Recent Development for long term modeling of CO_2 storage

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Introduction

Following the active R&D program initiated by ANR, several teams are currently actively involved in modeling CO_2 geological storages with different focus of interest in time (injection or storage period) and space (near well bore, full field, geosphere). Therefore, different tools are developed and used depending on the background of the modeling team (nuclear waste disposal, hydrogeology, oil&gas). This paper summarizes the recent developments of these teams and focuses on application to field scale rather than mechanistic modeling of the different processes involved.

Models

Most teams develop in part or fully their modeling tools. Thus, model development ranges from add-on to an existing tool such as TOUGHREACT (Xu and Pruess, 2001) , Cast3M (Le Potier, 1998 and Genty, 2000) up to development of dedicated tools such as COORES (Le Gallo et al 2006 and Trenty et al, 2006) or HYTEC (van der Lee et al., 2002, 2003).
The code uses different numerical approaches based upon finite volume (HYTEC, COORES, TOUGHREACT) or Mixed-Hybrid Finite Element (Cast3M) to solve the flow governing equations in 3-D. However, differences exist between the codes regarding multiphase flows (most of them are only 2 phase flow) and reactive transport (only one does not model it).
The coupling approaches between geochemical and flow equations are different in every code (HYTEC, COORES, TOUGHREACT) which rely on different geochemical modules. All geochemical modules integrate kinetic rate laws but different level of development exists regarding reactive surface modeling in precipitation/dissolution reaction or high ionic strength solution model (Debye-Hückel vs. Pitzer model). The feed back of mineral alterations on flow is mainly focused on permeability changes but other changes in flow parameters are computed for diffusion flux in HYTEC (Lagneau, 2000) and capillary pressure (COORES, TOUGHREACT).
Most of the codes assume compressible multiphase flow and a few of them currently account for hysteresis of relative permeability. Most of the available tools account for thermal effects.

The geomechanical impacts are mainly handled through external coupling with dedicated geomechanical software with various coupling algorithm. The main focus of the modeling team is not yet on geomechanical interactions but rather on geochemical interactions even though work is currently underway in various ANR projects e.g. Geocarbon Injectivity, Geocarbon Integrity.
To handle the necessary coupling, software platforms such as ALLIANCES (e.g.Montarnal, 2007) which was originally developed by the CEA, ANDRA and EDF to perform calculations of the long term evolution of radioactive waste disposal or ICARRE which is currently developed by IFP for oil industry calculations connecting third party software (reservoir and geosciences models) are started to be applied to CO2 storage modeling.
Besides featuring the implementation of different existing (stand-alone) codes (components), the platform main advantage is to provide a unified set of data, multi-domain computation, and coupling between some components (e.g. flow, mass and heat transport, geochemistry).

Applications

The modeling teams are focused on different modeling problems ranging from well scale to full field simulations and from injection period to storage life. This paper does not intend to thoroughly consider the various applications of the modeling tools to CO_2 geological storage but rather focus on key applications selected by the various contributing teams.

Well scale application

A simplified two-phase flow module has been developed for HYTEC to investigate the processes in the near-field of an injection well during the early phase of injection, using a 1D-radial geometry. The fluid-rock interactions are complex: they are controlled by rapidly changing saturation states (progression of the gas front). The progression of reacted water and of the desaturation front defines a moving reaction zone (Figure 1). The fast flow in the vicinity of the well, and the dilution of the velocity at larger distances from the well (radial propagation), leads to a decreasing propagation velocity of the reacting zone and its spreading out in time and space. Accordingly, slower reactions become important, causing a spatial zonation of the precipitates. Simultaneously, the solute composition is strongly modified along the flow path since all the previous reactions closer to the well alter the solution composition. Hence, the hydrodynamic and chemical processes are strongly coupled and simple reaction path simulations fail to describe the competition between kinetics of reactions and hydrodynamics.

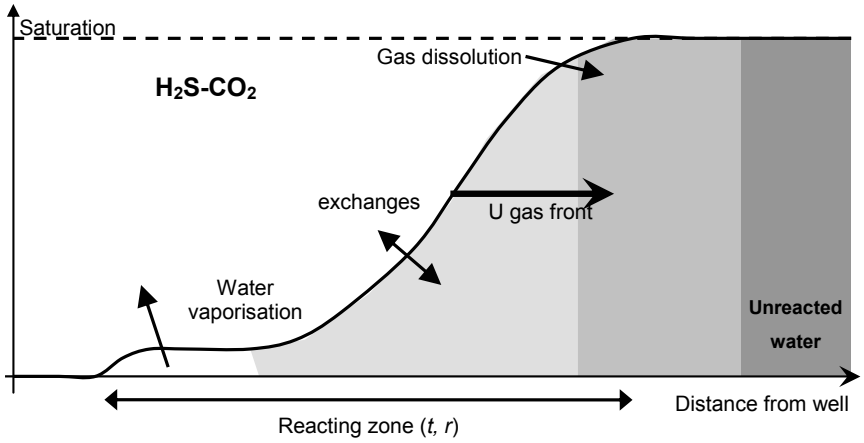

Figure 1 Schematic view of the reacting zone in the well injection simulation: reactions are bounded by the arrival of disequilibriated water (gas dissolution, previous mineral reactions) and the final disappearance of water (pressure drive followed by vaporization in the dry injected gas).

Aquifer hydrodynamics and upscaling

As large volume of CO_2 should be injected and as the expected plume lateral scale should be kilometric scale, it is probable that permeability will display spatial variability due to rock heterogeneity. Several numerical studies showed that large scale heterogeneities (facies heterogeneities) have a significant impact on the behaviour of the injected carbon dioxide (Johnson, 2001) (Flett, 2006).

Indeed, heterogeneities induce preferential flow-paths for the gas-like CO_2 plume which is pushed by the injection velocity field and submitted to strong buoyancy forces. It results in a lateral spreading of the CO_2 plume which in turn increases the contact surface between the plume and the host formation.

Moreover, Kumar et al. (2005) showed that horizontal to vertical permeability ratio has a significant impact on gas migration. These processes affect CO_2 dissolution in brine and carbon mineralization (Kumar et al, 2005). The intrinsic permeability value and the type of relative permeability curves are also very important (Doughty, 2004).

At the plume lateral scale, the numerical representation of small scale geological heterogeneities is out of reach and one must upscale the storage model. This is a classical problem in petroleum reservoir engineering. One of the main processes which have to be upscaled is the plume paths dispersion through permeable flow-paths resulting in a global spreading in all directions.

Consequently, one of the main modelling objective is to derive for large scale models effective permeability and macro dispersion tensors. This problem has been studied by numerous authors in several domains: in hydrology (Gelhar, 1993), hydrogeology (Sahimi, 1995) and oil reservoir engineering (Langlo, 1994, Christie, 1996).

The case of CO_2 migration in an heterogeneous porous media is quite more difficult: flow is non stationary, equations describing flow and transport are hardly non linear, several forces play an important part in the CO_2 migration such as those due to gravity, capillary pressure, CO_2 dissolution is important... The impact of heterogeneities on these processes and the way to upscale them has been tackled only recently (Panfilov and Floriat, 2004).

An upscaling methodology and initial results of an assessment of the impact of host-rock heterogeneity on CO_2 plume migration is presented. The CO_2 injection in the porous media is simulated with an incompressible two-phase flow model. As a detailed characterization of the geological formation is too difficult to obtain, the impact of aquifer heterogeneities on the CO2 plume migration is assessed in the framework of stochastic modelling through Monte Carlo simulations and ensemble averaging. The stochastic approach provides a statistical

description of the plume migration in terms of means and variances. 2-D grids simulate aquifer vertical sections with an injection point located at the bottom of the aquifer. In these first simulations, we neglected capillary pressure forces and CO_2 dissolution in water.

First, simulations of CO_2 migration in a homogeneous aquifer allowed to characterize the influence of the intrinsic permeability value on the plume migration, and in particular on its spreading. If the permeability is very low, buoyancy effects are negligible around the injection point and the bubble migration is piloted by the injection rate: it grows radially, according to the Buckley-Leverett theory. On the contrary, if the permeability is high, buoyancy effects become rapidly predominant, and plume migration becomes essentially vertical. In all cases, far enough from the injection well, migration bubble is buoyancy driven (Mugler and Mouche, 2006). These two behaviours are still present in the case of a heterogeneous aquifer: if the intrinsic permeability is low (injection driven case), the plume first spreads radially through permeable flow-paths and reaches rapidly the lateral limits. In a second step, it migrates in the low permeable strata. On the contrary, if the intrinsic permeability is high enough (buoyancy driven case) the plume rises vertically through strata distribution in a quasi 1D migration (Mugler and Mouche, 2006). These first simulations showed the importance of the intrinsic permeability: in the buoyancy driven case, the plume should occupy the top of the aquifer only; at the contrary, in the injection driven case, the plume should invade all the aquifer.

Second, Monte Carlo simulations of injection of CO_2 were performed in a 2-D heterogeneous aquifer. The host-formation intrinsic permeability is assumed to be a lognormal anisotropic random process. The domain extent is 20 λ_H wide and 27 λ_V high, where λ_H and λ_V are the horizontal and vertical correlation lengths, respectively, with $\lambda_H/\lambda_V=10$ and $\lambda_V=1$ m. The $\log_{10}$ permeability covariance is assumed to be exponential, with a mean $\log_{10}$ intrinsic permeability $<\log_{10}K>$ equal to -12.3 and a $\log_{10}$ standard deviation σ equal to one. Two hundreds realizations of permeability field were generated and these fields were used as input to the two phase flow model. The duration of each simulation was about two to three CPU hours. Figure 2 shows various CO_2 plume distributions obtained with 5 different realizations of the permeability field, after four days of injection. By comparison, (a) gives the CO_2 plume obtained with a homogeneous permeability K equal to 5×10^{-13} m^2 ($\log_{10}K=-12.3$). These various patterns illustrate the influence of heterogeneities on the behaviour of CO_2 which rises upwards and spreads through permeable flow-paths.

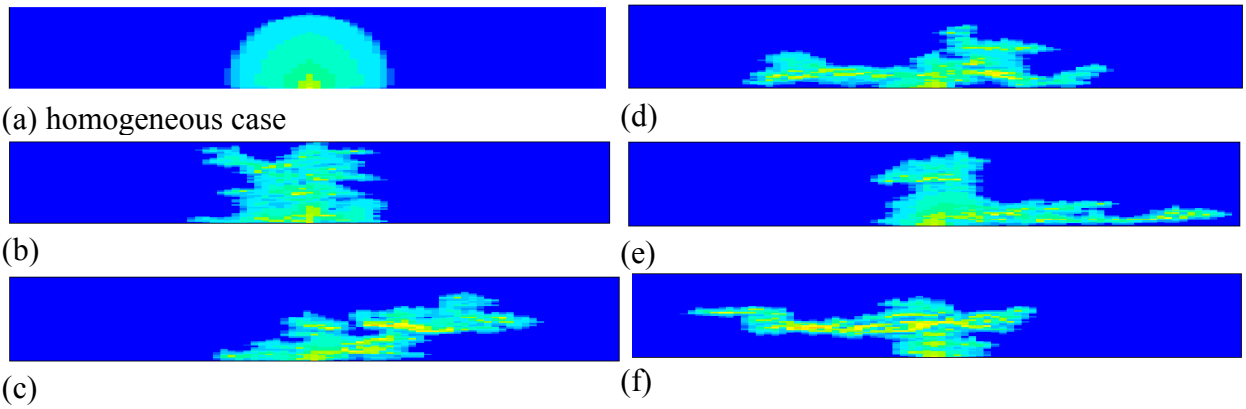

Figure 2 CO_2 saturation distributions after 4 days of injection, with $<\log_{10}K>$ = -12.3 and (a) σ=0 (homogeneous case) and (b)-(f) σ=1 (heterogeneous cases).

The different types of spreading obtained from Monte Carlo simulations may be quantified by a moment analysis of the CO_2 saturation spatial distribution (Gelhar, 1993). In the simple case where the solute transport equation is 1-D convection-dispersion type, the time derivative of the first spatial moment is equal to the flow velocity and the dispersion coefficient is proportional to the time rate of change of the spatial second moment (Gelhar, 1993). In our case, these relations are no more valid because of the presence of non linearities and gravity forces. For each Monte Carlo simulation, the horizontal and vertical second spatial moments around the center of mass are calculated . The time evolution of these 200 moments allow to quantify the CO_2 plume dispersion (see Figure 3).

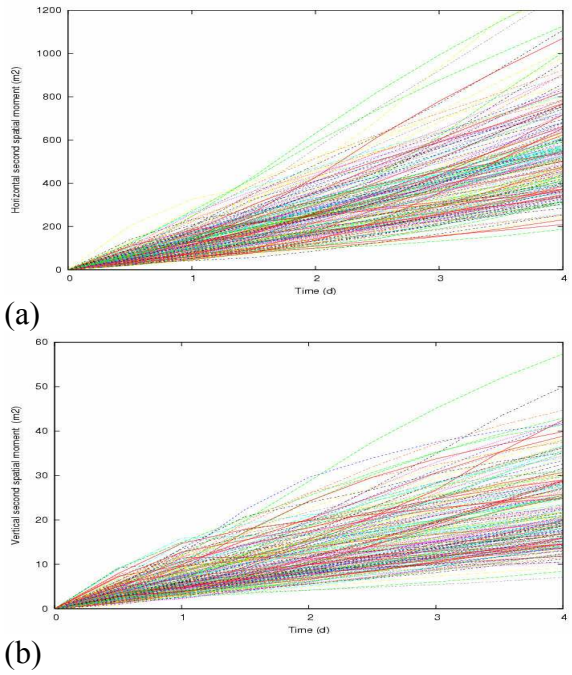

Figure 3 Evolution versus time of the second spatial moments of the 200 Monte Carlo simulations: (a) horizontal second spatial moments, (b) vertical second spatial moments.

The challenge is now to determine a homogeneous media equivalent to the heterogeneous one giving horizontal and vertical second spatial moments quite identical to the moments averaged over the 200 Monte Carlo simulations. Indeed, one of the final objectives of this work is to define equivalent migration parameters for large scale simulations, corresponding to those that would be obtained for an equivalent homogeneous media. Monte Carlo simulations and a moment analysis of CO_2 saturation distribution will allow us to define equivalent migration parameters for volumes of rock and sediment with sizes comparable to grid blocks used in large scale flow simulations (about tens to hundreds of meters). These scaled-up parameters will be used as input to a large scale flow model of CO_2 injection, with the aim of assessing the importance of accounting for the effects of rock and sediment heterogeneity on the behavior of injected supercritical CO_2.

Gas storage and geochemical impact

The K12-B field is a depleted methane reservoir located in the North Sea produced by Gaz de France Netherlands since the 80's. This field is one of the four sites of the CASTOR project funded by the European Commission within the 6th European Framework. Within the CASTOR project, a numerical modeling study on hydrodynamic and geochemical impact of the CO_2 injection at K12-B was developed (Audigane et al., 2007). Due to the complexity of

the multiphase system (CO_2 and CH_4 gas mixture and dissolution coupled with fluid rock geochemical interaction), a complete coupled simulation of the CO_2 injection into a methane gas field estimating at the same time the geochemical reactivity was divided in two separate simulations using (i) TOUGHREACT to estimate mineral trapping (case A) and (ii) using TOUGH2/EOS7C to estimate structural and solubility trapping (case B). The injection rate is chosen at 10 kg/s while production rate has been chosen arbitrary ten times smaller than injection rate at 1 kg/s for each producer K12-B1 and K12-B5 in order to limit the CO_2 breakthrough time.
This simulation was carried out assuming that the storage of large quantities of CO_2 was a primary objective. Results show that mineral trapping plays a minor role in terms of CO_2 storage. As the reservoir contained initially 13% of CO_2 in the gas phase, the geochemical system is equilibrated between fluid and rock minerals. Therefore, injection of CO_2 will not induce large modification of the system. As illustrated by Figure 4a for the pH field after 10 years of injection simulated values range from 4.40 to 4.58 with slight variations distinguished in four regions through the reservoir.

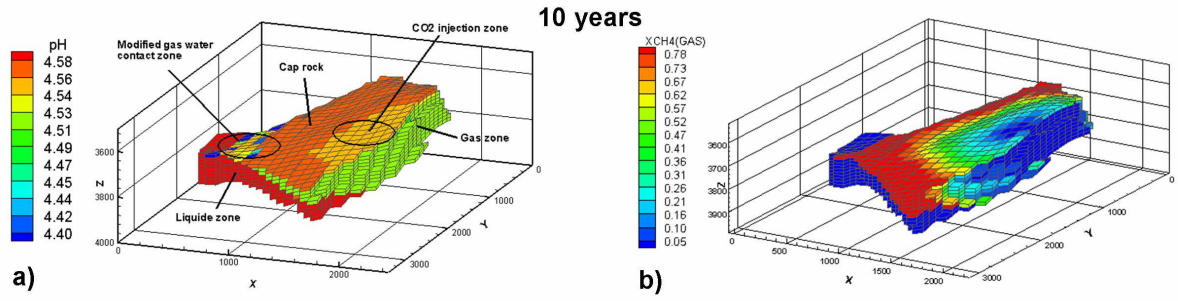

Figure 4 a) Case A: Four zones for pH field are distinguished: (i) the liquid phase saturated part, (ii) the gaseous phase, (iii) the cap rock and (iv) the gas water contact area within the cap rock, with a pH average value of 4.58, 4.51, 4.55 and 4.0, respectively. b) Case B simulation: methane gas field after 10 years of CO2 injection. The methane is also produced from two producers.

The simulation for Case B (Figure 4b) shows a relatively short CO_2 arrival time in the producers (60 days and one year) and a linear increase of reservoir pressure between 47 bar to 104 bar. Though, these breakthrough times are relatively short and therefore the prediction of the enhanced gas recovery efficiency is rather poor, the capacity of CO_2 storage remains good as only 20 % of the injected mass of CO_2 is produced from the reservoir.

Reactive transport modeling of the CO_2 injection into saline aquifers is well addressed when using TOUGHREACT. Nevertheless, when considering gas mixtures (impurities or gas reservoir), some simplifications are to be made. Either considering a gas phase constituted with pure CO_2 with geochemical fluid rock interactions, or using a EOS module able to handle the gas mixtures (CO_2, CH_4 S_2H…) but neglecting induced geochemical reactivity. The present case study is a perfect illustration of such limitation as two separate simulations had to be performed to complete a full study of the structural dissolution and mineral trapping occurring during the injection of CO_2 into the depleted methane reservoir.

Aquifer storage and geochemical impact

A 3-D saline aquifer is modeled (3000 x 6000 x 200 m) with about 50 000 grid blocks. The different sand bodies, with a permeability of 2500 mD and porosity of 35%, are separated by shaly layers with permeability of about 10 mD and porosity of 10%. The mineralogy is derived from literature (Nghiem et al, 2004). The mineral volume fractions are different in the

shale, kaolinite and k-feldspar rich, and sand, quartz rich. The aquifer water is initially at equilibrium with the rocks. CO_2 is injected at a rate of 1Mt/y for 40 years. The lateral boundaries of the model are at hydrostatic conditions and the top and base boundaries are assumed to be no-flow.
From the assumed initial mineral composition (7 minerals), aqueous species (8 chemical elements and 16 aqueous species), Figure 5 illustrates the geochemical alteration of the host rocks (sand and shale) link with the CO_2 plume evolution. The influence of geochemistry is quite minor as well since there is no significant porosity and consequently permeability variation (see Figure 5) computed over the whole storage life (1000 years). As illustrated by the pH variations (Figure 5), most of the geochemical changes occur within the CO_2-rich water region. This altered zone extends long after the CO_2 injection is finished since the CO_2-rich water migrates downward due to buoyancy. Figure 5 also illustrates the open lateral boundary condition (hydrostatic pressure) of the model as the CO_2-rich water spreads over the top of the aquifer. Due to the parallel kinetic reactions with different reaction rates, calcite mainly dissolves fairly rapidly in the reservoir while illite mostly precipitates over long storage time (Le Gallo et al, 2006).

Figure 6 illustrates the influence of capillary pressure of the shale barrier on the CO_2 distribution at the end of injection and end of storage life. Shale layers with significant pore entry pressure (capillary pressure) will induce a significantly different distribution of Free and thus dissolved CO_2 in the reservoir. The capillary properties and heterogeneities, i.e. rock type, significantly alter the CO_2 distribution and consequently the storage capacity of the aquifer (Le Gallo et al, 2006).

Future steps

Several research paths are pursued by the different modeling teams ranging from multi-domain computation to uncertainty/sensitivity analysis and model capability enhancements.
Future developments mainly concern the reactive multiphase flow both in fractures reactivated by geochemical/geomechanical processes and also in aquifer matrix where the impact of heterogeneities and consequently the impact of increased dispersion of injected CO_2 on the rate at which CO_2 dissolves in the formation waters and reacts with the host sediments to become permanently stored.

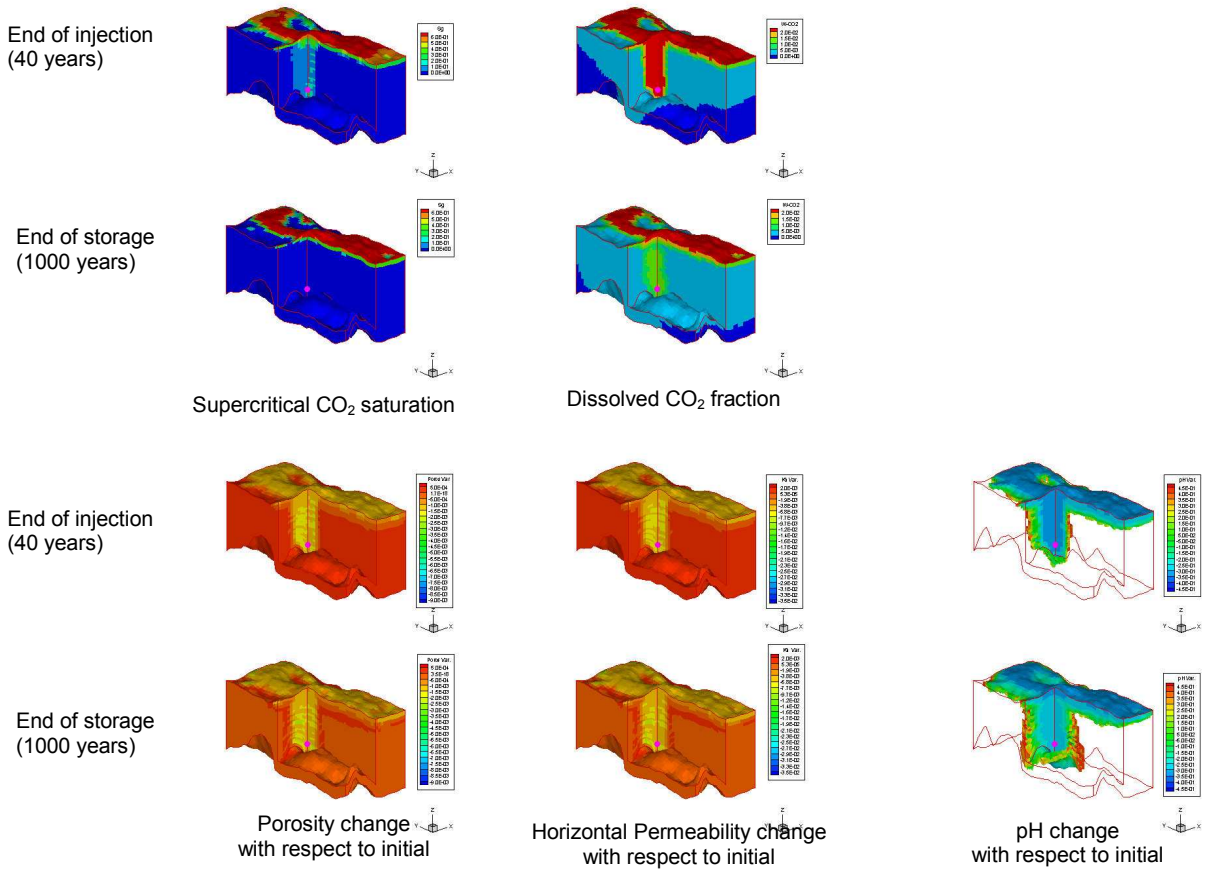

Figure 5 CO2 fraction free (upper left) and dissolved in the water (upper right), porosity (lower left), permeability (lower center) and pH (lower right) changes with respect to initial at the end of injection (40 years) above and at the end of storage (1000 years) below. The purple dot indicate the injection point

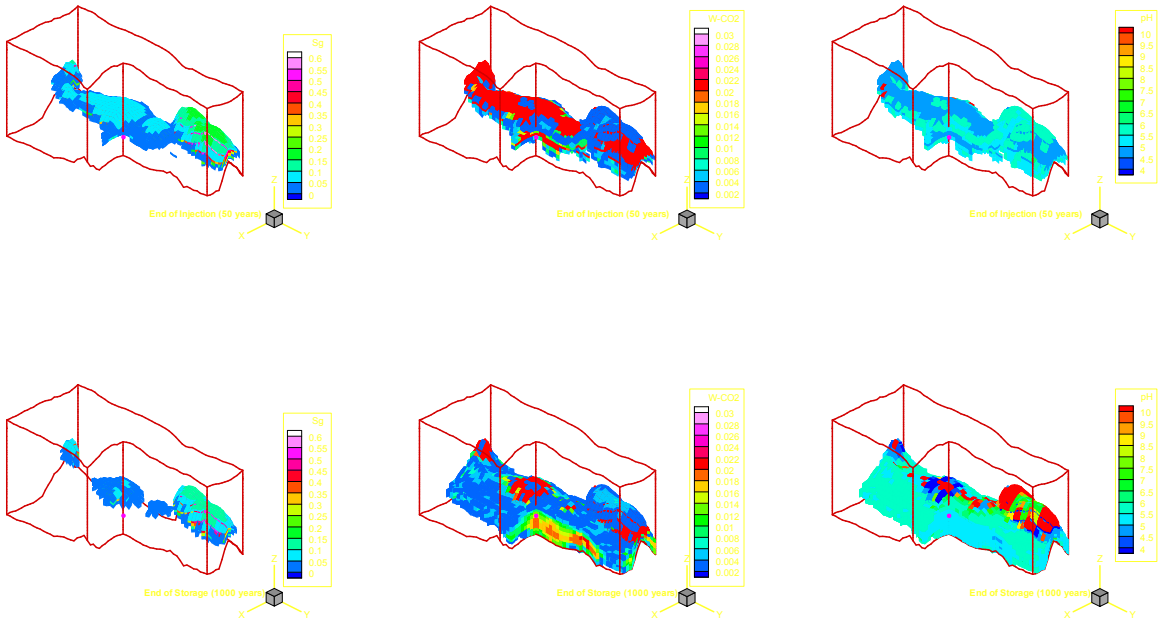

Figure 6 CO2 fraction free (left), dissolved in the water (center) and pH (right) at the end of injection (50 years) above and at the end of storage (1000 years) below assuming shale capillary barrier.

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