, the aqueous phase chemical reactions, mineral precipitation and dissolution.

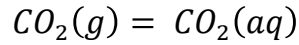
The modeling of CO₂ storage in saline aquifers involves the solution of the component transport equations, the equations for thermodynamic equilibrium between the gas and the aqueous phase, and the equations for geochemistry, which involve reactions between the aqueous species and mineral precipitation and dissolution.

There are essentially two approaches for solving the coupled system of equations: the sequential solution method and the simultaneous solution method. In the sequential solution approach, the flow equations and chemical equilibrium equations are solved separately and sequentially. Iterations are applied between the two systems until convergence is achieved. The simultaneous solution approach solves all equations simultaneously with Newton's method. The simultaneous solution approach is also referred to as the fully-coupled approach. The fully-coupled approach is the method used in the GEM simulator for modeling the CO₂ storage in saline aquifers (User's Guide Computer Modeling Group, 2009).

The GEM module for CO₂ sequestration was developed by Nghiem (2004). The simulation and modeling techniques for solubility, residual gas and mineral trapping are based on the equation of state compositional and greenhouse gas simulator with the geochemical option.

3.7.1 SOLUBILITY TRAPPING.

Gas solubility in brine is modeled as a phase equilibrium process and can be represented by the following chemical reaction:



Where (g) and (aq) represent the CO₂ in the gas and aqueous phases.

As dissolution of gas in liquid is very fast, these phases are assumed to be in thermodynamics equilibrium, which is governed by the equality of fugacity in the gas and aqueous phase:

$$f_{i,g} = f_{i,aq}, i = 1, \dots, n_c$$

The fugacity $f_{i,g}$ of component i in the gas phase is calculated from the Peng-Robinson equation of state PR_EOS (Peng, D,Y and Robinson, D,B, 1976). The fugacity $f_{i,aq}$ of component i of the gas in the aqueous phase is calculated using Henry's Law: (Li and Nghiem, 1986)

$$f_{iw} = y_{iw} \cdot H_i$$

Where H_i are the Henry's law constants which are affected by the pressure, temperature and salinity and are expressed as:

$$\ln H_i = \ln H_i^* + \frac{1}{RT} \int_{p^*}^p \bar{v}_i dp$$

Where,

H_i Henry's constant at p and T

R Gas Constant

$\bar{v}_i$ Partial molar volume of component i in solution.

Several correlations have been developed to calculate Henry's constant for many gases including CO_2 using the saturation pressure of H_2O , temperature and the effect of salinity (Bakker 2003). The GEM simulator uses correlations published by Harvey (1996) in order to do the calculations. Appendix B presents the

correlations to calculate the Henry's constants and the equation that take into account the effect of salinity in the constants.

3.7.2 RESIDUAL GAS TRAPPING.

Residual gas saturation is important for CO₂ trapping. Carbon dioxide is first injected into the aquifer displacing the water present in it (considering that CO₂ is not the wetting phase, this is a drainage process). After the injection has stopped, the water migrates again to the space where the gas was injected (imbibitions' process) and generates hysteresis. The residual gas saturation is the gas trapped when the water has imbibed into the rock from a state of irreducible water saturation to a state of zero capillary pressure. There are many residual gas trapping models. In this simulator the classical Land's model is used (Land, 1968). The Land's coefficient C is expressed as:

$$C = \frac{1}{S_{gt,max}} - \frac{1}{S_{g,max}}$$

Where, $S_{g,max}$ is the maximum gas saturation that could be attained and $S_{gt,max}$ is the maximum trapped gas saturation. The residual gas saturation for a given gas is:

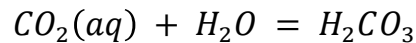
$$S_{gt}^*(S_{gi}^*) = \frac{S_{gi}^*}{1 + CS_{gi}^*}$$

To promote residual gas trapping is highly recommended to inject the CO₂ near the bottom of the aquifer in order to create more interaction between water and carbon dioxide while the CO₂ is flowing up due to density differences.

3.7.3 MINERAL TRAPPING.

This mechanism is potentially attractive because it can immobilize CO₂ for long periods of time, and prevent its easy return to the atmosphere.

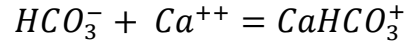
Chemical reactions occur between components in the aqueous phase and between minerals and aqueous components. Ortoleva et al (1998) presents the chemical reactions induced by CO₂ injection. First, CO₂ dissolves in water to produce the weak carbonic acid:



This is followed by rapid dissociation of carbonic acid to form:



The increased acidity induces dissolution of many of the primary host rock minerals, which in turn causes complexing of dissolved cations with the bicarbonate ion such as:



Under favorable conditions, the carbonate ion will react with the different metal ions present in the formation water to precipitate carbonate minerals. Reactions for the most common carbonate minerals are:

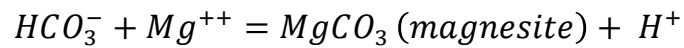
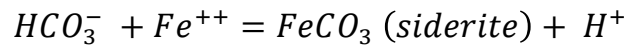
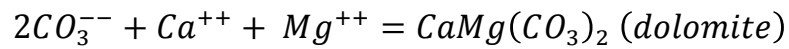
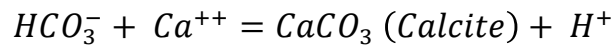
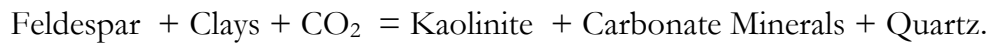


Table 3 presents some of the most common aqueous and mineral reactions that trap CO₂ through the dissolution and precipitation of minerals.

TABLE 3 – GEOCHEMICAL REACTIONS	
<u>Intra-aqueous chemical equilibrium reactions</u>	
1.	$\text{H}_2\text{O} \leftrightarrow \text{H}^+ + \text{OH}^-$
2.	$\text{CO}_2(\text{aq}) + \text{H}_2\text{O} \leftrightarrow \text{H}^+ + \text{HCO}_3^-$
3.	$\text{HCO}_3^- \leftrightarrow \text{H}^+ + \text{CO}_3^{--}$
4.	$\text{AlOH}^{++} + \text{H}^+ \leftrightarrow \text{Al}^{+++} + \text{H}_2\text{O}$
<u>Mineral dissolution/precipitation reactions</u>	
5.	$\text{Calcite} + \text{H}^+ \leftrightarrow \text{Ca}^{++} + \text{HCO}_3^-$
6.	$\text{Dolomite} + 2 \text{H}^+ \leftrightarrow \text{Ca}^{++} + \text{Mg}^{++} + 2 \text{HCO}_3^-$
7.	$\text{Chalcedony} \leftrightarrow \text{SiO}_2(\text{aq})$
8.	$\text{Kaolinite} + 6 \text{H}^+ \leftrightarrow 5 \text{H}_2\text{O} + 2 \text{SiO}_2 + 2 \text{Al}^{+++}$
9.	$\text{Illite} + 8 \text{H}^+ \leftrightarrow 5 \text{H}_2\text{O} + 0.6 \text{K}^+ + 0.25 \text{Mg}^{++} + 2.3 \text{Al}^{+++} + 3.5 \text{SiO}_2(\text{aq})$
10.	$\text{Siderite} + \text{H}^+ \leftrightarrow \text{Fe}^{++} + \text{HCO}_3^-$
11.	$\text{Annite} + 10 \text{H}^+ \leftrightarrow 3 \text{Fe}^{++} + \text{K}^+ + \text{Al}^{+++} + 3 \text{SiO}_2(\text{aq}) + 6 \text{H}_2\text{O}$
12.	$\text{Anorthite} + 8 \text{H}^+ \leftrightarrow \text{Ca}^{++} + 2 \text{Al}^{+++} + 2 \text{SiO}_2(\text{aq}) + 4 \text{H}_2\text{O}$

Table 3. Chemical and Mineral Reactions. From Nghiem (2009).

According to Nghiem (2004) mineral trapping is more effective in reservoirs that have large protons sink such as feldspar and clay mineral. The ions H^+ and HCO_3^- from the aqueous chemical equilibrium reactions, will react with the different minerals resulting in an overall reaction of the form (Bachu, 1996).



The same appreciation of Nghiem (2004) was done by Gunter et al. (2000), saying that from their experimental work, the sandstones (Siliciclastic) aquifers appear to be better trapping reservoirs for mineral trapping of CO_2 than carbonates aquifers.

Modeling of Chemical Equilibrium Reactions, as well as, mineral dissolution and precipitation reactions and their solutions methods were done by Nghiem (2009).

4. CASE STUDIES.

Different scenarios were evaluated in order to study the CO₂ movement inside the aquifer and the impact that every trapping mechanism has in the carbon dioxide sequestration.

4.1 BASE CASE – STRUCTURAL TRAPPING.

A base model was built using the CMG-GEM simulator. The properties mentioned in Chapter 3 as well as the RESCUE model from GRIDGEN were used to build this model. In this case, injection of carbon dioxide in a supercritical state is performed and the only mechanism included is the structural trapping.

A compositional model was created using two components: CO₂ and C1. The C1 component is added as a trace component (trace-component is usually a gaseous component such as C1 or another CO₂-like component with properties identical to those of CO₂), so the gas phase exists in each grid block because this component is not soluble in the aqueous phase (solubility is set to zero for C1) and gas phase properties are continuously calculated.

After the model ran for 25 years, 50,759 MMScf of CO₂ were injected , which is around 2.9 millions of tons of CO₂ (1 Ton = 14.7 Mscf). The injectivity of the well was good enough to accomplish the injection objective of CO₂.

After the simulation was completed, the CO₂ had migrated about 1,430 feet in the horizontal plane, and had migrated up and reached layer 25 which is the top layer of Navajo Formation. Layer 24 represents the bottom layer of the seal and free gas CO₂ did not migrate into the seal. Figures 9 and 10 present the CO₂ saturation around the well and the shape of the CO₂ plume after 25 years of simulation (Keep in mind that the bottom 6 layers correspond to the Navajo Sandstone as is showed in Figure 10).

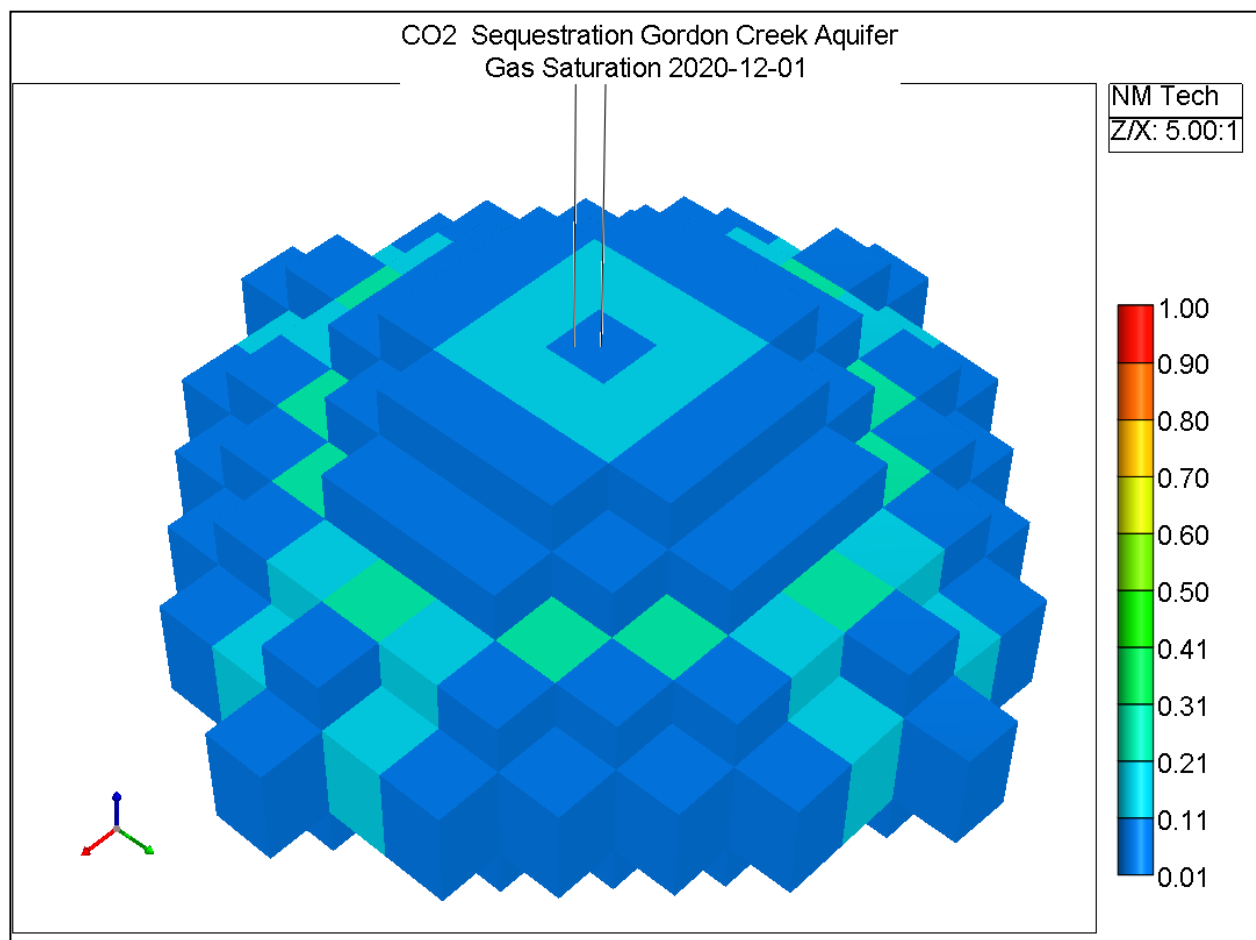


Figure 9. CO₂ Saturation graph in 3DView after 25 years of Simulation.

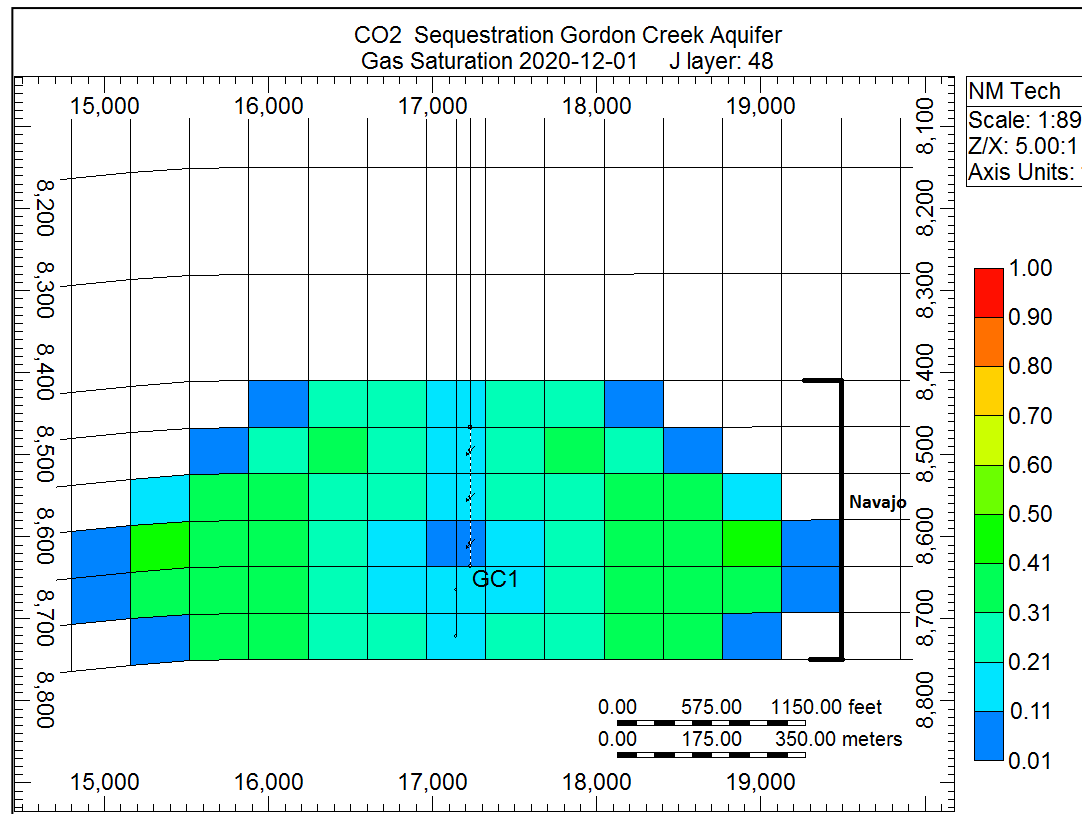
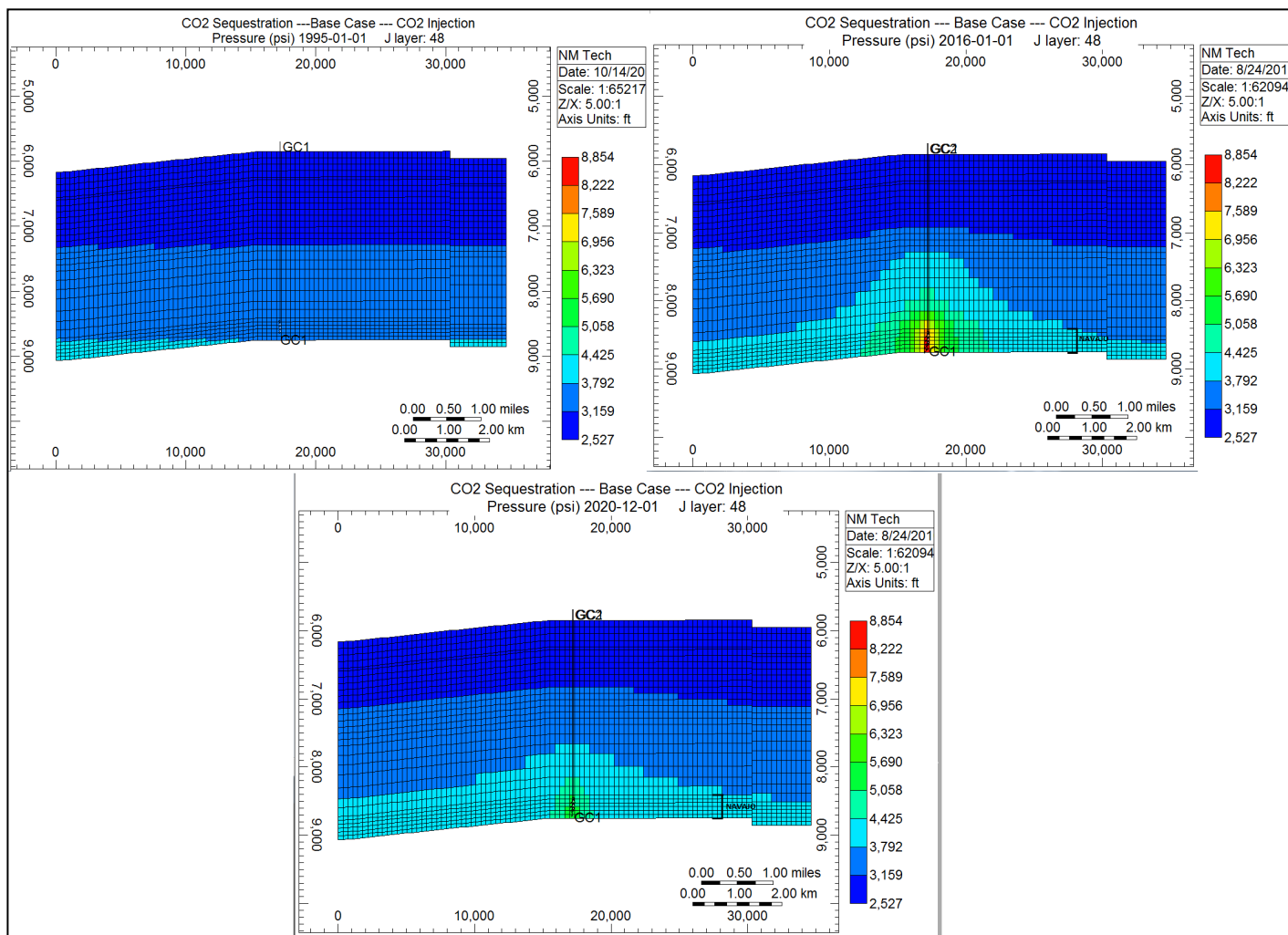


Figure 10. CO₂ saturation graph. Base Case Model.

The pressure in the reservoir changed due to the injection of water and CO₂.

The biggest changes were observed around the well. Pressure changes were observed not only in the Navajo Sandstone, but also in the seal formation above it, which implies that there is communication between the formations. Figure 11 shows the pressure changes around the wellbore after the simulation was completed. Maximum values of 8,854 psi were observed during the simulation around the wellbore, which is lower than the expected fracture pressure for the zone (9000 psi).



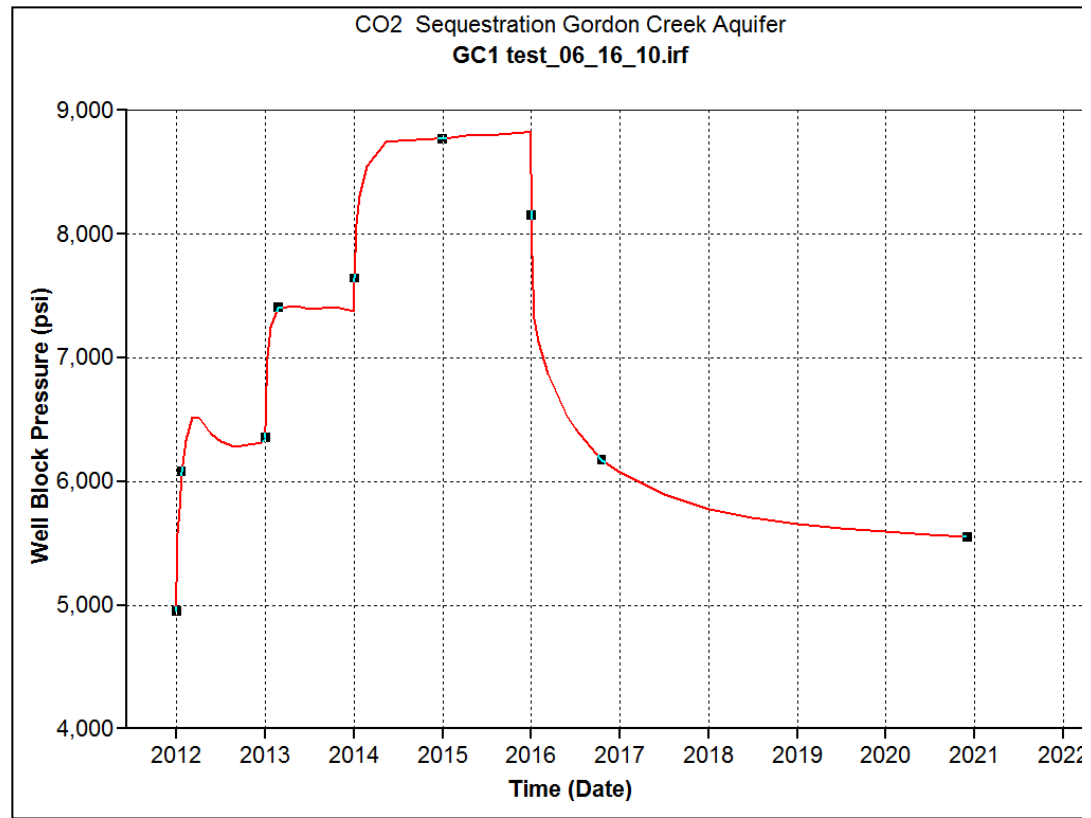


Figure 12. Well Block Pressure. Base Case.

Figure 12 also shows the pressure around the wellbore through time and confirms that the pressure does not reach the fracture pressure of the formation.

4.2 CASE2. STRUCTURAL TRAPPING - RESIDUAL GAS TRAPPING

Residual gas trapping in the model is simulated using a value for the maximum residual gas saturation. Including this value into the simulator, when the gas is contacted by water after the CO₂ injection, some gas will get trapped into the pores while saturation of water increases.

Some studies have been made to calculate the maximum residual gas saturation (S_{grm}). Holtz (2002) and Kumar (2005) state that rock and pore type can have a strong influence in the value of S_{grm} , and variations in carbonate rock types can also affect it. According with Holtz' study, S_{grm} increases with an increase in clay content in sandstones and decreases with sorting and grain size.

A study of petro-physical properties concluded that porosity is the property that most influences the values of S_{grm} . The following correlation was developed by Holtz to calculate the S_{grm} and was used in this study to calculate this value:

$$S_{grm} = 0.5473 - 0.969 * \phi$$

An average value for the S_{grm} for the Navajo Formation was calculated using the values of porosity available. A value of 0.4 for the S_{grm} was calculated and included in the model.

After the simulation, it was found that the CO_2 saturation around the well after 25 years is higher at the bottom part of the aquifer and the free gas CO_2 has not migrated upwards as much as it did in the Base Case due to the gas trapping in the bottom grid blocks. Figure 13 presents the gas saturation around the well and the shape of the plume.

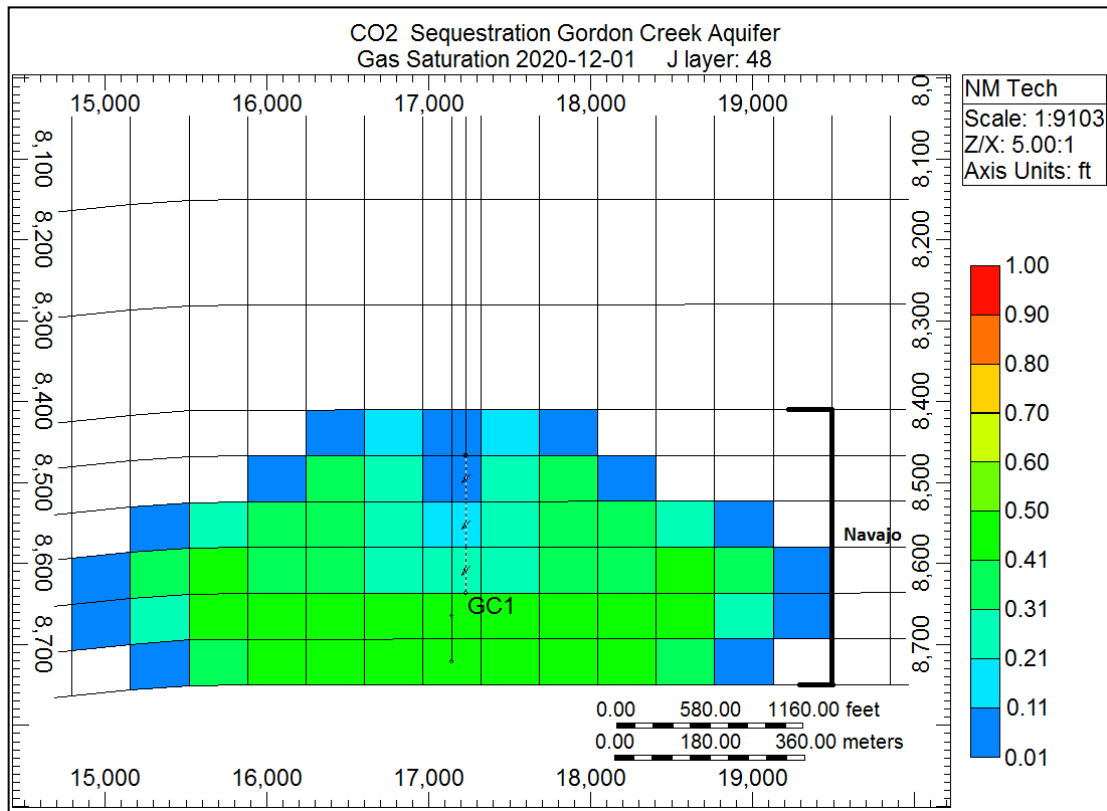


Figure 13. CO₂ saturation graph. CO₂ Injection + Gas Trapping.

Less CO₂ reached the upper layer of the Navajo Formation and contacted the seal, which implies that some of the CO₂ was trapped in the pores by hysteresis and was kept immobile in the bottom layers. This implies that there is a less risk of CO₂ gas leakage through the seal formation. Figure 14 shows the CO₂ saturation around the well for the Base Case (left picture) and the case involving gas trapping (right picture).

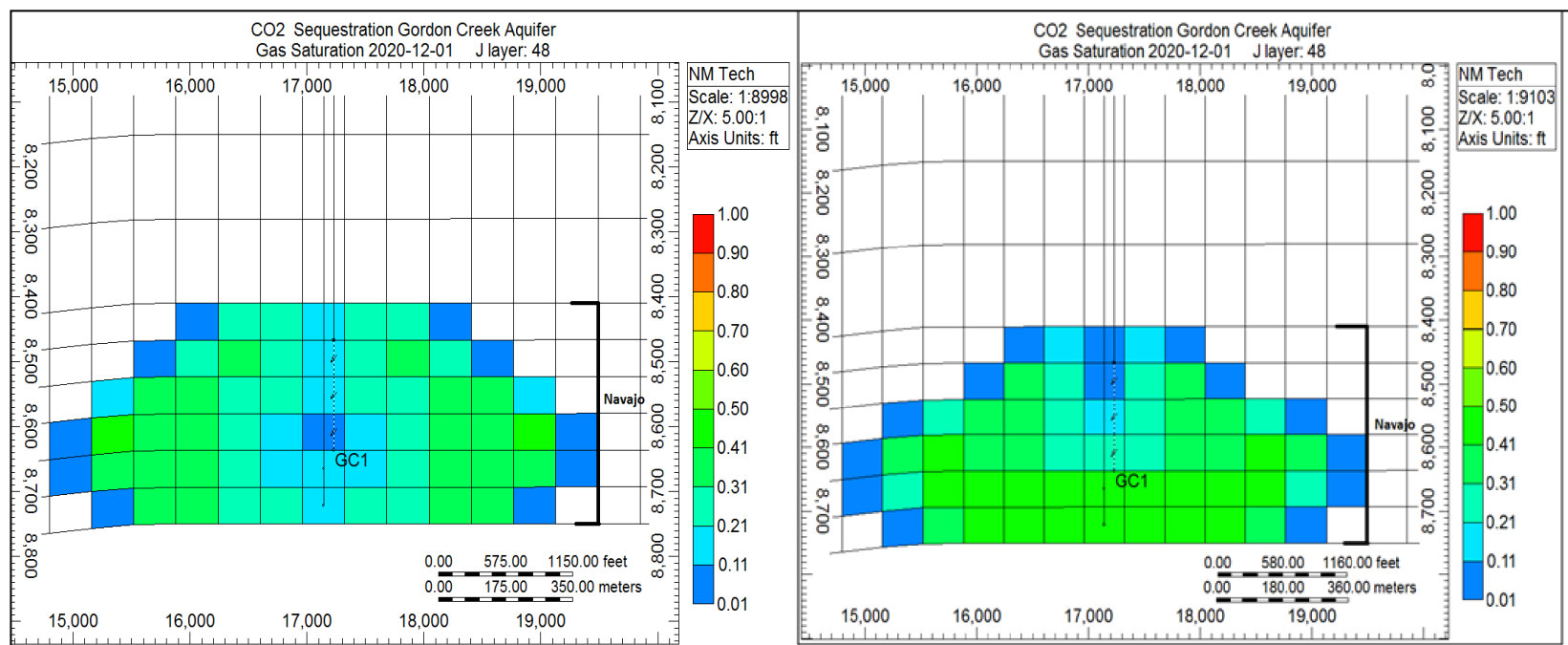


Figure 14. CO₂ saturation graph. Base Case (left) and CO₂ Injection + Gas Trapping Case (Right).

Figure 15 shows the cumulative injection of CO₂ and the contribution of each mechanism in the total amount of CO₂ trapped. In the Base Case all the CO₂ injected was trapped in a supercritical state; after the gas trapping was included v see that a large amount of that CO₂ was stored as immobile gas. Figure 16 presents the percentage of CO₂ trapped by each mechanism. It shows that about 35 % of the CO₂ has been trapped by the gas trapping mechanism and the rest (65%) still exists as a mobile CO₂, which is a good result for a very short simulation.

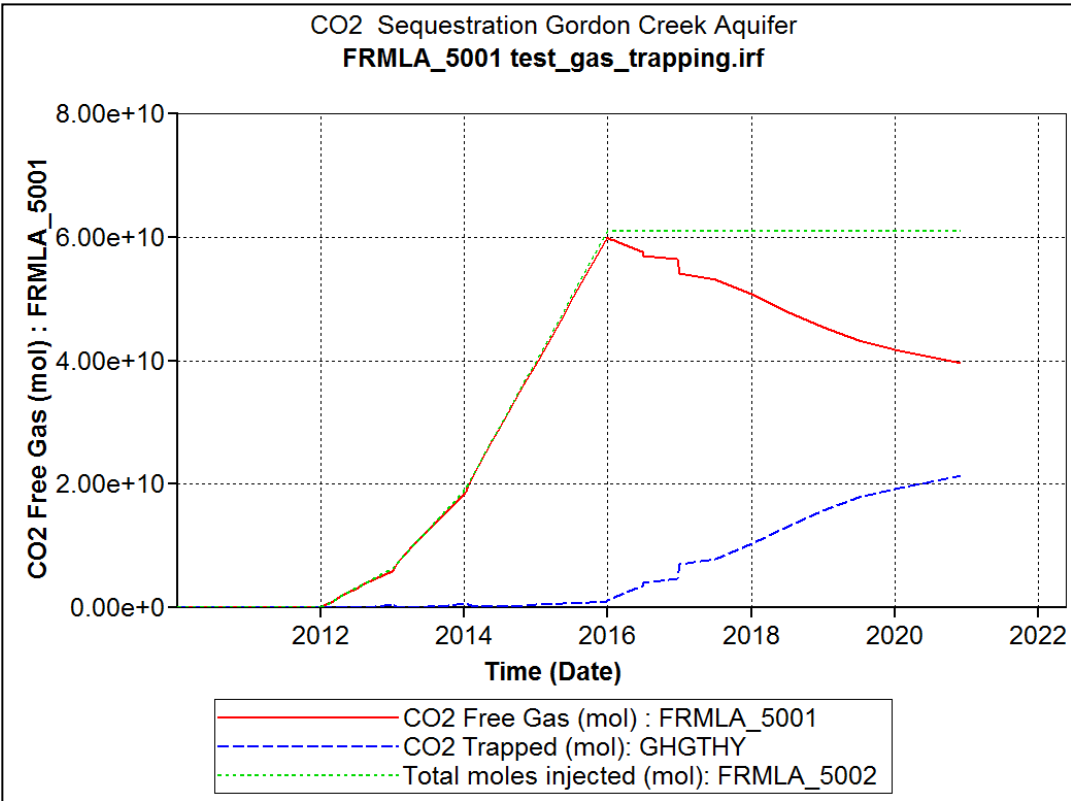


Figure 15. CO₂ trapping mechanisms contribution, Case 2.

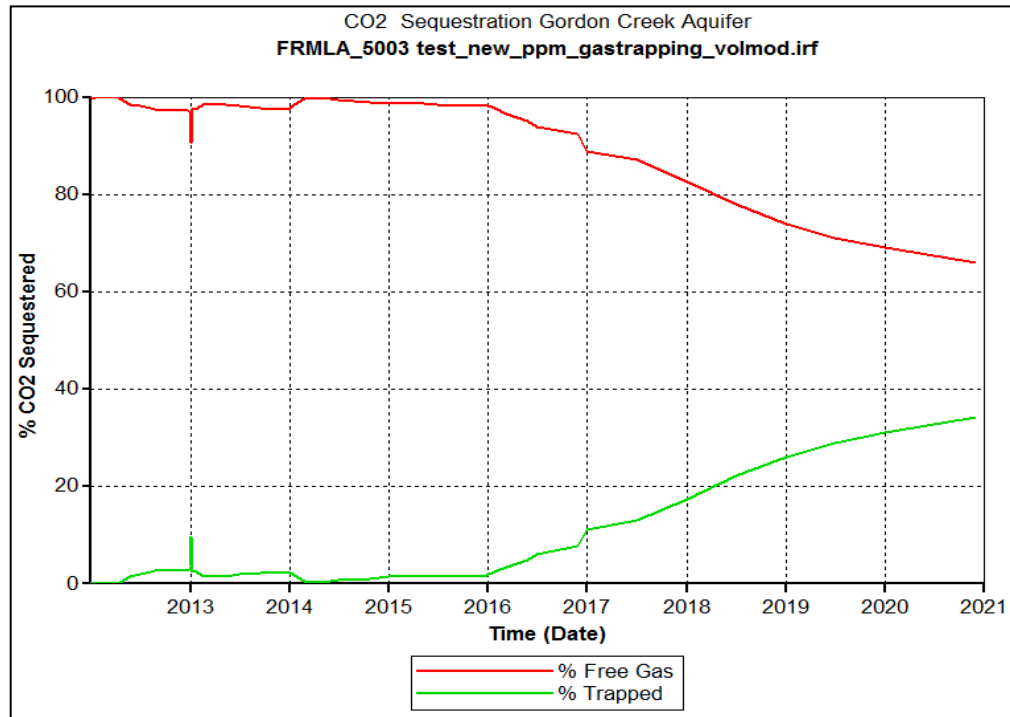


Figure 16. Percentage of CO₂ Sequestered, Case 2.

Figure 17 shows the pressure around the wellbore. The results are similar to the ones obtained in the Base Case; the pressure around the wellbore does not exceed the fracture pressure of the formation and the maximum value observed is less than 9000 psi. In this case the high values of pressure around the wellbore at the end of the simulation are due to the gas trapped in the pores when water is injected after the CO₂ which produces an additional increase in pressure. For that reason the final pressure at the end of the 25 years is higher than the pressure obtained in the Base Case.

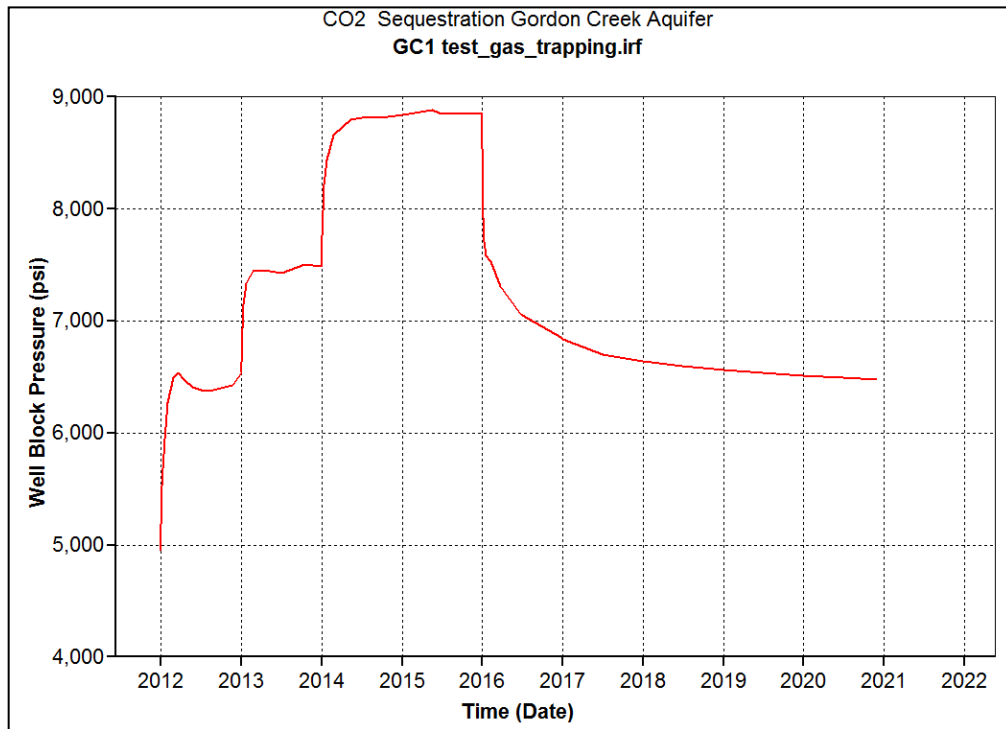


Figure 17. Well Block Pressure. Case2.

4.3 CASE 3. STRUCTURAL TRAPPING - RESIDUAL GAS TRAPPING – SOLUBILITY IN WATER

For case 3 the solubility trapping mechanism is included in the model as well as the gas trapping and seal trapping mechanisms.

The Henry's coefficients for the CO₂ and C1 needed to include solubility were calculated using the WinProp module available on CMG. Winprop is the equation of state multiphase equilibrium and properties determination program available in CMG. This program is used to generate component properties for the

compositional simulator (GEM) and calculate in this case the parameters needed to simulate the CO₂ solubility in water.

The Henry coefficient for C1 is not included in the calculation and is set to zero to avoid the solubility of this component in the aqueous solution (C1 is only a trace component and does not need to be included in the calculations). For the solubility calculation in this model, the Harvey's correlation has been used.

Figure 18 presents the gas saturation around the well after the simulation was done. According to the graph most of the CO₂ has been trapped at the bottom of the Navajo formation and the amount of free CO₂ reaching the seal is very low. It is also important to mention that the gas saturation around the well in the layers 25-28, where the injection of water continued after the injection of CO₂ stopped, is zero. The CO₂ has been displaced horizontally and upwards by the water and by dissolution, leaving no gas around the well and showing that in this case the dissolution prevails over the gas trapping mechanism.

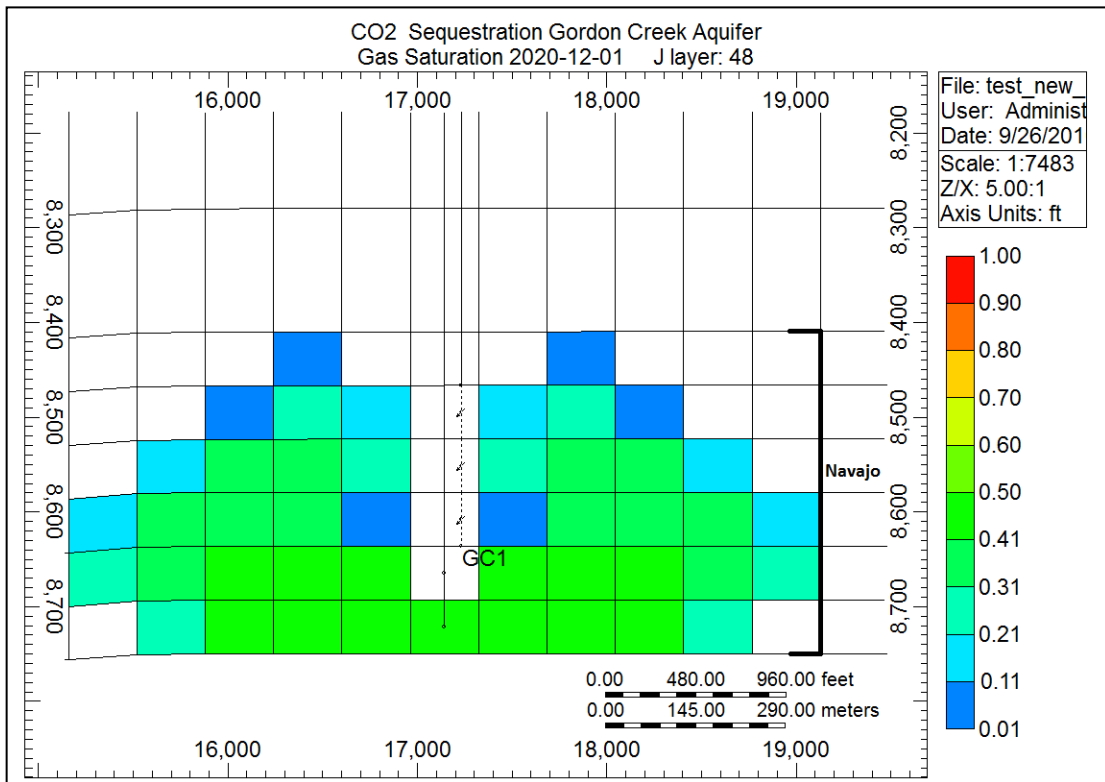


Figure 18. CO₂ saturation graph. CO₂ Injection + Gas Trapping.

Figure 19 is a comparison of gas saturation between the Base Case (left), the case including gas trapping (right) and the case including solubility (bottom). After the solubility and gas trapping were included, most of the gas stays at the bottom of the formation and with this, the free CO₂ is safely stored underground. It is also important to mention that the gas saturation at the outer edges of the plume is higher for case 3, implying that the lateral gas movement is higher than in previous cases.

The dissolution of CO₂ into water increases constantly through time and more CO₂ is dissolved when water is injected after the CO₂ injection period.

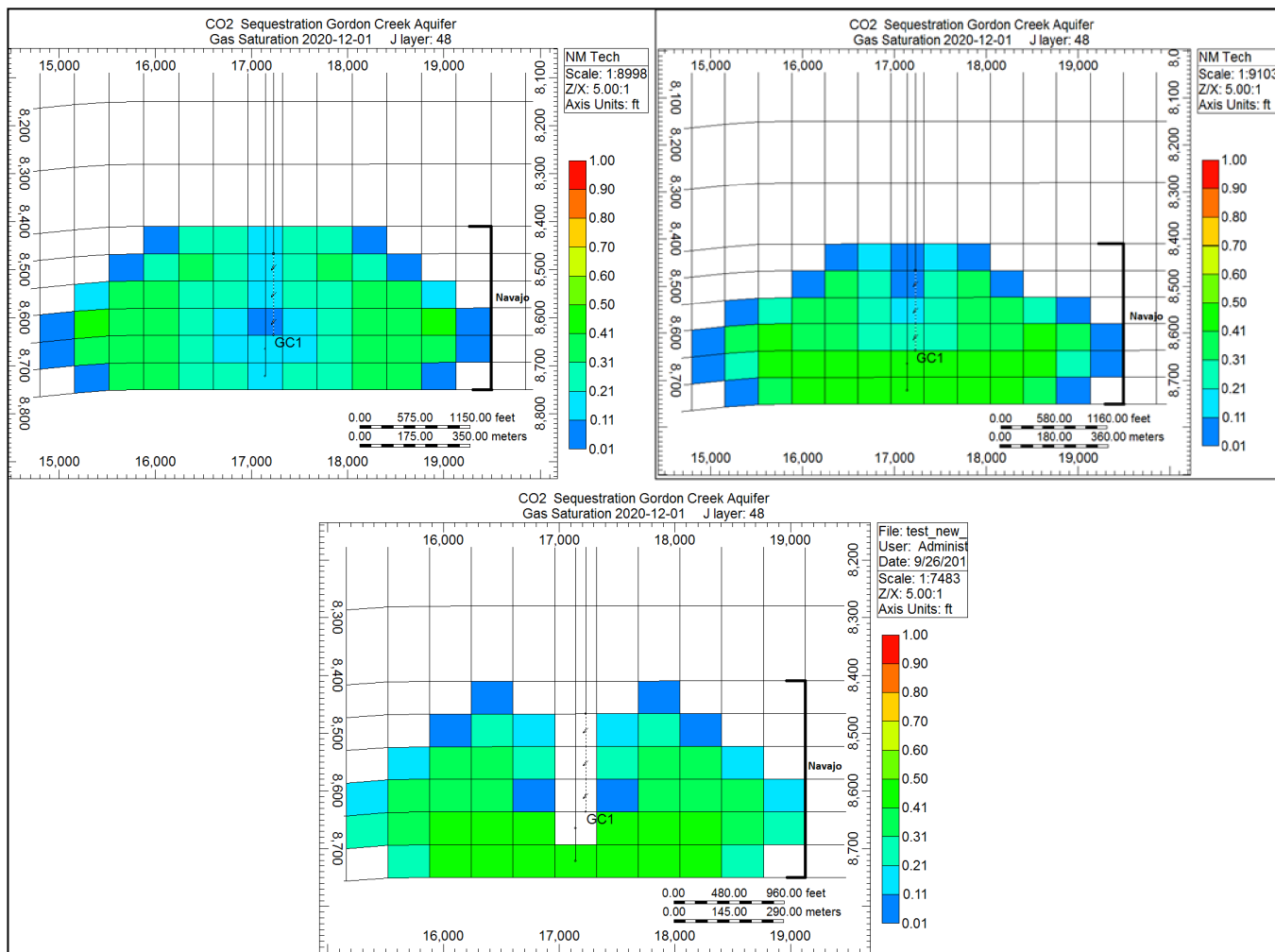


Figure 19. CO₂ saturation for the first 3 cases.

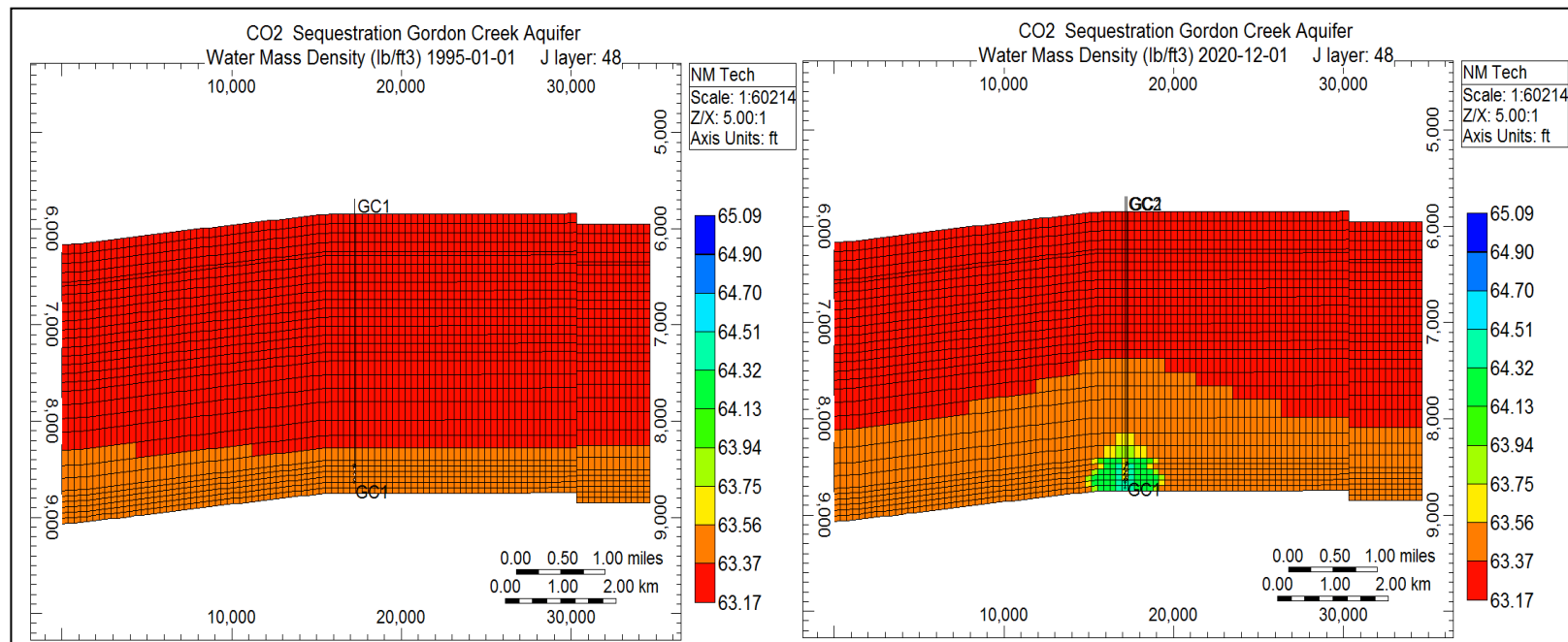


Figure 20. Water Mass Density changes.

Figure 20 presents the changes associated with the water mass density around the wellbore. These changes are related with the dissolution of CO₂ into the water. On the left side of the figure, the initial water mass density is presented. Constant values in almost all the formations are shown. After the CO₂ injection, the water mass density increases and big changes in this property are observed around the wellbore, which indicates that large amounts of CO₂ are in constant reaction with the formation water and CO₂ is dissolved into it.

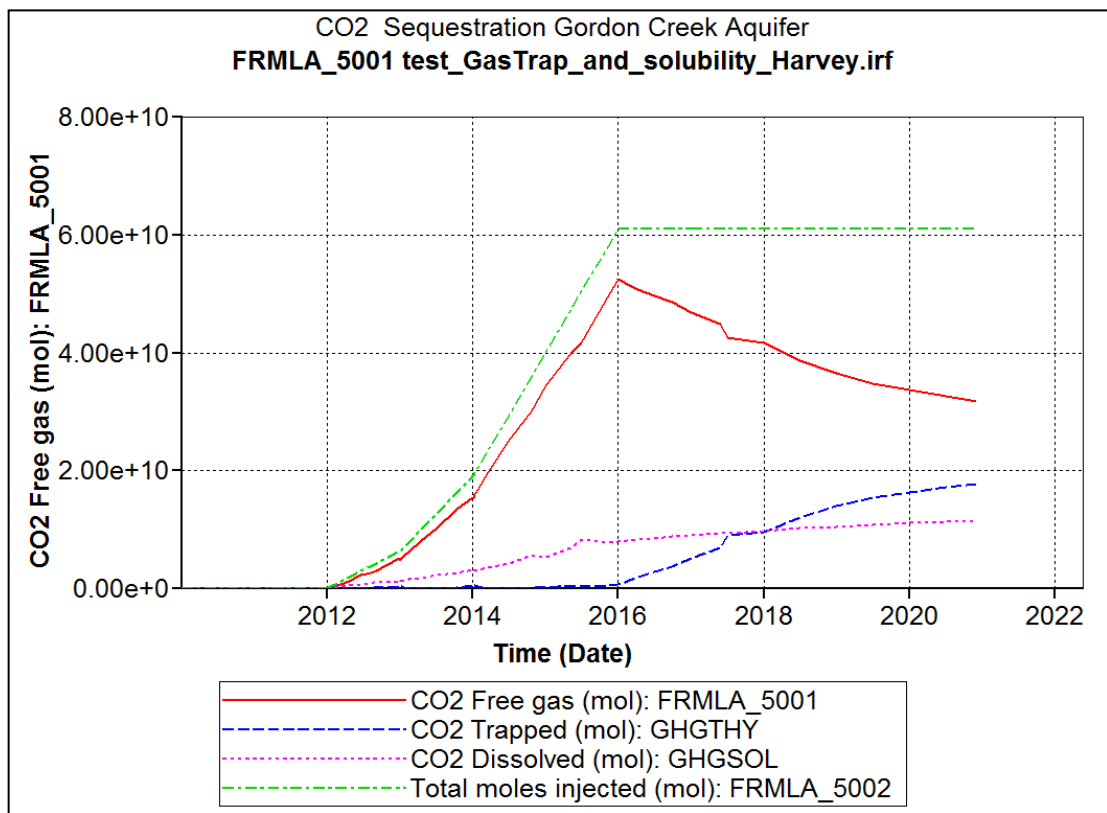


Figure 21. CO₂ trapping mechanisms contribution. Case 3.

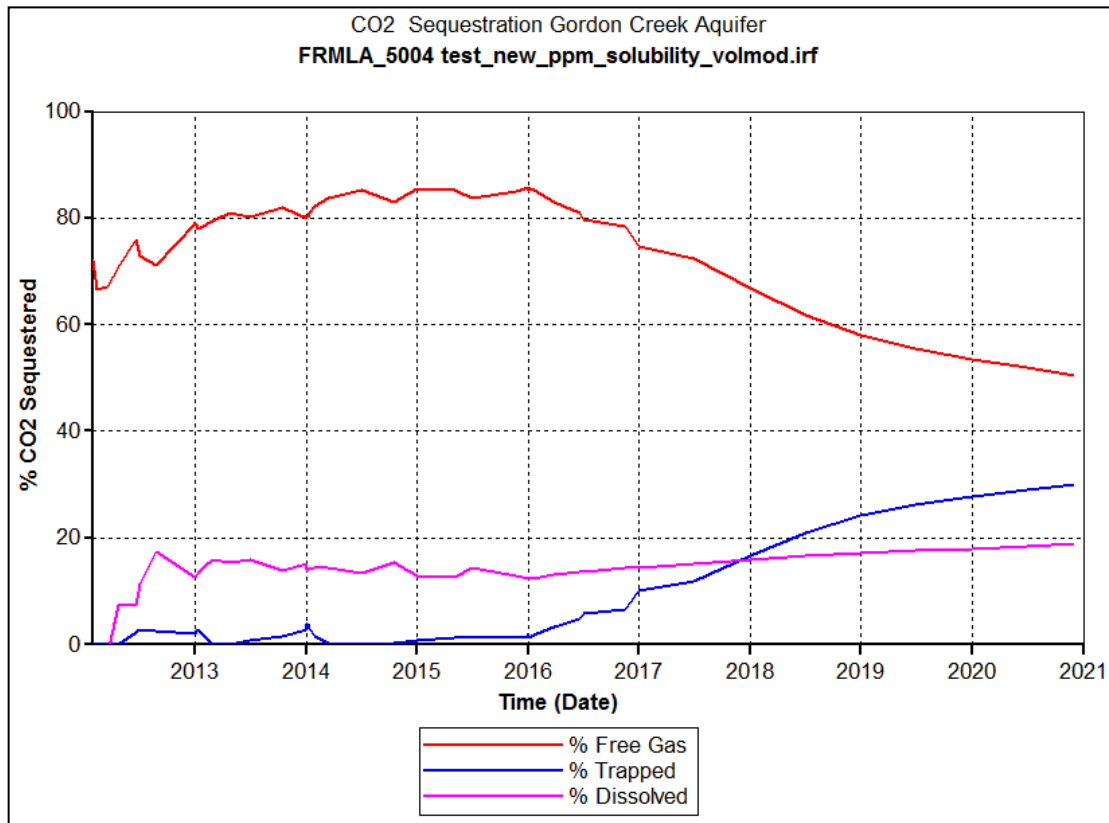


Figure 22. Percentage of CO₂ Sequestered. Case 3.

Figure 21 presents the amount of CO₂ trapped using the solubility mechanism, as well as, gas trapping and CO₂ in supercritical stage. We can see that most of the CO₂ is still mobile but a significant quantity of this CO₂ has been trapped for the other mechanisms. Figure 21 shows that residual gas trapping starts to be more important after the CO₂ injection has stopped and water alone is injected into the formation and CO₂ is displaced and trapped into the pores by hysteresis.

CO₂ trapping using the solubility mechanism increases slowly and the final amount of gas trapped is less than that which is trapped by residual gas saturation.

Figure 22 also presents the percentage of CO₂ trapped for each mechanism. The figure shows that around 50% of the gas is still mobile, 31% has been trapped by residual gas mechanism and around 19% has been trapped by dissolution in water. For a 25 year period of time, the amount of CO₂ trapped by residual gas trapping and dissolution in water is considerably high, and with that behavior big quantities of CO₂ are expected to be trapped for those mechanisms when simulations for longer periods of time are performed.

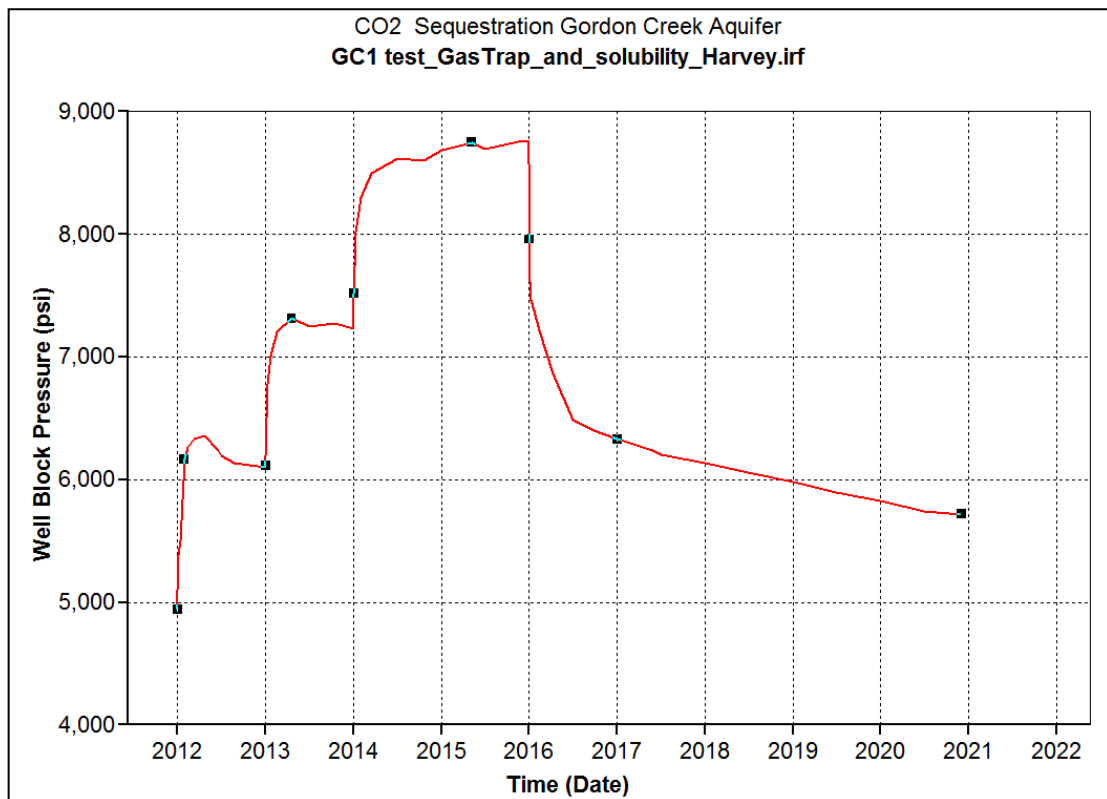


Figure 23. Well Block Pressure. Case3.

Figure 23 presents the pressure around the wellbore. Values lower than 9000 psi, which is the fracture pressure for the formation, are observed. It is observed that the well block pressure at the end of the simulation for this case is lower than the pressure in case 2 (above 6000 psi), the reason for this could be that there is less gas present as free gas around the wellbore because most of the CO₂ in that zone (wellbore) is dissolved into water.

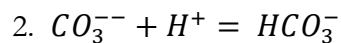
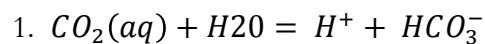
4.4 CASE 4. STRUCTURAL TRAPPING – RESIDUAL GAS TRAPPING – SOLUBILITY IN WATER - MINERALIZATION.

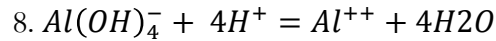
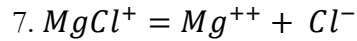
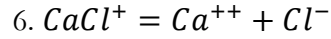
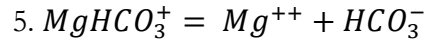
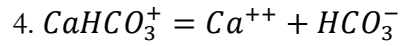
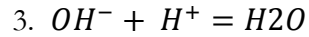
Before including the mineralization as a gas trapping mechanism in the simulation model, properties related with the aqueous phase and the minerals present in the rocks should be entered.

Winprop module is used to enter information related with the rock and the brine properties, and calculate the different parameters used in the simulation model.

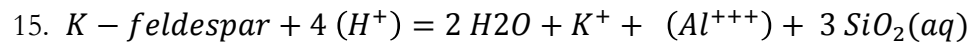
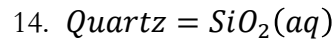
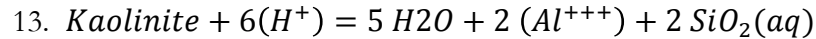
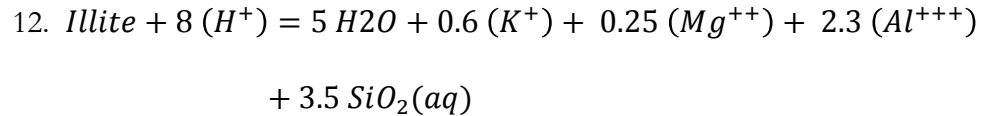
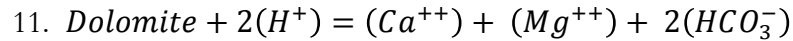
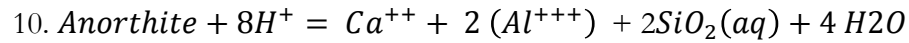
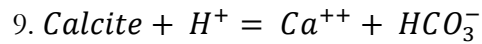
The following Aqueous and Mineral reactions were included in the model:

- Aqueous Species Reactions.





- Mineral Species Reactions.



Water analysis in the Navajo Formation was done by River Gas Corporation. The Total Dissolved Solids (TDS) present in the water were obtained. This information, as well as the molality calculations of the brine, are parameters needed in Winprop.

Table 4 presents the results of the water analysis done on a water sample obtained from the Navajo Formation. Cations and anions encountered in the sample are listed below.

PRODUCTION WATER ANALYSIS		
Cations	mg/L	as:
Calcium	397	(Ca++)
Magnesium	158	(Mg++)
Sodium	17990	(Na+)
Iron	0	(Fe ++)
Manganese	0	(Mn++)
Anions	mg/L	
Bicarbonate	1600	(HCO ₃ ⁻)
Sulfate	1540	(SO ₄ ⁻⁻)
Chloride	31309	(Cl ⁻)
Gases		
Carbon Dioxide	0	(CO ₂)
Hydrogen		
Sulfide	0	(H ₂ S)
Total Dissolved Solids (TDS)	58004	Mg/L

Table 4. Water Analysis.

The mineral dissolution and precipitation reactions are simulated using a rate law equation. Nghiem (2004) presents a complete analysis of the equations used in the simulator in order to model the mineral trapping.

The Reaction Rate Constants(K_{β}), Reference Temperatures for those constants, Reactive Surface Area for minerals ($\hat{A}_{\beta}$) and the Activation Energy ($E_{a\beta}$)for each reaction are needed.

The reaction rate constants are normally reported in the literature (Nghiem 2004, Xu 2000) at a reference temperature (Usually 25°C). The Activation Energy values were taken from literature as well as the Reaction Surface areas (Nghiem 2004).

Table 5 shows the values for each of the parameters for the mineral reactions included in the model. The table also presents the initial volume fraction of the minerals present in the rock. The mineral volume fractions of the Navajo Sandstone were taken from Parry et al (2009) who reported the mineralogy for various core samples of the Navajo Sandstone in the area. Average values were taken for each mineral and were included in the model.

Reactions	Log K β at 25°C (mol/ (m2 s)	$\Delta\beta$ (m2/m3)	Ea β (J/mol)	Volume Fraction.
<i>Calcite</i> + $H^+ = Ca^{++} + HCO_3^-$	-8.79588	88	41870	0.0088*
<i>Anorthite</i> + $8H^+ = Ca^{++} + 2 (Al^{+++}) + 2SiO_2(aq) + 4 H_2O$	-12	88	67830	0.0088*
<i>Dolomite</i> + $2(H^+) = (Ca^{++}) + (Mg^{++}) + 2(HCO_3^-)$	-9.2218	88	41870	0.0176
<i>Illite</i> + $8 (H^+) = 5 H_2O + 0.6 (K^+) + 0.25 (Mg^{++}) + 2.3 (Al^{+++}) + 3.5 SiO_2(aq)$	-14	26400	58620	0.0233
<i>Kaolinite</i> + $6(H^+) = 5 H_2O + 2 (Al^{+++}) + 2 SiO_2(aq)$	-13	17600	62760	0.0035
<i>Quartz</i> = $SiO_2(aq)$	-13.9	7128	87500	0.7874
<i>K - feldspar</i> + $4 (H^+) = 2 H_2O + K^+ + (Al^{+++}) + 3 SiO_2(aq)$	-12	176	67830	0.0385

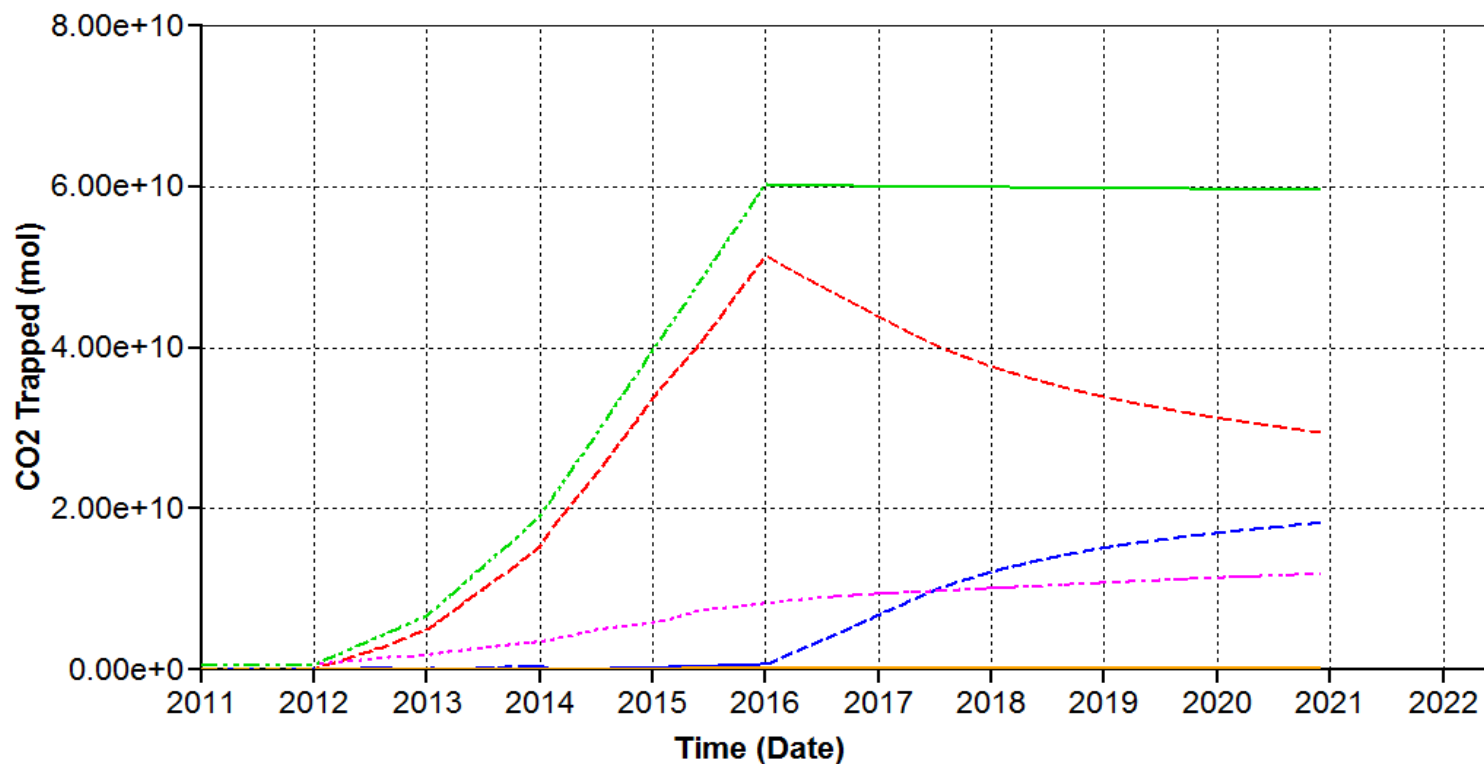
Table 5. Mineral Dissolution / Precipitation Reactions.

(*)Assumed Values.

After the parameters for the mineralization mechanism were generated in Winprop, the simulation was run for a period of 25 years.

After the simulation, it was found that the mineralization does not play an important role in the CO₂ sequestration for the time analyzed in the model (25 years). As observed in several studies Kumar (2004), Basbug et al., (2007) the mineralization is a long term mechanism and takes hundreds to thousands of years to have considerable effect in CO₂ trapping. Meanwhile, some

CO2 Sequestration Gordon Creek Aquifer
FRMLA_5001 test_all.irf



- Free Gas (mol): FRMLA_5001
- CO2 Trapped (mol): GHGTHY
- CO2 Dissolved (mol): GHGSOL
- CO2 Mineral (mol): GHGMNR
- Total Moles Injected (mol): FRMLA_5002

gas trapping due to mineralization was observed. Figure 24 presents the amount of CO₂ sequestered by mineralization, as well as, for the other mechanisms mentioned before.

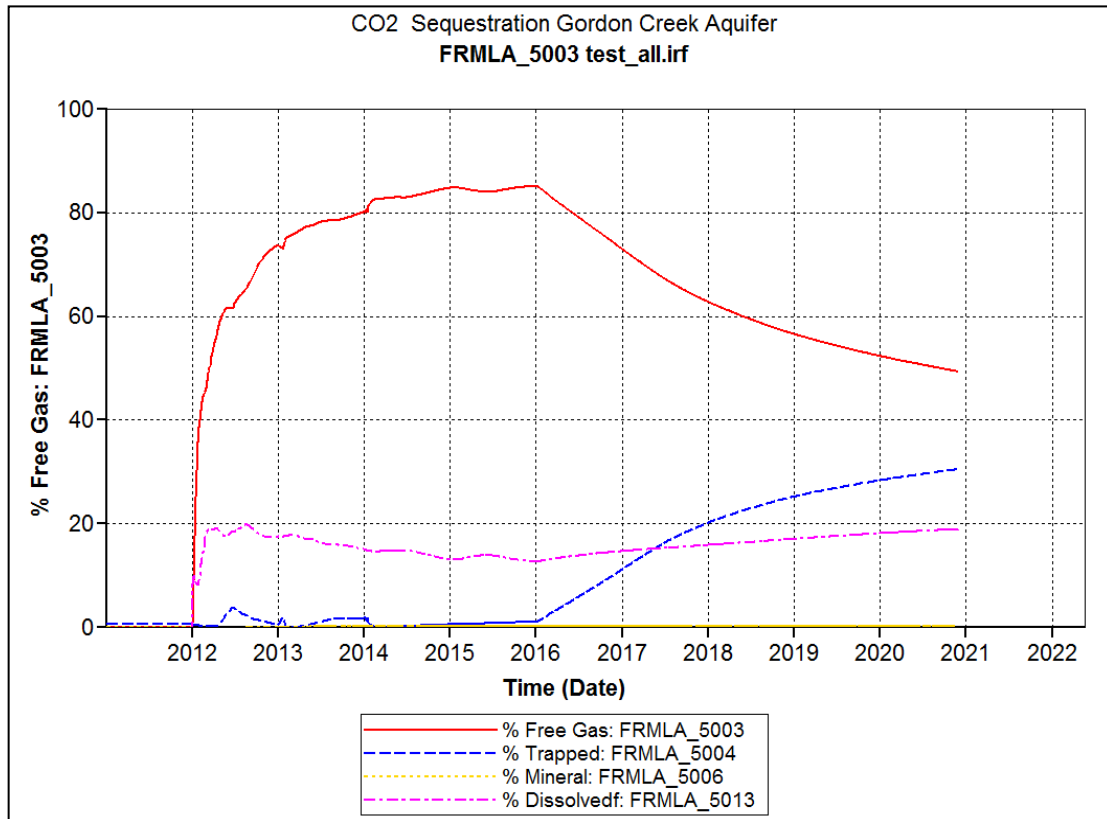


Figure 25. CO₂ trapping mechanisms contribution.

Figure 25 shows the percentage of CO₂ sequestered by each of the mechanisms. The figure shows that the percentage of free gas has been reduced to 50% in 25 years. Gas trapping mechanism is also an important mechanism because it traps around 30% of the CO₂ that was injected in a short period of time. This value

should increase once the CO₂ continues to spread out in the reservoir and contacts more brine. CO₂ trapped by dissolution increases slowly but still represents 19% of the CO₂ trapped in a period of 25 years.

Mineralization is a slow process that needs long periods of time to capture significant CO₂ as it precipitates; for a 25 year simulation, around 0.29% of the CO₂ injected was trapped by mineralization. This value should increase when a simulation for longer periods of time is performed.

Most of the precipitates compounds that contribute to the 0.29% of the total CO₂ trapped by mineralization are related to Dolomite. Figure 26 presents the Mineral Moles Changes for the Dolomite, Calcite and Kaolinit.

By convention positive values represent precipitation, while negative values represent dissolution. Figure 26 shows only Dolomitic precipitates. There is a considerable amount of Kaolinite and Calcite in dissolution but they have not been precipitated. For the rest of minerals included in the simulation, very low amounts of dissolution are observed. Longer simulations are required to see if mineralization precipitates for other minerals are observed.

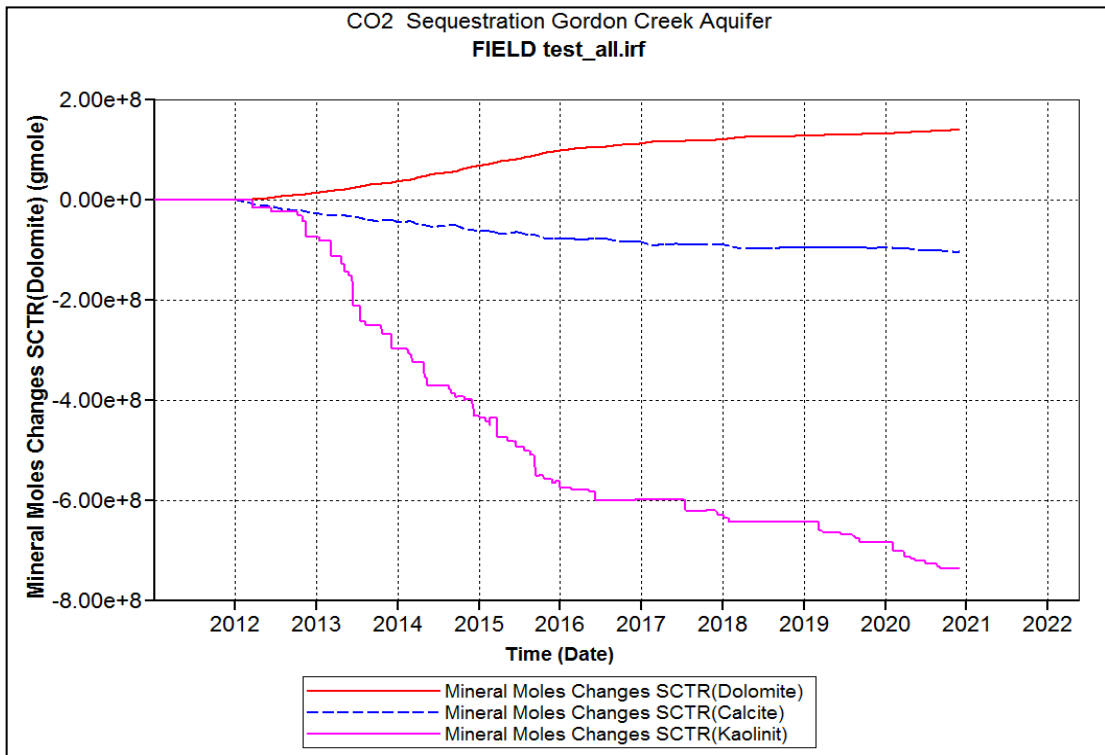


Figure 26. Mineral Trapping Precipitates quantities. .

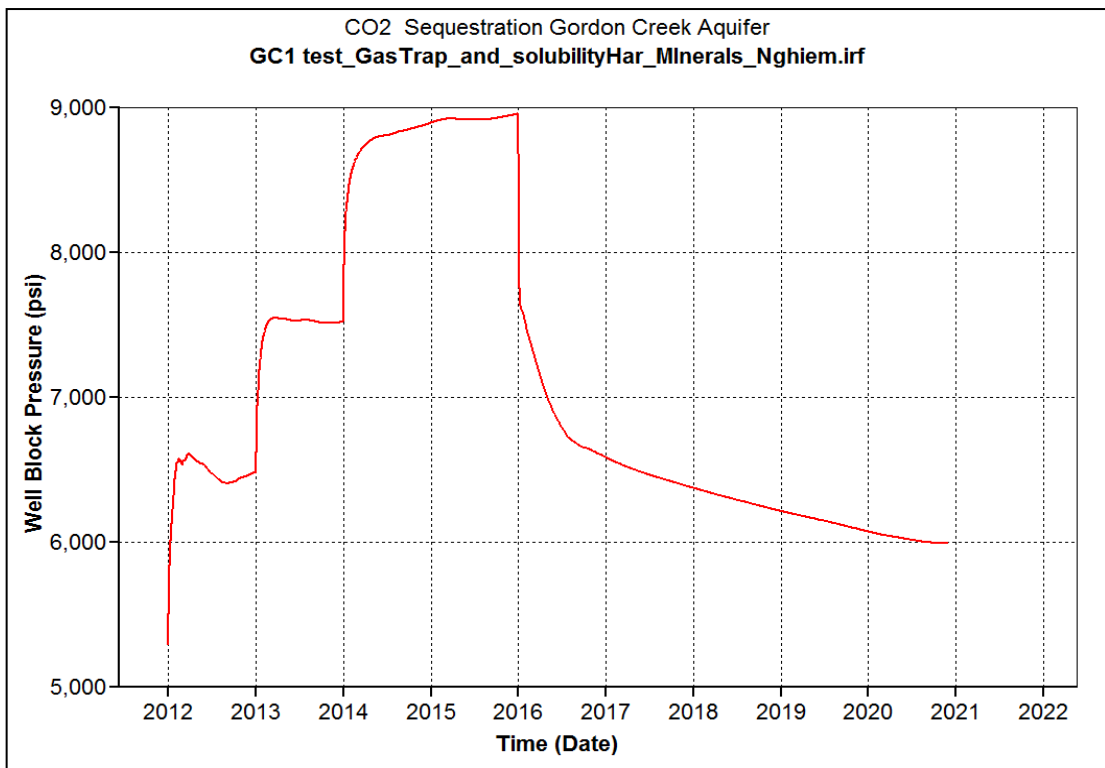


Figure 27. Well Block Pressure. Case4.

It is important to mention that the run time for this case was seven times the time spent by the Case number 3 (this model was successfully completed in around 5.6 days). Convergence problems were observed during the simulation. To solve those problems some work in tuning and optimization was performed. The parameters used to solve convergence problems are mentioned in Appendix C, which also presents a step by step procedure to build a CO₂ Sequestration model.

Another parameter that has to be analyzed is the pressure around the wellbore (Figure 27). As shown in previous cases, the pressure does not exceed the fracture pressure for the Navajo, but the values obtained in this case are higher and very close to 9000 psi. These values could be explained because of the dissolution and precipitation of minerals such as Dolomite and Kaolinite in the blocks around the wellbore can cause a small restriction to fluid flow, leading to an increase in pressure around the wellbore. This effect should be directly analyzed in future work. Figure 28 presents the Dolomite precipitate and dissolution saturation around the wellbore. Dissolved dolomite is present around the wellbore primarily as a precipitate in the model.

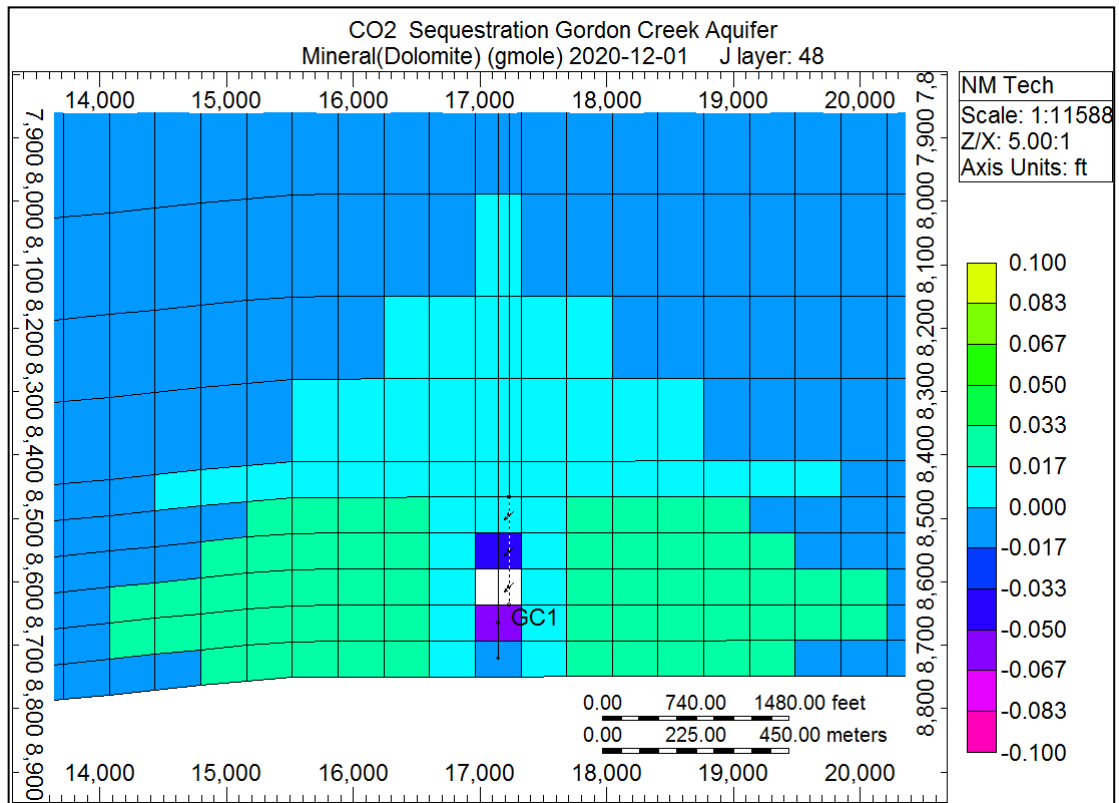


Figure 28. Dolomite Precipitate content. Case4.

Due to the time spent by the software to run this case (almost 5.6 days) it was not possible to run the model for longer periods of time including the mineralization. Problems with convergence were found and have to be solved in future studies. To overcome this problem and have some idea about how the rest of the mechanisms behave for longer periods of time, Case 3 was simulated for a period of 1000 years. Figure 29 presents the CO₂ trapped for each of the mechanisms (seal, residual gas and solubility trapping) after 1000 years of simulation. The amount of free gas CO₂ after that time is very low which indicates that the rest of the trapping mechanisms are very effective and can trap CO₂ safely for longer

periods of time. The free gas amount will be reduced when the effect of mineralization for long periods of time can be included.

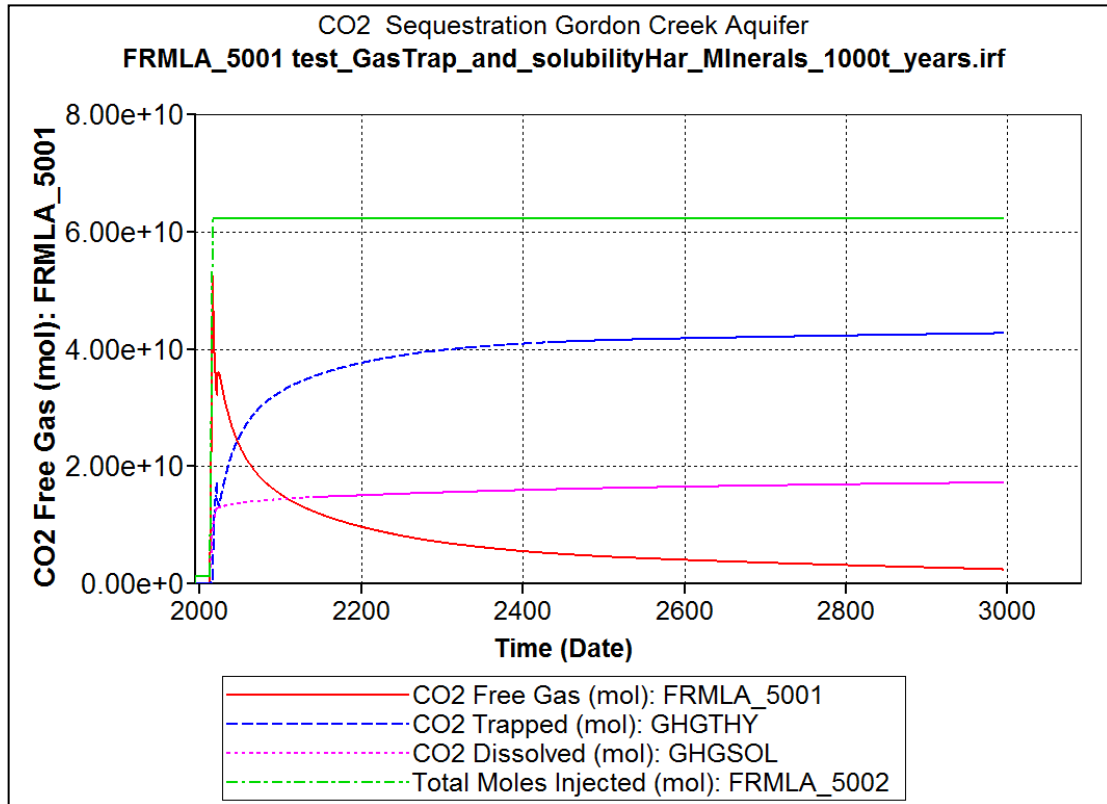
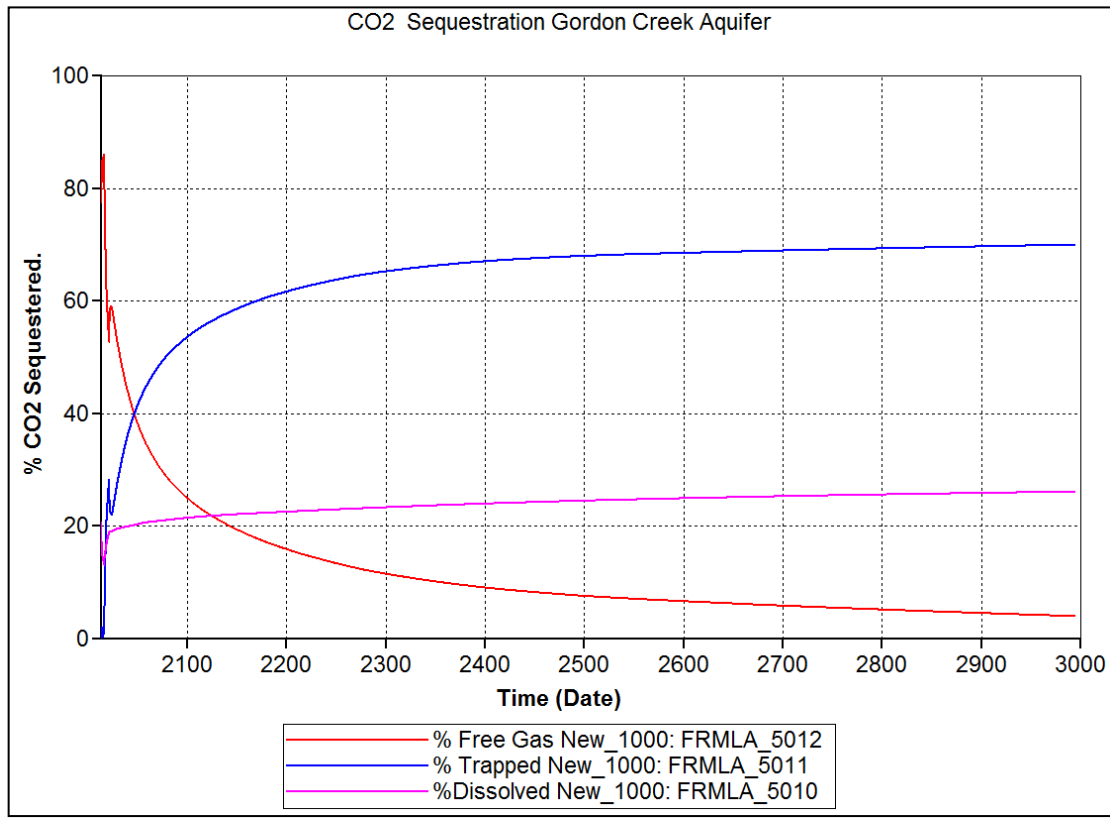


Figure 29. CO₂ trapping mechanisms contribution 1000 years, Case3.

Figure 30 shows the amount of CO₂ present in each mechanism as a percent of the total amount of CO₂ injected. As it was mentioned above, the amount of free CO₂ has been reduced drastically and at the end of the 1000 years simulation, 4% of CO₂ still remains mobile; around 70% was trapped by the residual gas mechanism and 26% by dissolution in water.



With these results, it is shown that CO₂ can be trapped securely by different mechanisms underground for long periods of time. The amount of mobile CO₂ in the aquifer is reduced to a very low value after one thousand years.

5. SENSITIVITY ANALYSIS

The influence of different parameters in the CO₂ storage capacity for each of the mechanisms mentioned before can be analyzed.

Uncertainty is present in each value entered or calculated in the simulation model. An estimate of how these values affect the total amount of CO₂ sequestered is an important matter that can help to refine the model and focus attention on those variables that are most sensitive.

The total amount of CO₂ sequestered by gas trapping and solubility will be the objective values for this study. These two trapping mechanisms are a safe way to keep the CO₂ away from the atmosphere and for that reason the main objective is to maximize them. Sensitivity Analysis on the following parameters are performed:

Parameters to be analyzed
Salinity
Temperature
Residual Gas Saturation
Initial Pressure

Table 6 Parameters to be analyzed in Sensitivity Analysis.

The first part of the Sensitivity Analysis consists of running simulation experiments, where the parameters present in table 6 are modified using low and

high values. A qualitative picture of the effect of each of these parameters in the objective functions is obtained.

In order to accomplish this first step the CMOST Software developed by Computer Modeling Group (CMG) was used. This software allows changing different inputs in the model and determines how sensitive the objective functions are.

The software uses only two values for each parameter (high and low values), for that reason the sensitivity relationship is considered linear, which may not be true in practice and is something that has to be improved in the program.

A full fractional sampling method was used to accomplish this analysis and a total of 16 simulations were completed.

The values used for this Sensitivity Analysis are presented in Table 7.

Parameter	Values	
	Low	High
Salinity (ppmvol)	20000	120000
Temperature (F)	100	180
Residual Gas Saturation	0.15	0.55
Initial Pressure (psi)	3400	4000

Table 6. Parameters values for Sensitivity Analysis

The following tornado charts show the results obtained in the Sensitivity Analysis performed with CMOST using the amount of CO₂ dissolved in water and trapped by residual gas saturation as the objective functions.

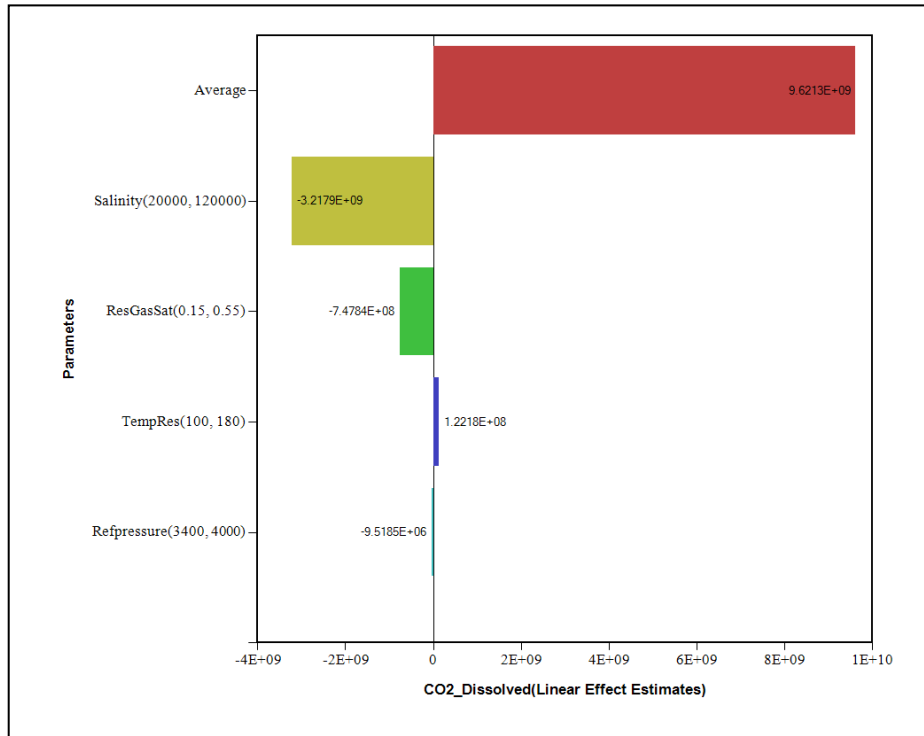


Figure 30. Sensitivity Analysis for CO₂ Dissolved

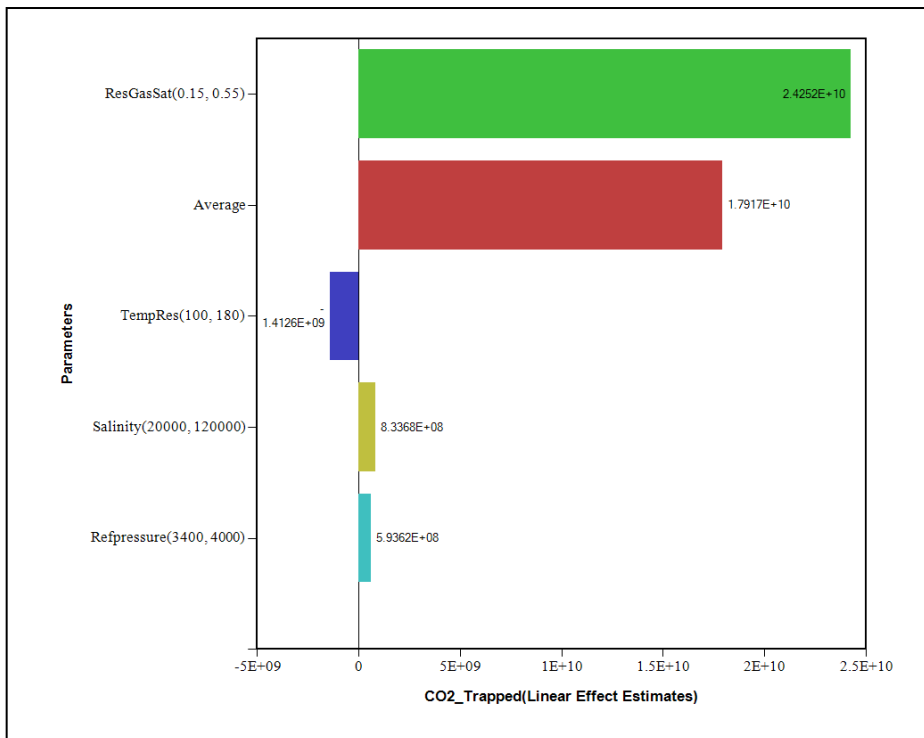


Figure 31. Sensitivity Analysis for CO₂ Trapped

Figure 30 presents the Tornado Chart for the CO₂ dissolved objective function. According with the graph, from the parameters analyzed, the brine salinity is the one that has more impact in the total amount of CO₂ trapped by this mechanism. The residual gas saturation is a parameter that also affects the CO₂ dissolved in water but to a lower degree. Temperature and Pressure do not seem to have a big impact on the CO₂ dissolved. According with these results more information about the brine salinity can help to improve and refine the model.

Figure 31 presents the Tornado Chart for CO₂ trapped by residual gas saturation. In this case, as expected, the residual gas saturation plays a very important role in the amount of trapped CO₂. The influence of this parameter is high and a correct determination of this value is a critical aspect that must be understood when building CO₂ sequestration models as the Gordon Creek project is executed and new data is acquired. The rest of parameters do not significantly affect final volumes of CO₂ trapped by residual gas saturation.

The Sensitivity Analysis only considers two values and a linear sensitivity relationship. However, the relationship between each parameter and the objective function is not generally linear. Therefore further analysis needs to be done in order to evaluate how each mechanism behaves when parameters are modified in a specific range of values. One method to evaluate this consists of running

simulations to evaluate only one parameter at a time, while all other parameters are kept constant. Six different values for each parameter were used and a total of 24 simulations were done in order to accomplish this analysis. The CO₂ trapped due to dissolution in water and residual gas trapping were the focus of this analysis. The impact of each parameter in the CO₂ free gas phase (Super Critical State) was also studied.

Effect of Water Salinity.

Figures 32, 33 and 34 present the results obtained when brine salinity values are changed from a value of 20000 ppm to a value of 120000 ppm.

Figure 32 shows that the CO₂ trapped by residual gas trapping in the aquifer increase with an increase in the salinity.

Figure 33 presents the effect of salinity in the amount of CO₂ dissolved in water. This graph shows that an increase in salinity (holding other properties constant), produces a decrease in the amount of CO₂ dissolved in water. This result agrees with previous experimental works done by various researchers that show a decrease of CO₂ dissolved in water increasing salinity.

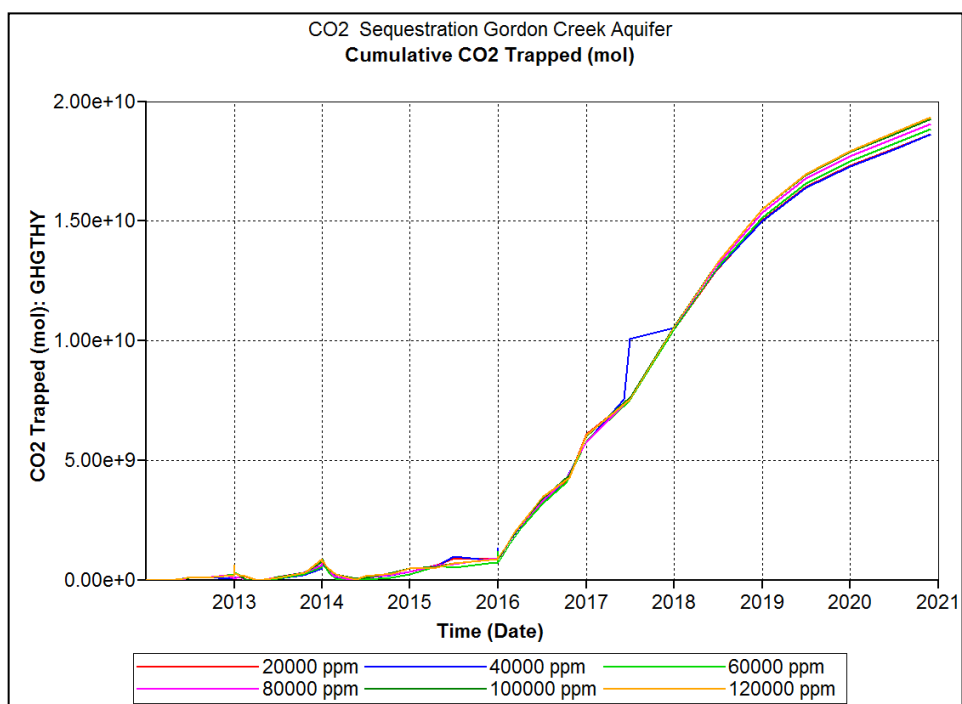


Figure 32. CO₂ Trapped using different Salinities.

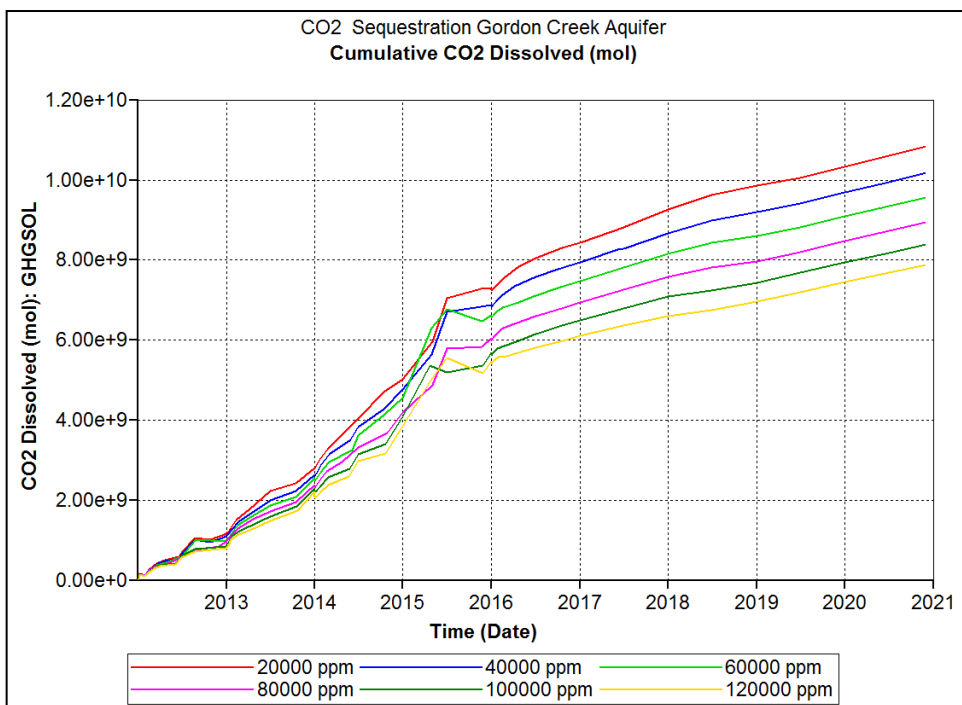


Figure 33. CO₂ Dissolved using different Salinities.

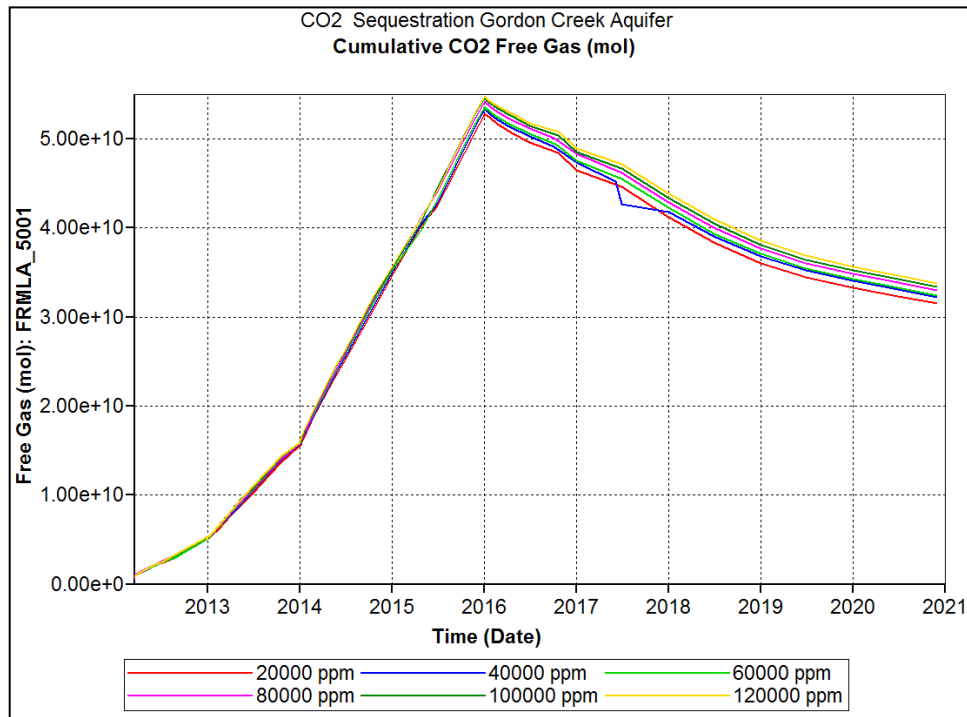


Figure 34. CO₂ Free Gas using different Salinities.

Another factor to study is the impact of the water salinity on the total amount of free CO₂ in the aquifer. Figure 34 shows that an increasing salinity increases free CO₂. This increase in CO₂ trapped as a free gas is due to a considerable decrease in CO₂ dissolved in the water, the increase in the CO₂ trapped by residual gas saturation does not play an important role in the overall amount of free CO₂.

Effect of Temperature.

An increase in temperature in the aquifer leads to a decrease in the CO₂ trapped by Residual Gas Saturation (Figure 35). Increases in temperature may increase the

mobility of the CO₂ which could react with more water in the reservoir. For that reason, the CO₂ dissolved into the water may increase with an increase in temperature. This behavior can be observed in early stages of the simulation in Figure 36, meanwhile, after 2018 the trapping for the low temperatures becomes higher and a reverse behavior is observed, showing that the CO₂ solubility in water decreases with temperature which is the normal behavior that should be expected. Due to the reduction in gas dissolved and trapped by residual gas saturation, the free gas shows a slight increase with temperature as it can be seen in Figure 37.

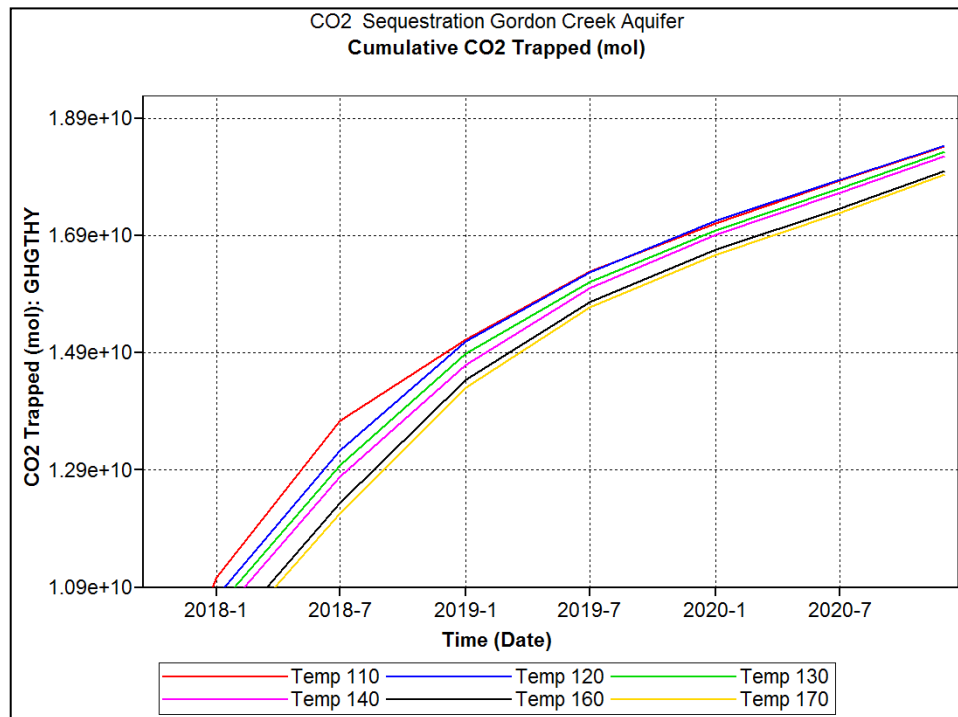


Figure 35. CO₂ Trapped using different Temperatures.

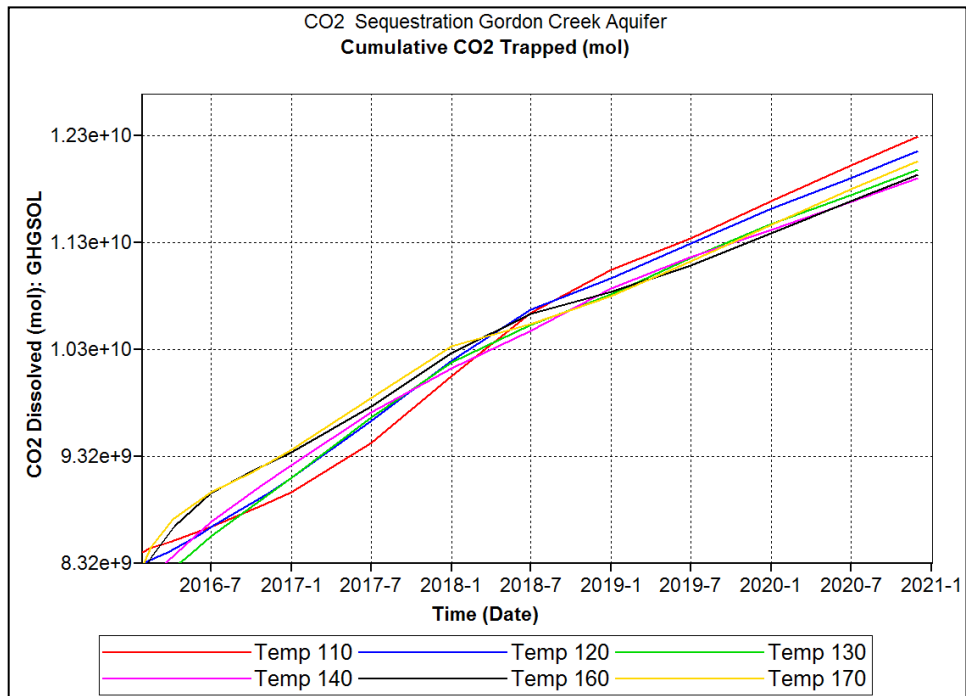


Figure 36. CO₂ Dissolved using different Temperatures.

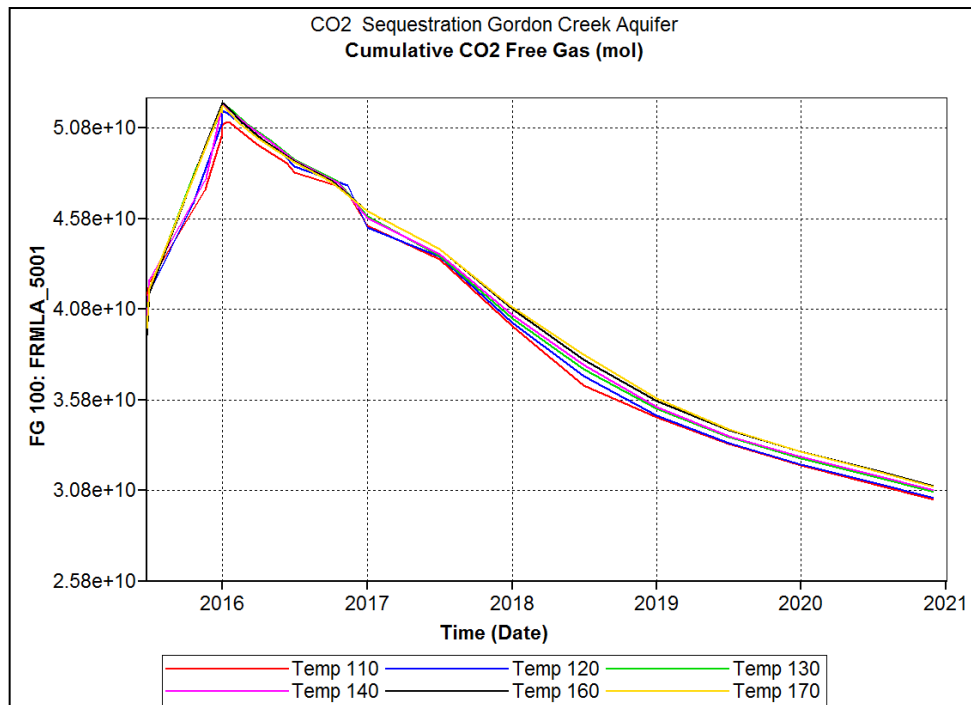


Figure 37. CO₂ Free Gas using different Temperatures

Effect of Residual Gas Saturation.

As expected, CO₂ trapped by residual gas saturation rises with an increase in residual gas saturation (Figure 38). The increase in the amount of CO₂ trapped is dramatic and this confirms the results of the sensity studies shown in Tornado Charts. A small change in the Sgr can bring considerable changes in the gas trapped, which implies that the Gas trapping mechanism is very effective.

Figure 39 shows the effect of the increase of Sgr in the Dissolved CO₂. A decrease in Sgr implies an increase in the CO₂ Dissolved; this can be explained because at lower Sgr the plume can travel further and the CO₂ which is mobile at small saturations, can be contacted by water and get dissolved.

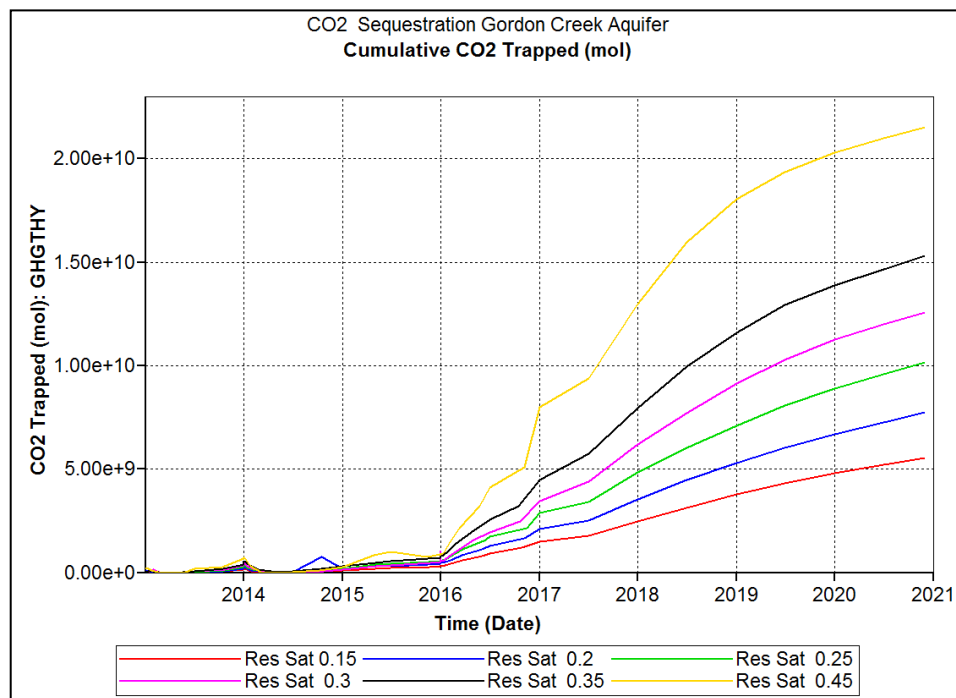


Figure 38. CO₂ Trapped using different Sgr.

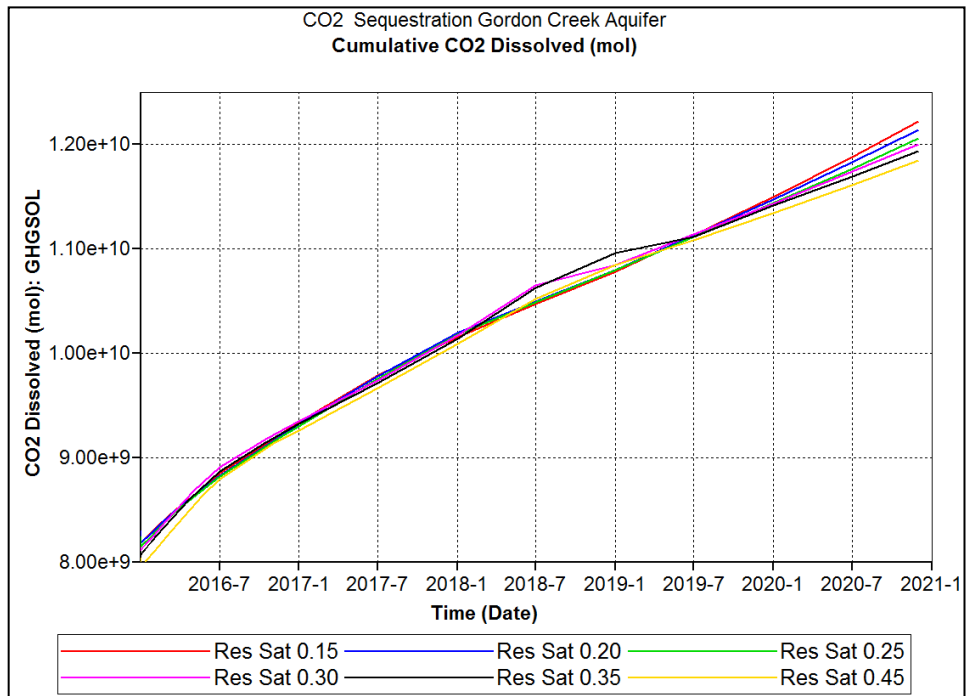


Figure 39. CO₂ Dissolved using different Sgr.

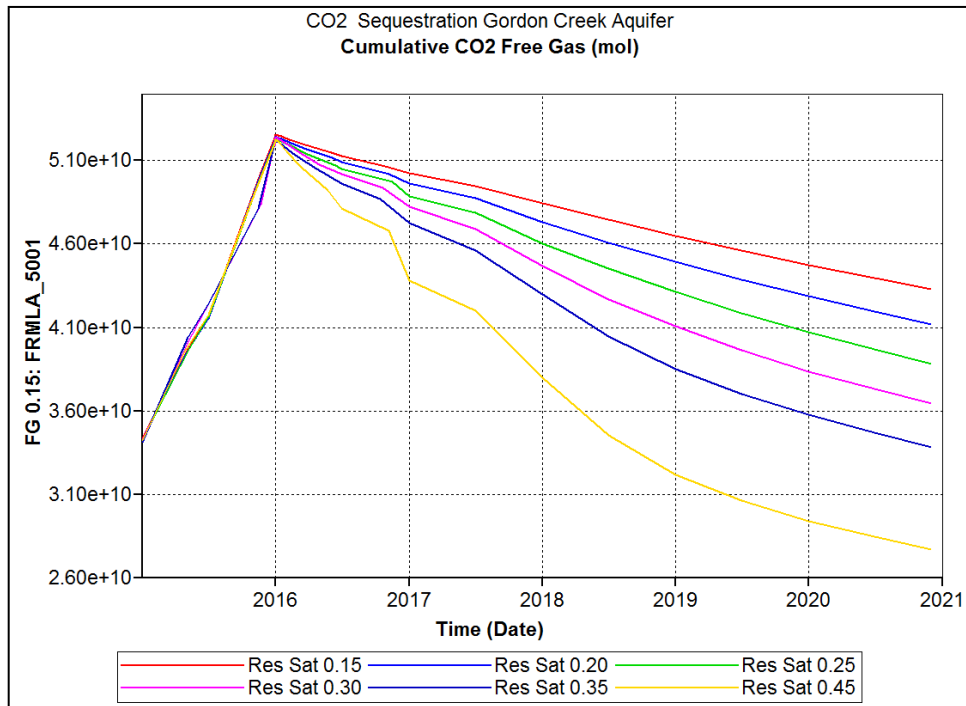


Figure 40. CO₂ Free Gas using different Sgr.

Figure 40 shows a decrease of CO₂ as a free gas due to an increase in residual gas saturation. If the values obtained for the amount of free CO₂ present in the aquifer for $S_{gr} = 0.15$ and $S_{gr} = 0.45$ are compared, a reduction of around 35% of the mobile CO₂ was observed in a short period of time. This result confirms that the gas trapping mechanism is very effective and significant efforts should be made to get the best value of S_{gr} for the aquifer present in Navajo Sandstone.

Figure 40 also shows that the values of mobile CO₂ before 2016 are similar which implies that the real effect of the residual gas saturation mechanism starts when the CO₂ injection is ceased and the hysteresis process of water displacing CO₂ into the aquifer starts.

Effect of Pressure.

When initial pressure is increased from a value of 2500 psi to a value of 5000 psi, the free CO₂ is less mobile in the aquifer, and when displaced by water in a hysteresis process, more CO₂ remains trapped by the residual gas trapping mechanism. This behavior can be clearly observed in Figure 41. A slight increment in CO₂ trapped is observed with increments in pressure.

Figure 42 shows that, in general, the amount of CO₂ dissolved into water decreases with increments in pressure. When the pressure increases, the

solubility of water and CO₂ decreases and less CO₂ is dissolved. This behavior, while not clearly illustrated earlier in the simulation becomes obvious after several years.

Due to the incrementally increasing CO₂ trapped by residual gas saturation and dissolution in water, the free CO₂ gas decreases as pressure is increased. Figure 43 shows this behavior.

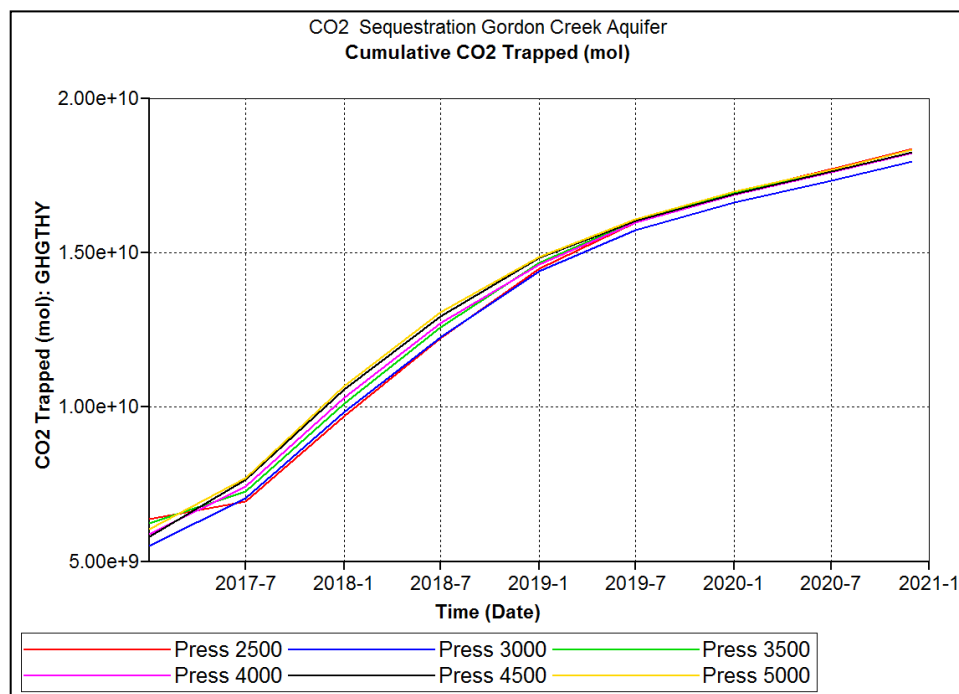


Figure 41. CO₂ Trapped using different Pressures

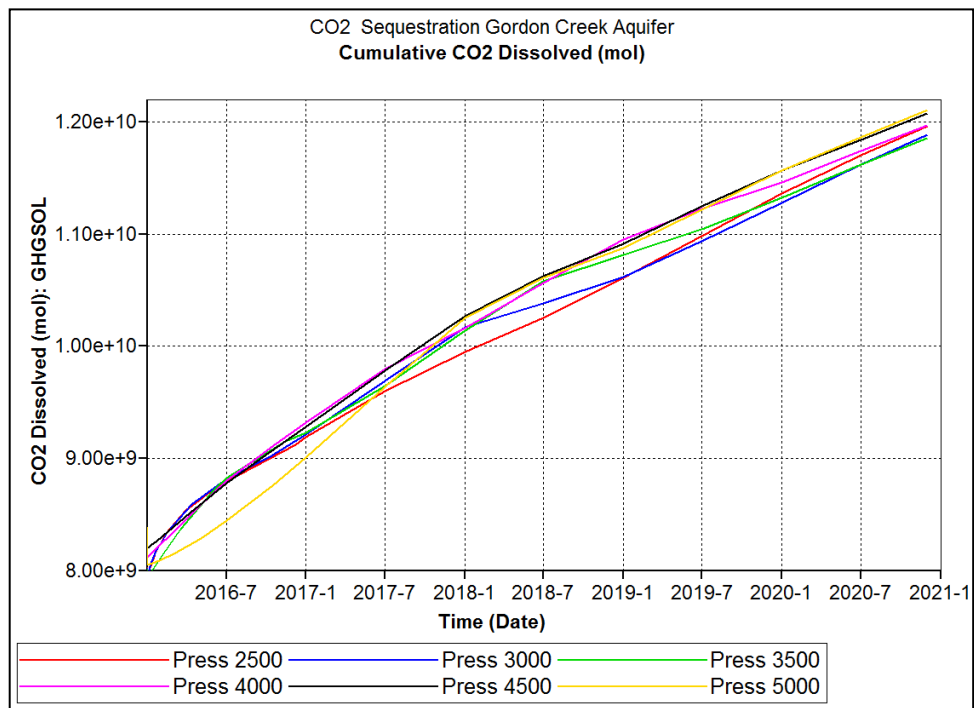


Figure 42. CO₂ Dissolved using different Pressures

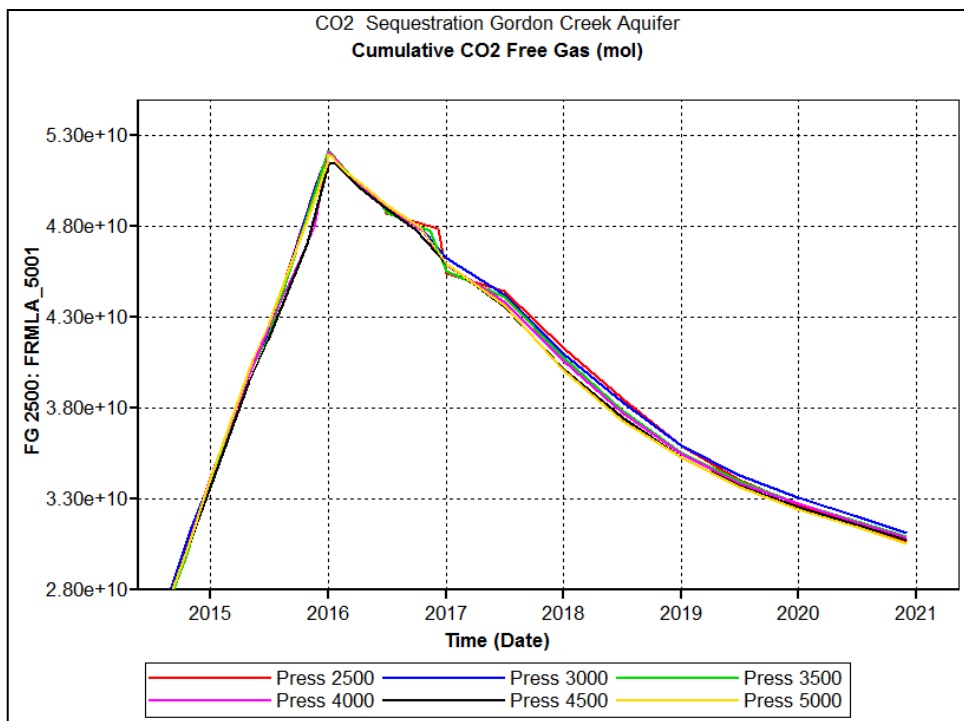


Figure 43. CO₂ Free Gas using different Pressures.

6. CONCLUSIONS AND FUTURE WORK

Carbon dioxide sequestration in aquifers is one of the most promising ways to trap CO₂ underground for long periods of time.

Characterization of the Gordon Creek Navajo aquifer helped to understand the effect of some of the petro-physical properties on the amount of CO₂ trapped. Further research is needed to get better values for each of the parameters included in this study and provide the most realistic scenario possible for the pilot project.

Each of the trapping mechanisms included in this project played an important role in the CO₂ sequestration and their effects always should be incorporated in modeling efforts. Various conclusions were obtained during this project and are summarized as follows:

- There are four main trapping mechanisms that have to be considered whenever a CO₂ sequestration project is modeled. Seal trapping, residual gas trapping, solubility in water, and chemical reactions trapping (Mineralization) are these mechanisms. Each one of them is important in keeping CO₂ underground for long periods of time. Mineralization is the

mechanism with the highest storage security but also takes longest period of time to sequester a significant quantity of carbon dioxide.

- A total of 50,759 MMScf of CO₂ were injected. (This is about 2.94 million of tons of CO₂ injected in supercritical state). The goal of injection for the four year period was verified as possible by this model.
- The injected CO₂ migrated laterally about 1,430 ft. In all studied cases CO₂ did not penetrate the seal formation, which means that CO₂ reached the top of the Navajo Formation but did not migrate into the seal.
- For Case 1, when only the seal trapping mechanism was considered and all the CO₂ was present in supercritical state. A considerable quantity of CO₂ reached the bottom of the seal formation and the CO₂ saturation at the top layer of Navajo Sandstone was around 0.3. At the top layer of Navajo Sandstone CO₂ had migrated laterally around 770 ft. This case represents a worst case scenario for trapping mechanisms
- Case 2 includes the gas trapping and seal trapping mechanisms in the CO₂ sequestration simulation. A value of 0.4 for the residual gas saturation was

used. After the simulation, less gas reached the top of the structure compared to Case 1, and around 35% of the total gas injected is trapped in the pores, with the rest mobile (Supercritical state).

The residual gas saturation trapping mechanism initiates when the gas injection is stopped and water imbibes the blocks that are saturated with CO₂ leaving gas trapped in the pores. For that reason, CO₂ trapped by this mechanism is observed after the CO₂ injection is concluded.

- Case 3 includes the residual gas trapping, seal trapping and solubility mechanisms. As a result of the simulation 50% of the CO₂ is present as a free gas, 31% remains trapped in the pores and 19% is trapped by dissolution in water. There is a considerable reduction of free gas in a very short time in this model.
- Case 4 shows that mineralization is a very long term effect as was observed in previous studies. Only 0.29% of the CO₂ injected is trapped by Mineralization in a period of 25 years, with Dolomite being primary precipitant. Longer simulations than possible in the time allotted to this study are needed to analyze the effect of mineralization in this aquifer.

- For the one thousand year simulation, it was shown that the free CO₂ at the end of the simulation was reduced to 4%, while the CO₂ trapped by residual gas saturation increased to a value of 70% and the amount of CO₂ dissolved in water was 26%. This indicates that the mechanisms analyzed in this study are an effective way to keep the CO₂ safely underground at Gordon Creek.
- Sensitivity Analysis using Tornado Charts showed that the residual gas saturation is a very important parameter that highly affects the total CO₂ trapped by residual gas saturation. The rest of the parameters studied do not notably affect the amount of trapped CO₂.
- Tornado Chart shows that the amount of CO₂ dissolved in water is strongly affected by the brine salinity. Other parameters affect to a lower degree the total amount of CO₂ dissolved in water.
- An increase in salinity implies that the amount of CO₂ trapped increases and the CO₂ dissolved in water decreases. Increasing salinity increases the amount of CO₂ present in the aquifer as free gas.

- The amount of CO₂ trapped by residual gas saturation decreases with an increase in temperature while the amount of CO₂ dissolved in water increases for early stages of simulation but after that, the amount decreases with temperature increase. As a result of this, the total amount of CO₂ as free gas increases with temperature.
- Residual gas saturation plays an important role in CO₂ sequestration. The calculation of this value is crucial and has to be refined in order to get more realistic results. According to the sensitivity analysis, the amount of CO₂ trapped increases with an increase in the residual gas saturation, on the other hand, the CO₂ dissolved in water decreases with an increase in Sgr. As a result of the dramatic increase of trapped CO₂ the CO₂ present as free gas shows a decrease..
- Increasing pressure results in an increase in the amount of CO₂ trapped and CO₂ dissolved in water. Due to this increase the amount of CO₂ as free gas is decreased at higher pressures.
- The formations of interest for this study were the Navajo and Carmel Formations. Navajo Formation is sandstone that has relatively low values of porosity and permeability according to the log analysis.. No cores were

available for this study in order to get another value of these parameters to be able to compare results. It would be useful to have core and new logs of the area of interest to have a better idea of these parameters and update the model.

- A Simulation grid was built using the best known structure contours and the GRIDGEN Software. This preliminary model included a fault. More information is needed regarding the geology and structures present in the Navajo Sandstone. The possibility of an non-fault bounded anticline has not been completely eliminated and more characterization work is needed.
- Due to the lack of information coming from cores, relative permeability curves were taken from old studies in other formations. Laboratory measurements of these curves could help to get a better idea of the rock-fluid interaction inside the aquifer. Capillary pressure values are also required to include the effect of hysteresis in a more realistic way.
- A better characterization of the geochemistry of the formation should be made. The values included in the model when mineralization was added have to be analyzed to get a more realistic estimate of the reactions that

take place between the minerals in the rock and the water with the CO₂ injected.

- Due to the big difference in pressure between the aquifer and the seal above it, the seal provided by the cap rock could be breached and flow across the breach may occur. Further investigation regarding this phenomenon has to be included in the model to determine the amount of CO₂ that can migrate from the aquifer to the seal formation and to the Entrada Formation.
- This study presents a manual in the appendices that can be used to build a CO₂ sequestration model in the Computer Modeling Group Software.

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APPENDIX A.

A table with some of the petro-physical properties calculated using LESA is presented.

	Porosity	Permeability		Porosity	Permeability
Layer	(Fraction)	(md)	Layer	(Fraction)	(md)
1	0.08	0.195	16	0.0101	0.007
2	0.064	0.2	17	0.011	0.007
3	0.12	1.968	18	0.101	0.713
4	0.113	0.776	19	0.0955	1.147
5	0.056	0.071	20	0.0783	0.176
6	0.039	0.084	21	0.0697	0.0935
7	0.045	1.055	22	0.0697	0.0935
8	0.042	0.43	23	0.061	0.011
9	0.0418	1.769	24	0.0459	0.097
10	0.0428	0.323	25	0.0888	4.017
11	0.031	0.553	26	0.0857	0.463
12	0.0387	0.221	27	0.0992	1.622
13	0.0208	0.083	28	0.1554	7.888
14	0.028	0.011	29	0.1524	6.07
15	0.0321	0.032	30	0.1434	3.129

APPENDIX B.

The Henry's law constant at P and T is given by:

$$\ln H_i = \ln H_i^* + \frac{1}{RT} \int_{p^*}^p \bar{v}_i dp$$

The Henry's constants are used to calculate the solubility of CO₂ in water.

Some correlations have been developed to calculate these constants. Harvey (1996) developed some correlations which have the form:

$$\begin{aligned} \ln H_i^s = & \ln p_{H_2O}^s + A(T_{r,H_2O})^{-1} + B(1 - T_{r,H_2O})^{0.355} (T_{r,H_2O})^{-1} \\ & + C[\exp(1 - T_{r,H_2O})](T_{r,H_2O})^{-0.41} \end{aligned}$$

Where

H_i^s Henry's constant for component i at the saturation pressure of H₂O (MPa)

$p_{H_2O}^s$ Saturation pressure of H₂O in MPa at T (K)

T_{c,H_2O} Critical temperature of H₂O (K) (647.14 K)

T_{r,H_2O} Reduced temperature of H₂O. Is defined by $T/T_{c,H_2O}$

The values of the parameters A, B and C for the gases of interest are presented in the following table:

Gaseous Solute	A	B	C
CO ₂	-9.4234	4.0087	10.3199
N ₂	-11.6184	4.9266	13.3445
H ₂ S	-5.7131	5.3727	5.4227
CH ₄	-11.0094	4.8362	12.522

The saturation pressure $p_{H_2O}^s$ of water is calculated from the Saul and Wagner (1987) correlation:

$$\ln \left(\frac{P_{H_2O}^s}{P_{c,H_2O}} \right) = \frac{T_{c,H_2O}}{T} (a_1 \tau + a_2 \tau^{1.5} + a_3 \tau^{3.5} + a_4 \tau^{3.5} + a_5 \tau^4 + a_6 \tau^{7.5})$$

Where,

P_{c,H_2O} Critical pressure of H₂O (22.064× 10⁶ KPa)

$$\tau = \frac{T}{T_{c,H_2O}}$$

The values for the coefficients are:

a_1	-7.85823
a_2	1.83991
a_3	-11.8711
a_4	22.6705
a_5	-15.9393
a_6	1.77516

In the Henry's law, the $\bar{v}_i$ has to be calculated. For CO₂ the correlation used is:

$$\bar{v}_{CO_2} (cm^3/mol) = 37.51 - 9.585 \times 10^{-2}T + 8.740 \times 10^{-4}T^2 - 5.044 \times 10^{-7}T^3$$

The effect of Salinity was described by Bakker (2003). The correlations that presented are:

$$\ln \frac{H_{salt,i}}{H_i} = k_{salt,i} m_{salt}$$

Where,

$H_{salt,i}$ Henry's constant of component i in brine.

H_i Henry's constant of component i at zero salinity

$k_{salt,i}$ Salting-out coefficient for component i

m_{salt} Molality of the dissolved salt (mol/kg H₂O)

The value of $k_{salt,i}$ can be calculated using the following correlation:

$$k_{salt,CO_2} = 0.11572 - 6.0293 \times 10^{-4}T + 3.5817 \times 10^{-6}T^2 - 3.7772 \times 10^{-9}$$

APPENDIX C.

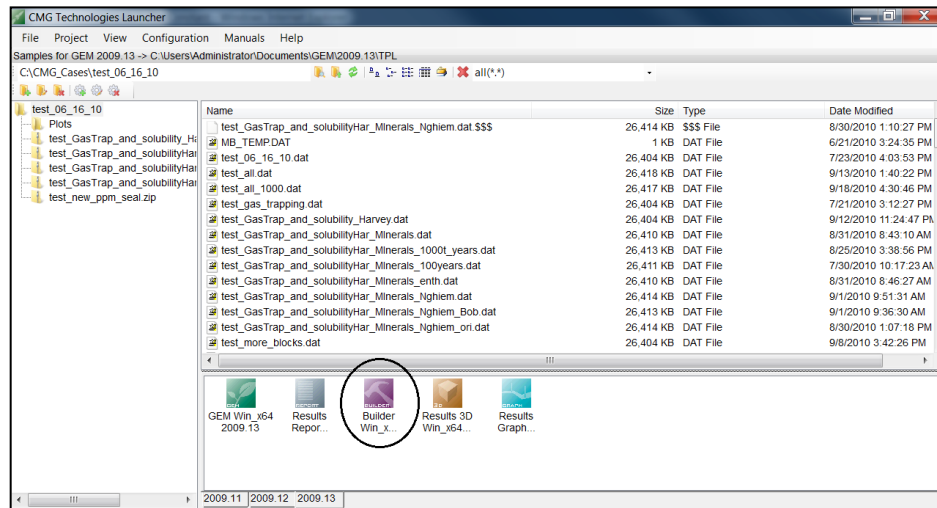
MANUAL

“HOW TO BUILD A MODEL IN CMG FOR CO₂ SEQUESTRATION”

The objective of this Appendix is to develop a procedure for building a CO₂ Sequestration model using the CMG Software. Some tips learned during this work are presented to benefit future studies.

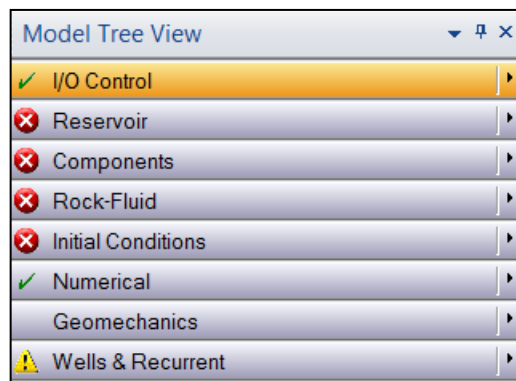
All trapping mechanisms of CO₂ studied during this project are included in this manual. Information related with convergence problems and possible solutions are also presented.

1. In order to start building the model, the application has to be opened using the icon for the CMG Launcher. The following figure shows the Launcher window and the link to the Builder, which is the module to build the model.

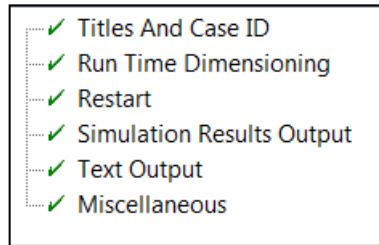


2. After the Builder is open, a new window comes up and the type of simulator (GEM), the working units (Field), type of Porosity (Single Porosity) and simulation start Date (01/01/1995) have to be selected. After that information is provided, the main window of Builder is opened. The information mentioned above cannot be changed once it is entered into the Builder. If changes are required, then a new Builder model has to be created.

3. In the left part of the Builder window, the Model Tree View is presented. This tree has different labels that allow the user to input all the information related to the model. Whenever the minimum information of one label is entered, the label changes from  symbol to  symbol. Once all the tabs have the green symbol, the model can be run. The information needed to build a model is divided into the following categories:



4. Click on the Input/output Control tab (**I/O Control**). After the user clicks on this, the following options appear below the Model Tree View



5. Double click on the Title and Case ID and provide the information required.

6. Double click on the Restart option and activate the “Enable Restart Writing” option. Click on the  symbol and accept the date of the start of the simulation and then click OK.

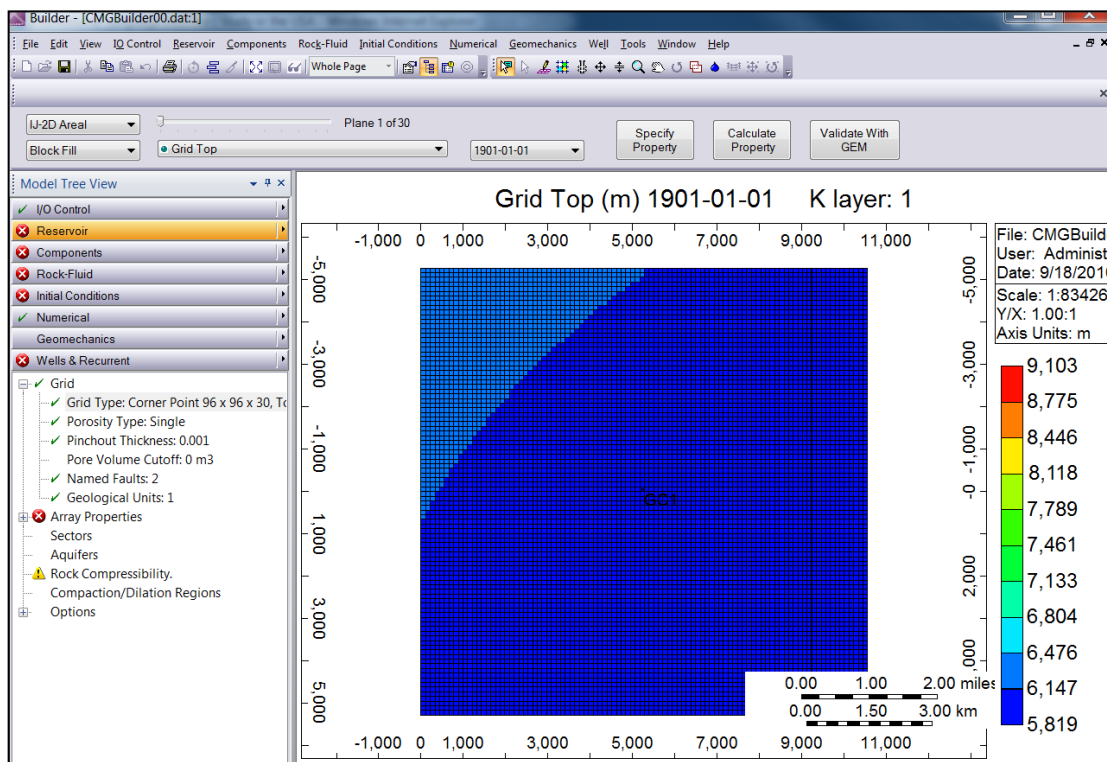
7. Click on the **Reservoir** tab in order to enter the information related to the grid and the array properties for the model. For this study the grid was created outside of CMG and imported as a Rescue file.

To create or import a grid, click on the arrow next to the Reservoir label and click on “create grid” option. If the grid is in Rescue format, click on “Open Rescue File” and choose the .bin file that contains the grid.

After you have selected the file, the program runs a validation to see if the Rescue file can be imported and gives the user a summary report.

A mapping of properties from the Rescue file to the CMG model has to be done before the user click OK.

8. After the grid and properties are imported, the user should be able to see the grid in the Builder Window.



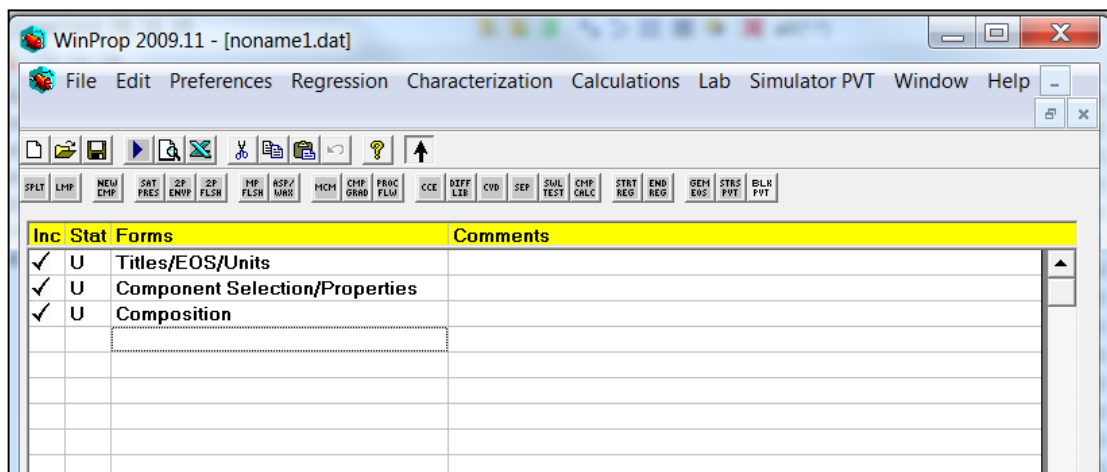
If some property values are missing and are not imported from the Rescue file, the user should double click on the “Array Property” option and enter each value. Values for the whole grid or for each layer can be entered. For this study information of Porosity and Permeability for each layer were provided.

9. Double click on the Rock compressibility option and enter values of Rock compressibility and reference pressure, then click OK.

Now the user should have a green check mark for the Reservoir label.

10. The next section to analyze is the Components section.

For the CO₂ sequestration models, compositional models are used. In order to create this fluid model the user needs to use the WinProp module. From the Launcher, double click on the WinProp icon. The following window will appear:

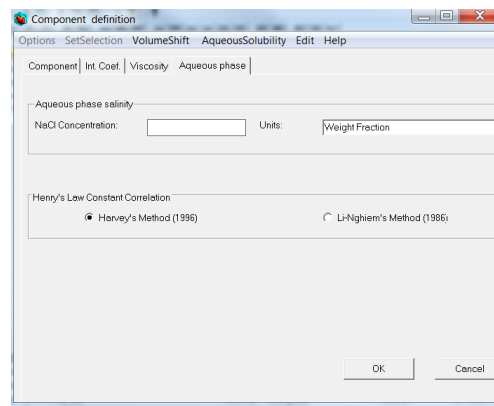


11. Double click in the “Titles/EOS/Units” and enter the Title and the Units for your calculations.

12. Double click in the “Component Selection/Properties”. The component Definition window will appear. Click on “Options”, “Insert Library Components” and then select the CO₂ and C1 components.

The C1 component is a trace component that allows the gas phase to exist in each grid block and with this the gas phase calculations are performed continuously.

13. To include solubility into the model, click on the “Aqueous phase” tab and select the Harvey’s Method, then click OK.



14. Double click in the Composition option in the WinProp main window. Enter the following values for the components and then click OK.

Component	Primary	Secondary
Sum	1.000000	0.000000
CO2	0.001	0.0000
C1	0.999	0.0000

Note: Do not enter very low values for the CO₂; otherwise the simulator will have convergence problems. It is highly recommended to use the values mentioned above.

15. In the Winprop window, click in the “Simulator PVT” option and select the “CMG GEM EOS MODEL” option. Then double click the option and enter the following information:

Write CMG GEM EOS model data

Help

Comments:

File Selection

☐ Print detailed component properties to WINPROP_TEST_ALL.OUT

☒ Print component properties for GEM to WINPROP_TEST_ALL.GEM

Reservoir temperature for GEM fluid model (deg F):

☐ Write solid model parameters for GEM ☐ Use Rowe-Chou aqueous density correlation

☐ Write component heating values for GEM ☐ Use Kestin aqueous viscosity correlation

☐ Include H2O in GEM component list

Solubility Parameters

☒ Print aqueous phase component solubility parameters

☐ Print solubility parameters from a previous calculation

☒ Recalculate solubility parameters at T and P below

Temperature (deg F):

Pressure (psia):

Interaction Coefficient Table

☒ Lower triangular format

☐ Upper triangular format

GEM-GHG Parameters

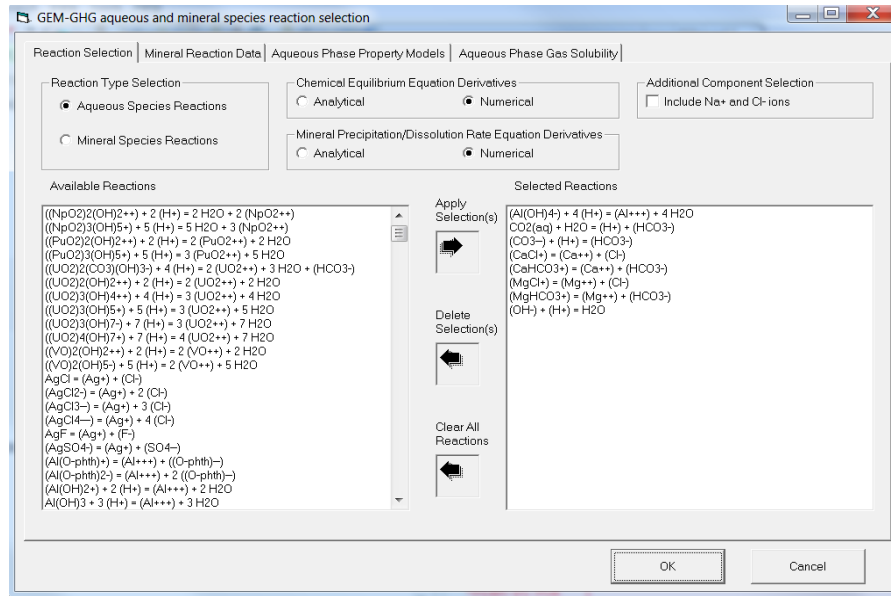
☒ Print GEM-GHG parameters

Select Reactions

OK Cancel

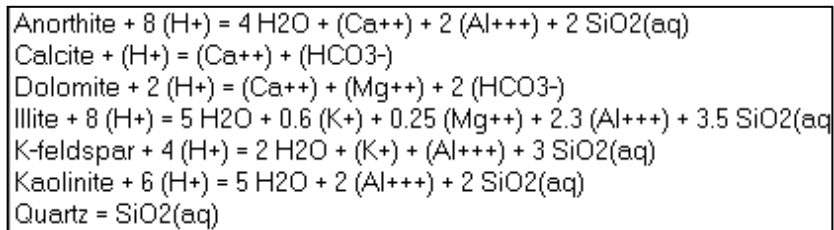
If the solubility mechanism is analyzed, the “Print aqueous phase component solubility parameters” option has to be checked.

16. In order to include the Mineralization option, the “Select Reactions” option on the right hand side of the figure shown above has to be selected. After the user double clicks on that option the following window should appear:



Click in the “Aqueous Species Reactions” box and introduce the Aqueous reactions showed above (these are the reactions chosen for this study).

17. Click the “Mineral Species Reaction” box and select the Mineral reactions that will be used in the model. For this study the reactions included are:



18. In the Mineral Species Reaction Selection, click on the “Mineral Reaction Data” and introduce the information related with Reactive Surface Area, Rate Constant, Activation Energy and Reference Temperature shown below:

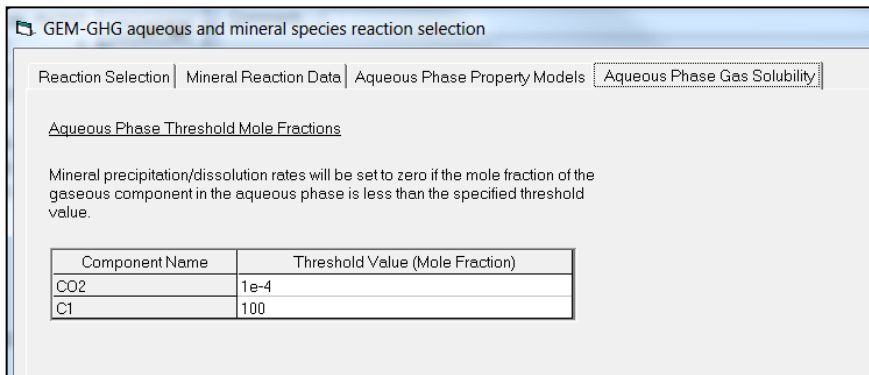
Mineral Reaction	Reactive Surface Area (m2)	Log10(Rate Constant) at Tref (mol/m2.s)	Activation Energy (J/mol)	Reference Temperature (deg C)
Anorthite + 8 (H+) = 4 H2O + (Ca++) + 2 (Al+++) + 2 SiO2(aq)	88	-12	67830	25
Calcite + (H+) = (Ca++) + (HCO3-)	88	-8.79588	41870	25
Dolomite + 2 (H+) = (Ca++) + (Mg++) + 2 (HCO3-)	88	-9.2218	41870	25
Illite + 8 (H+) = 5 H2O + 0.6 (K+) + 0.25 (Mg++) + 2.3 (Al+++) + 3.5 SiO2(aq)	26400	-14	58620	25
K-feldspar + 4 (H+) = 2 H2O + (K+) + (Al+++) + 3 SiO2(aq)	176	-12	67830	25
Kaolinite + 6 (H+) = 5 H2O + 2 (Al+++) + 2 SiO2(aq)	17600	-13	62760	25
Quartz = SiO2(aq)	7128	-13.9	87500	25

☒ Reduce permeability as a function of porosity change due to mineral precipitation according to Carman-Kozeny equation.

OK Cancel

19. Click on the Aqueous Phase Property Models and select the B-Dot Model for the Aqueous Phase Activity Model. Information regarding the Aqueous Phase Salinity also needs to be entered. (For this case a constant salinity was used.)

20. Click on the “Aqueous Phase Gas Solubility” tab and enter the following parameters then click OK until the user reaches the main window



This option will set the precipitation/Dissolution rates for the C1 to zero. Remember that C1 is just a trace component and results for C1 are not needed.

21. Now is time to save the WinProp model using the  link and run it using the  link. After you have run the model, a *****.gem** file will be created in the same folder where you saved the Winprop model. This file will have all the fluid model information required by the simulator.

22. Close the Winprop module and return to the Builder main window.

23. The information created in Winprop has to be included in the model. To do that, click in the arrow next to the Components tab and click on the “Import Winprop generated Model” option, then select the .gem file and click Open.

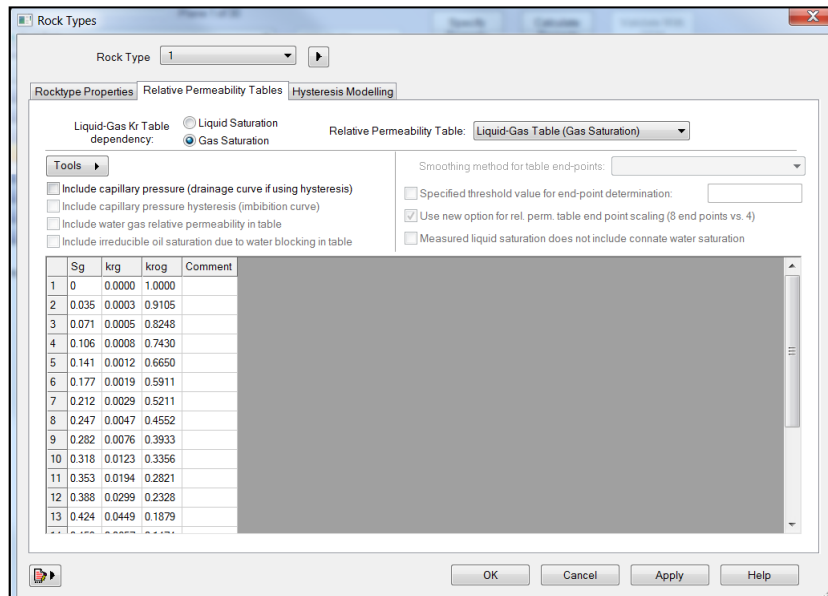
24. The Components tab now should have a green check mark, information regarding Water properties should be also entered in the “Properties of Water” option inside the Components label. Values for Density, Compressibility and Viscosity are needed.

25. The “Reservoir” label should be red again. This is because the gas compositions of the fluids present in the model have to be entered. That information will be entered later on in the “Initial Conditions” section.

26. The next section that has to be analyzed is the “Rock Fluid” tab. In this section, the user needs to double click in the “Rock Fluid Types” section and select the “New Rock Type” option that is located inside the  link. This will create a new Rock type.

27. Relative Permeability curves need to be entered for the Rock type that was created.

For a CO₂ –Water model, information about relative permeability of a Gas-Water system is needed. Meanwhile, CMG asks for a Water-Oil relative permeability table, so a “Fake” table should be entered.



To enter the Gas-Water table, the “Liquid-Gas Table (Gas Saturation)” option has to be selected (see figure above) and the Gas saturation box has to be checked. By default, GEM will use this curve as the Drainage curve. If you want to include Capillary pressure you have to check the “Include capillary pressure” box. (For this case no P_c was included).

28. To include the Gas Trapping mechanism, a value for maximum residual gas saturation is needed. To enter this value click on the “Hysteresis Modeling” tab inside the Rock Types Window and check the “Model Hysteresis effect in gas relative permeability. Krg values” box and enter Sgr of 0.4, then click OK.

29. Double click in the “Initial conditions” option in “Initial Conditions” tab. In the Calculations Method tab select the VERTICAL_DEPTH_AVE and WATER_GAS options.

30. In the “Init Region Parameters” tab, enter the information related with Reference pressure and depth, water saturation below water-oil contact and the gas composition for each component, then click OK. Do not enter very low values of ZGAS for the CO₂; otherwise you will have convergence problems. The values shown in the following figure are recommended. Now this section should have a green check mark.

Initial Conditions

Calculation Methods **Init Region Parameters** Advanced Parameters

Initialization Region: **Region 1**

Initialization Region Parameters
Initialization Region Type 1 is not defined. Grid depth range: 5818.86 to 9159.84 ft

Reference Pressure and Depth
 Pressure (REFPRES): 3700 psi
 Depth (REFDEPTH): 8540 ft

Phase Contact Depths
 Water-Oil Contact (DWOC):
 Gas-Oil Contact (DGOC):
 Water-Gas Contact (DWGC): 5400 ft

Capillary Pressure at Phase Contacts
 Gas-Oil capillary pressure at the gas-oil contact (GOC_PC):
 Water-Oil capillary pressure at the water-oil contact (WOC_PC):

Water Saturation
 Below Water-Oil Contact (SWOC): 0.999

Critical Depth
 Depth at which the phase identity, oil or gas, of a single-phase fluid is determined (CDEPTH):

Oil Zone and Gas Cap Compositions

	Comp.	Oil Zone (ZOIL)	Gas Cap (ZGAS)
1	CO2	0.0	0.0001
2	C1	0.0	0.9999
Total:		0.	1.

OK Cancel Apply Help

31. The “Numerical” section is where the user defines all the parameters that the simulator will use when the model is running. These parameters help avoid numerical non-convergence and in time step selection.

The following configuration can be useful whenever you have a simple model, if you still have convergence problems you may try one of the two sets of keywords shown below:

a. For simple cases, in the “Numerical Controls” section, enter the following parameters and then click OK.

```
* DTMIN 0.001
*DTMAX 31.
*NORM PRESS 10000 **Kpa
*NORM SATUR 0.1
*NORM GMOLAR 0.1
*MAXCHANGE PRESS 50000 **Kpa
*MAXCHANGE SATUR 0.9
*MAXCHANGE GMOLAR 0.9
*CONVERGE MAXRES NORMAL (1E-3)
*ITERMAX 100
*AIM THRESH 0.01
*NORTH 30
```

These values can also be entered manually in the .DAT file (This is the input file where all the information about the model is stored.)

Note: This could be a good time to save all the information that we have entered.

To do that, go to “File”, “Save As”, enter the name of the file and the location and press Enter. The user will see that a .DAT file is created.

b. If the model does not converge with the parameters mentioned above, then the following keywords can be used:

```
*NORM *PRESS 1000
*NORM *SATUR 0.05
*NORM *GMOLAR 0.005
*NORM *AQUEOUS 0.3
*MAXCHANGE *SATUR 0.8
*MAXCHANGE *GMOLAR 0.8
*CONVERGE *PRESS 1.E-05
*CONVERGE *HC 1.E-04
*CONVERGE *WATER 1.E-04
*CONVERGE *MAXRES 5.E-05
*PRECC 1.E-06
*NORTH 80
*ITERMAX 200
*DTMIN 1.E-06
*DTWELL 0.1
*DTMAX 75
```

Most of the time this set of keywords works best with most of the CO₂ sequestration models.

32. The last section that has to be completed before we can run the model is the “Wells & Recurrent” tab. For this study the well was imported from the Rescue file, but an explanation of how to create wells is presented.

- To begin this, the user has to double click in the “Dates” option. Once there, click on the “Add a range of dates” link and enter the Dates for your simulation and the desired step, then click OK and the user will see that new dates are created.
- Go to the last date and check the “Set STOP” box, so a Stop card is created in that date, then click “Close.”
- Right click in the “Wells” option and select “New.” The following window should appear:

The screenshot shows a "Create New Well" dialog box. The title bar reads "Create New Well" and the subtitle is "Global Composition(C1) 1901-01-01". The dialog is divided into several sections. The "ID & Type" section has a "Name" field containing "Well-2". The "Constraints" section has a checkbox "Add multiple wells numbered" with input fields "1" and "10" and the text "The name is used as a base and numbers are appended." The "Wellbore" section has a "Type" dropdown menu set to "Undefined". The "Group" section has a dropdown menu set to "<None>" with the text "3rd or 2nd level group with no other groups attached to it". The "Fraction" section has a checkbox and an input field "0" with the text "use to multiply well rates and index". Below these sections, there are two dates: "Simulation start date: 1901-01-01" and "Definition date: 1901-01-01". At the bottom, there is a checkbox "Add wells using a drilling schedule of" with input fields "1" and "2" and the text "wells every months". The bottom of the dialog features four buttons: "Add new well", "OK", "Cancel", and "Help".

- In the figure shown above, enter well ID, well type (Injector or producer) and the Definition date of the well. For this case of CO₂ sequestration, the user has to select INJECTOR.
- Click on the “Constraints” tab and enter the constraints for your well.
- Click on the “Injected Fluid” and select SOLVENT, and then specify the mole fraction of CO₂ as 1.0 and click OK.
- Once the well has been defined, the perforations locations have to be entered. In the Tree View, expand the “Wells” option and then select the “*** -PERF” option (** is the Definition date of the well). Go to the “Perforations” tab and then select the location of the cells for each perforation. The user can also add perforations with the mouse directly into the model, and then click OK.

Well Completion Data (PERF)

Well & Date: GC1 1995-01-01 INJECTOR

General Perforations Rel Perm.Options

Perforated grid blocks: Use trajectory perf intervals... Add perms with the mouse Begin

#	User Block Addr.	Connect to	Form facto.	Status	Ref Layer	WI (md/ft)	Length (ft)	Block Top
1	48 48 26	Surface	1	Open	29.149	56.666	8466.491	
2	48 48 27	1	1	Open	102.115	56.665	8523.157	
3	48 48 28	2	1	Open	496.6	56.665	8579.823	

Reset Well OK Cancel Apply Help

- Double click in the well name in the tree view to open the Well Event window. In there, click on the “Options” tab and check the WELLINIT

Option and select ITER from the dropdown list.

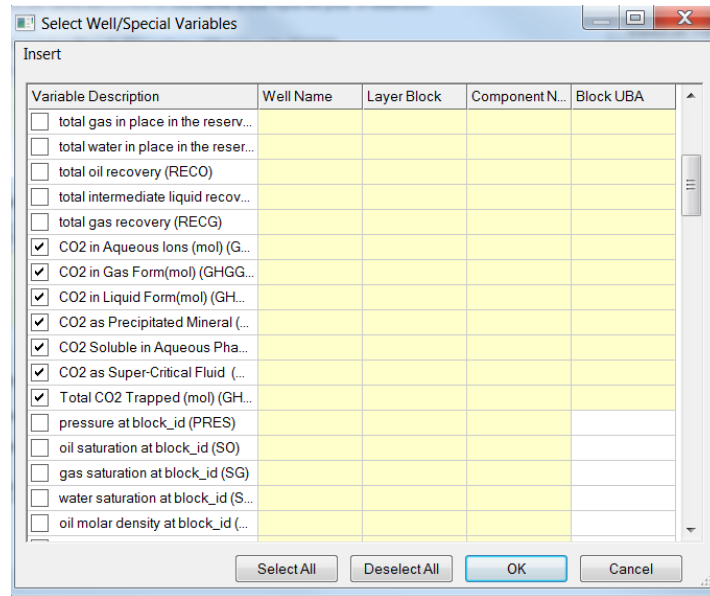
- To SHUT-IN the well, the user has to go to the date wanted in the Well Events window and then under “Options” check the “Status” option and select Shut-in.

After the user enters all this information, the “Wells & Recurrent” tab should have a green check mark.

33. Output arrays that the user wants have to be defined in the “I/O Control” tab. Click on the “Simulation Results Output” and then click on the “Select” tab, in the OUTSRF section. Some properties are already defined by default, but the following have to be selected:

☒ Component molality in aqueous phase of 'OH-' (MOLALITY)	☒ Gas saturation (SG)
☐ Component molality in aqueous phase of 'Al(OH)4-' (MOLALITY)	☒ Water saturation (SW)
☒ Change in mineral moles of 'Dolomite' (MINERAL)	☒ Pressure (PRES)
☒ Change in mineral moles of 'Illite' (MINERAL)	☐ Datum Pressure (DATUMPRES)
☒ Change in mineral moles of 'K-feldsp' (MINERAL)	☐ Pressure drop from time zero (DROP)
☒ Change in mineral moles of 'Kaolinit' (MINERAL)	☐ Trapped oil saturation (TSO)
☒ Change in mineral moles of 'Quartz' (MINERAL)	☐ Oil molar density (RHOO)
☒ Change in mineral moles of 'Calcite' (MINERAL)	☒ Gas molar density (RHOG)
☒ Change in mineral moles of 'Anorthit' (MINERAL)	☐ Gas phase mole fraction in o/g system (FRG)
☐ Triggers the output of Block Face based phase velocities for construc	☐ Capillary pressure for water (PCW)
☒ Temperature (TEMP)	☐ Capillary pressure for gas (PCG)
☒ Gas saturation for Krg hysteresis (SGHYS)	☐ Oil relative permeability (KRO)
☒ Residual gas saturation for Krg hysteresis (SGRHYS)	☒ Gas relative permeability (KRG)
☒ Dynamic trapped gas saturation for Krg hysteresis (SGDTHY)	☒ Water relative permeability (KRW)
☐ Matrix-Fracture transmissibility multiplier (TRANSMF)	☐ Viscosity (VISO)
☐ Aqueous phase salinity (molality) (SALIN)	☐ Gas viscosity (VISG)
☒ Porosity change due to mineral reactions (DPORMNR)	☐ Oil molecular weight (MWO)
☐ Water viscosity (VISW)	☐ Gas molecular weight (MWG)
☒ Oil phase resistance factor (RFO)	☐ Oil mass density (DENO)
☒ Component molality in aqueous phase of 'CO2' (MOLALITY)	☒ Gas mass density (DENG)
☐ Component molality in aqueous phase of 'C1' (MOLALITY)	☒ Water mass density (DENW)
☒ Component molality in aqueous phase of 'H+' (MOLALITY)	☒ Current porosity (POROS)
☒ Component molality in aqueous phase of 'Ca++' (MOLALITY)	☒ Permeability in each direction (PERM)
☐ Component molality in aqueous phase of 'Cl-' (MOLALITY)	☐ Saturation pressure (SATP)
☒ Component molality in aqueous phase of 'Mg++' (MOLALITY)	☐ Interfacial tension between oil and gas (SIG)
☒ Component molality in aqueous phase of 'Al+++ ' (MOLALITY)	☐ Solid mass and adsorbed mass; resistance factor (SOLID)
☒ Component molality in aqueous phase of 'K+' (MOLALITY)	☐ Adsorbed mass fraction of 'CO2' (ADS)
☒ Component molality in aqueous phase of 'SiO2(aq)' (MOLALITY)	☐ Adsorbed mass fraction of 'C1' (ADS)
☒ Component molality in aqueous phase of 'HCO3-' (MOLALITY)	☒ Velocity vectors of oil, water and gas at reservoir conditions. (VELOCRC)
☒ Component molality in aqueous phase of 'CO3--' (MOLALITY)	☒ Global mole fraction of 'CO2' (Z)

34. Click on the  symbol in order activate the output for the well related parameters and select the following arrays:



35. Save all the changes and exit the Builder.

36. Before we run the simulation some keywords have to be added manually in the .DAT file. The actual version of CMG does not allow entering these parameters through the interface, so the user has to do it manually opening the .DAT file in any Text Editor.

- Delete the *HENRY-CORR-C1 keyword. This keyword represents the solubility calculations for the C1 component and we do not need it.
- Insert the INVENTORY- CO2 in the I/O section of the dataset, which means that you can insert it below the WRST TIME keyword.

- Insert the following keywords at the end of the Model section:

```
*OGW_FLASH *NO_H2OVAP
*TRACE-COMP 2
*CO2-AQU-FACT
0. 0. 0. 0. 0. 0. 0. 1. 1. 0. 1. 0. 0. 0. 1.
*CO2-MNR-FACT
2. 0. 0. 0. 0. 1. 0.
```

The values entered for the TRACE-COMP 2 and *CO2-MNR-FACT are specific for each model, depending on the mineral and aqueous reactions entered in the model. For more information on these keywords please read the GEM User's Guide.

- The last modification that has to be done before we can run the model consists of adding the Molality of the aqueous components and the Volume fraction of minerals. Add the following keywords at the end of the Initial section (just before the NUMERICAL keyword).

```
*MOLALITY-AQUEOUS-PRIMARY
1e-07 0.009905684 0.883113 0.006501 1e-07 1e-07 1e-07
*VOLUMEFRACTION-MINERAL
0.0176 0.0233 0.0385 0.0035 0.7874 0.0088 0.0088
```

Note: The values for each keyword represent the molality of each of the aqueous components and the Volume Fraction of each of the Mineral components. The values entered here are specific for this study.

37. In order to run the simulator, the user has to go to the Launcher main window and drop the .DAT file into the GEM Simulator link.



Press the “Submit Job” button and the simulation will start.

When the simulation is finished, the following files will be created:

- *.out file (This is the output file of the simulation)

- *.irf file (Index Results file)

- *.mrf file (Main Results File)

- *.rst file (Restart file)

- *.log file (Log run file)

The .irf and .mrf file are used to see the results in the RESULTS 3D and RESULTS GRAPH modules.