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Reactive Transport of CO2 in Saline Aquifers with implicit geomechanical analysis

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Abstract

Geological storage of CO_2 in saline aquifers is a promising way to reduce the concentration of the greenhouse gas in the atmosphere. Injection of CO_2 will, however, lead to dissolution of minerals in regions of lowered pH and precipitation of minerals from transported ions in regions of higher pH. The geomechanical implications of these changes on the stability of the reservoir are of crucial importance in the evaluation of potential injection reservoirs. The possible injection rate for given over-pressures of the injected CO_2 depends on the porosity and permeability of the rock matrix in the vicinity of the injection well. Local fracturing in this region can be a tool for increasing the injection flow rate but a geomechanical analysis will be needed in order to make sure that this fracturing will not affect the geomechanical stability outside this limited region to a significant degree. This paper presents a new rewritten version of RetrasoCodeBright (RCB) for simulations of CO_2 storage in saline aquifers. An advantage of this code compared to other codes is the *implicit* geo-mechanical module. The code has been rewritten to account for non-ideal gas through corrections of gas density and gas solubility in all transport terms. Newton-Raphson method used to solve the flow and mechanics in RCB has been improved so as to improve convergence even under high gas injecting pressures. A 2D hydro-chemical-mechanical problem is used to illustrate the modified RCB code. This particular test case is chosen as a block of pure calcite embedded in top or bottom sections with mineralogy similar to that of the Utsira formation. The test case is designed so as to investigate horizontal migration and injection is controlled by a pressure difference between injection on the right hand side (140 bar) and a constant pressure (100 bar) on the left hand side of the system. For this particular test case the Soave Redlich Kwong (SRK) equation of state has been applied for compressibility factors and fugacity coefficients but can easily be replaced with more accurate equations of state for CO_2. The simulated results show as expected a significant buffering effect which slows down the mineral erosion close to the injection zone and for the specific example the only region which appear to have potential geomechanical implications of the injected CO2 is close to the left side of the block where the difference between stress and overpressure indicate region of instability after 100 years of injection.

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1. Introduction

  The geological storage of greenhouse gas in deep saline aquifers can be one of the most promising options to reduce the concentration of CO_2, the major greenhouse effect contributor, in the atmosphere (Haszeldine, 2004). Saline aquifers are water bearing porous layers of sandstone or limestone in the subsurface and by far they are the volumetrically largest, and widespread, proposition for large-scale CO_2 storage. Currently there are four functioning CO_2 sequestration projects in the world; two in Norway, one in Algeria, and one in Canada. Statoil, Norway's largest oil company operates the two CO_2 sequestration projects in Norway; the Sleipner project and the Snohvit project. The Sleipner project has been running since 1996. One million tonnes of CO_2 are captured from the Sleipner natural gas field and then stored every year. The CO_2 is stored in a sandstone formation called Utsira, more than 800 meters below the sea floor. A special platform was built in order to treat the natural gas coming from Sleipner, extract the CO_2 and inject it back underneath the ocean. Natural gas production, CO_2 capture and CO_2 storage is all done on the Sleipner T platform since the Utsira formation, where the CO_2 is injected, is located above the Heimdal formation, where the natural gas is located. Production wells and the injection well are separated by about 1700 meters in depth and over 1000 meters in distance. The second CO_2 sequestration project in Norway is the Snohvit project, located in the Barents Sea. This project is based on the liquified natural gas (LGN) factory on the island of Melkoya. From the Snohvit field off-shore, the natural gas is brought by pipelines to the LGN plant on Melkoya where it is cooled to liquify it. Before this happens, CO_2 in the natural gas is extracted and sent back to the Snohvit field where it is injected into a sandstone formation called the Tubaen formation, 2500 meters below the sea floor and under the gas-containing layers. Here, over 700,000 tonnes of CO_2 will be stored yearly. This project started production in October 2007. In Algeria, Statoil, as well as Sonatrach and BP are funding a CO_2 sequestration project. This project, in connection with In Salah Gas, uses similar separating methods as the Sleipner project. Since starting in 2004, injected CO_2 volumes have increased from 186,000 tonnes to 687,000 tonnes in 2007, and expected to reach 1.2 million tonnes per year. In this project, CO_2 is stored in the same formation as the natural gas is found, but at a considerable distance from the producing regions. With this concept, the same cap rock that keeps the natural gas from leaking will also function as sealing for the injected CO_2. The Weyburn CO_2 Enhanced Oil Recovery project is located partly at the Weyburn oil field, southwest of the city of Regina in the Saskatchewan province in Canada and partly at the Great Plains Synfuels Plant near Beulah, North Dakota. In 1999, these two companies decided to form a partnership where waste gas (mostly CO_2) from the production of the synthetic natural gas from the Great Plains Synfuels Plant in North Dakota would be transferred through 330 km of pipeline to the Weyburn field where it would be injected 1400 m underground into the natural gas reservoir for storage and Enhanced Oil Recovery (EOR). Currently, it is predicted that the CO_2 EOR project will produce 130 million more barrels of oil and 20 million tonnes of CO_2 stored long-term or permanently . In addition to the running industrial full scale projects a number of research programs are active worldwide. As of now, there are seven regional partnerships for carbon sequestration in the U.S. Big Sky Carbon Sequestration Partnership includes Montana, Idaho, Wyoming, and South Dakota. BSCSP is looking at geological sequestration as well as terrestrial sequestration including changing management practices of the land. Currently, the BSCSP is looking at conducting two geological demonstration projects; in mafic rock formations and sedimentary rock saline aquifers. These projects would help to predict long-term effects of CO_2 storage in these formations as well as the sites' operational needs. The BSCSP is also looking at conducting pilot projects demonstrating possible terrestrial sequestration in the region. The Plains CO_2 Reduction Partnership includes Wisconsin, Minnesota, Iowa, Missouri, North Dakota, South Dakota, Nebraska, part of Montana and Wyoming, and four Canadian provinces. PCOR is currently conducting four CO_2 sequestration field validation projects, as well as developing two commercial-sized, long-term demonstration projects. The Zama field demonstration in Northwestern Alberta, Canada involves improved oil recovery, CO_2 sequestration, and elimination of elemental sulfur accumulation, since both CO_2 and H_2S are produced together from pinnacle reef structures in the Zama field. A field validation test in an un-minable lignite seam is being conducted in Northwestern North Dakota. In this case, CO_2 is sequestered into a lignite coal seam where the CO_2 molecules become physically attached to the coal, as well as replacing coalbed methane, which can then be brought to the surface. A deep oil reservoir field test will be implemented in western North Dakota to determine validity and productivity of CO_2 sequestration and EOR. Last, PCOR will maintain a managed wetland to show potential practices of terrestrial CO_2 sequestration. The Midwest Geological Carbon Sequestration

Consortium includes Illinois, Indiana, and Kentucky. The MGSC was just awarded their phase III project which consists of a large-scale demonstration including capture of CO2 from Archer Daniels Midland's ethanol plant in Decatur, Illinois, and storage of the captured CO2 in the Mt. Simon sandstone, a saline reservoir. MGSC is looking at capturing and storing one million tonnes of CO2 over a period of three years. This project may also include possible EOR. Midwest Regional Carbon Sequestration Program includes Indiana, Kentucky, Maryland, Michigan, Ohio, Pennsylvania, West Virginia, and New York. The MRCSP is working on three small-scale CO2 injection field test sites and three terrestrial sequestration projects. Southeast Regional Carbon Sequestration Partnership includes Alabama, Arkansas, Florida, Georgia, Louisiana, Mississippi, North Carolina, South Carolina, Tennessee, Texas, Virginia, and some counties in Kentucky and West Virginia. Currently, SECARB is working on four field validation projects. The Gulf Coast Stacked Storage Project includes long-term CO2 storage in saline-bearing formations as well as EOR. The saline-bearing formation proposed for injection is the lower Tuscaloosa Formation in southwestern Mississippi. Potential depth for injection is 3140 m with injection rates between 90,700 and 454,000 tonnes per year. The second field validation test, Central Appalachian Basin Coal test, consists of injecting 907 tonnes of CO2 into four coal seams in the Pocahontas Formation and four coal seams in the Lee formation in Virginia and southern West Virginia. In the third field validation test, Black Warrior Basin Coal test, SECARB is looking at sequestration in coalbed methane reservoirs and Enhanced Coalbed Methane Recovery. The test involves injecting 907 tonnes of CO2 into three different coal seams, Black Creek, Mary Lee, and Pratt coal zones in Tuscaloosa County, Alabama. The fourth field validation test, Saline Reservoir Field test in Mississippi consists of injecting 2722 tonnes of CO2 at about 2621 m in the Lower Tuscaloosa Massive Sand unit in Jackson County, Mississippi. Southwest Regional Partnership on Carbon Sequestration (SWP) is made up of all or part of Arizona, Colorado, Kansas, Nevada, New Mexico, Oklahoma, Texas, Utah and Wyoming. SWP has many projects going right now, including EOR projects in the Permian Basin in Texas and Paradox Basin in Utah, and an enhanced coalbed methane project and a possible terrestrial sequestration site in San Juan Basin in New Mexico. Currently, the SWP is working on a major deep saline sequestration project in Farnham Dome in central Utah. This project will start in 2008 and consist of 900,000 tonnes of CO2 stored per year for the next four years. The West Coast Regional Carbon Sequestration Partnership includes Washington, Oregon, California, Nevada, Alaska, Arizona, and British Columbia in Canada. Right now, WESTCARB is starting on their phase III project; an integrated oxy-combustion CO2 capture and large-volume storage test. This project involves capturing CO2 from the Clean Energy Systems' oxy-combustion power plant and injecting 226,800 tonnes of CO2 per year for four years into a saline basin in San Joaquin Basin in the Central California Valley. WESTCARB also has two phase II projects; one in the Thornton gas field in California, and one in northern Arizona. The Thornton gas field project involves two test injection sites, one in a saline zone in the McCormick sandstone, and one in a depleted gas reservoir in the Middle Capay shale above the McCormick sandstone. Both involve injection 2000 tonnes of CO2. The second phase II project, located in northern Arizona, involves injecting into a promising saline formation in the Colorado Plateau. Reservoirs vary significantly in terms of mineral compositions. Some CO2 storage reservoirs, like for instance Utsira, contains only small amount (3% Calcite) of quickly dissolving carbonates, such as sandstone or limestone (calcite is the main chemical element). In that case the reactive flow module is allowed to take the assumption that the reactions do not affect the fluid flow significantly except for trivial porosity/permeability changes as estimated from "accepted" / common correlations. Other reservoirs which have been put forward as potential reservoirs for storage of CO2 contain up to 11% calcite. Dissolution and transport of the ions resulting from dissolution of these minerals by reactions with CO2 may lead to precipitation of similar minerals in regions of higher pH, thus providing mineralization of CO2 and storage for geological time scales. Significant content of these minerals will lead to a buffering of the system for some time due to the balance between the released carbonate ions and corresponding shifts in the dissociation reactions for CO2. But eventually the erosion caused by reactions with CO2 will become significant and the question is whether or not the geological formation will be geo-mechanically stable. Dissolution of the calcite (and other quickly dissolving minerals) in such reservoirs will increase the porosity significantly and might result in local collapse of sediments. The situation might even be worse if the calcite is distributed in between the others minerals in a fashion that dissolution might lead to not only increased porosity but dissolution of larger particles into smaller. The dynamic nature of the couplings between mineral dissolution, corresponding buffering effects and changes in geo-mechanical properties of the reservoir makes is necessary to evaluate the reservoir continuously in terms of mechanical stability. This analyses needs to be conducted for time

periods beyond the active injection period, until the reservoir as whole has reached a state where the accumulated CO2 is distributed enough and/or precipitated into new minerals in regions of higher pH.

2. Reactive transport modeling

The time scale for evaluation of storage safety vary worldwide but a number of 10000 years frequently pop up in the discussion of long term storage safety. These long time scales challenge our current level of understanding of the whole storage system, which involves implicit couplings between fluid flow, reactions and potential implications for geomechanical stability. Most of the reservoir simulators used for studies of CO2 storage up to now have been based on finite volume algorithms and there are correspondingly no implicit bridges to the geo-mechanical analyses. Recently some of these simulators have been extended with a finite element library which enables external couplings to geo-mechanical analysis tools. Whether these explicit couplings are satisfactory in terms of capturing the dynamic coupling between the reactive transport and the corresponding geo-mechanical implications remains unverified. In view of the discussion above it is desirable to develop a reservoir simulator which has implicit coupling between reactive flow and the geo-mechanical analysis. In the work presented here code RCB (RetrasoCodeBright) has been chosen as the software platform. RCB is the result of coupling two codes: CodeBright and Retraso. CodeBright (COupled DEformation of BRIne Gas and Heat Transport) was designed for the thermo-hydraulic-mechanical analysis of three-dimensional multiphase saline media (Olivella et al., 1996). In other words, CODE-BRIGHT permits the modeling of deformation, mechanical processes and heat transport in multiphase. Retraso (REactive TRAnsport of SOlutes) is a code for solving reactive transport problems (Saaltink et al., 1997). The Retraso part of the code has a built in state of the art geochemical solver and in addition capabilities of treating aqueous complexiation (including redox reactions) and adsorption. The density of CO2 plumes which ccumulate under traps of low permeability shale or soft clay depends on depth and local temperature in each unique storage scenario. The difference in density and the density of the groundwater results in a buoyancy force for penetration of CO2 into the cap rock. And even if the solubility of water into CO2 is small dissolution of water into CO2 may also lead to out-drying. Mineral reactions between CO2 and shale minerals are additional effects which eventually may lead to out-drying and embrittlement. Linear geo-mechanics may not be appropriate for these effects. In particular clay is expected to exhibit elastic non-linear contributions to the geo-mechanical properties. Different types of non-linear models are already implemented in the CodeBright part of the code and the structure of the code makes it easy to implement new models derived from theory and experiments. Basically, in the coupled code RCB, a CodeBright module calculates the flow properties (Darcy flux of liquid and/or gas, saturation, temperature, density, displacements, etc.) and passes it to a Retraso module for the calculation of reactive transport and impact of geochemistry on the fluid flow (Saaltink et al., 1997, Saaltink et al., 2004). In the current version we have extended the code from ideal gas to handling of CO2 according to the SRK equation of state (Soave, 1972). This equation of state is used for density calculations as well as the necessary calculations of fugasities for the CO2 phase as needed in the calculation of dissolution of CO2 into the groundwater. See also Hellevang & Kvamme (2007) for more details. Other alternative equations of state can easily be implemented to replace SRK. The mathematical equations for the system are highly non-linear and are solved numerically (Saaltink et al., 2004). The numerical approach can be viewed as divided into two parts: spatial and temporal discretization. Finite element method is used for the spatial discretization while finite differences are used for the temporal discretization. The discretization in time is linear and the implicit scheme uses two intermediate points, $t^{k+\varepsilon}$ and $t^{k+\theta}$ between the initial t^k and final t^{k+1} times. The iterative scheme (Olivella et.al., 1996, Olivella et.al., 1997) in the original code solved using a Newton-Rhapson approach. This scheme has been modified through the introduction of a relaxation factor approach according to the algorithms of Nakata and Fujiwara (1993), in which we obtain the proper relaxation factors by combining the general tendency method (Nakata and Fujiwara, 1993) and time step reduction method.

3. Simplified model system and sensitivity study

In lack of real field data for relevant systems with significant reactivity we present some examples from a simplified model, which are part of a larger sensitivity study. The 2D model is consists of a 1000 m long (x-direction) and 1000 m high (y-direction) block. 100 m at and 100 m at bottom has limited reactivity, modeled as 3% Calcite and 97% Quarts with a porosity of 35% initially and subject to change with mineral dissolution and mineral

precipitation. For this reference case we also present some geomechanical results in figure 4 below. In these simulations we have used a poroelastic model with Young Modulus equal to 1000 MPa and Poissons ratio equal to 0.3. The middle zone is varied in terms of Calcite and Quartz content as well as porosity. The calculation of volume fraction and surface reactive area of calcite and quartz in the whole formation is adapted according to the paper by S.P.White (2002). Kinetic geochemical reactions are assumed for all fluid-mineral reactions.

Vol. fraction of calcite	0.97	0.97	0.97	0.5	0.1
Vol. fraction of quartz	0.03	0.03	0.03	0.5	0.9
porosity	0.1	0.2	0.3	0.1	0.1

Tab.1 Parameters variations for sensitivity study

In RetrasoCodeBright the rates of mineral dissolution or precipitation is calculated according to the general expression of Lasaga et al. (1994) (Saaltink et al., 1997):

$$r_m = \sigma_m \zeta_m \exp\left(\frac{E_{a,m}}{RT}\right) \sum_{k=1}^{N_k} k_{mk} \prod_{i=1}^{Ns} a_i^{P_{mki}} \left(\Omega_m^{\theta_{mk}} - 1\right)^{\eta_{mk}}$$

(1)

Where r_m is the mineral dissolution rate (moles of mineral per volume of rock and unit time), k_m is the experimental rate constant (in the same unites), Ω_m is the saturation ratio, which is the ratio between the ion activity product and the solubility product defined in eqn.(13).

$$\Omega_m = \frac{1}{K_m} \prod_{i=1}^{Nc} a_i^{v_{mi}^p}$$

(2)

where the log Ω_m value is known as the saturation index SI_m. The system reaches the minimum free energy at equilibrium when $\Omega_m = 1$ or $SI_m = 0$. The parameters θ and η must be determined from experiments. The term inside the parenthesis, called the far-from-equilibrium function, decreases the reaction rate in a non-linear way, as the solution approaches to equilibrium. The term $a_i^{p_i}$ accounts for the catalytic effect of some species (particularly of H+) and the value of p_i is determined by fitting experimental data. For reactions which are slow at ambient conditions the experiments are carried out at temperatures which are sufficiently high to result in dissolution within reasonable reaction times. Scaling of the rate constants are normally done through the Arrhenius equation:

$$k_m = k_0 \exp(\frac{-E_{a,m}}{RT})$$

(3)

where k_0 is a constant and $E_{a,m}$ is the apparent activation energy of the overall reaction process, which for most minerals range from 30 to 80 kJ/mol (Lasaga, 1984). Parameters k_0 and $E_{a,m}$ are determined from experiments performed at different temperatures. All kinetic parameters for the systems in this study was collected from Mucci and Morse (1983).

4. Results and discussion

In the sensitivity study we are running two sets of simulations. One set with realistic gravity and another set without initial gravity in terms of initial pressure defined according to pressure of initial fluid column. The case without initial gravity will correspond an extreme test case where the flow will be dominated by horizontal flow due to for

instance shale layers. Figures 1 and 2 show the results of a test case in which the initial pressure is 100 bar all over the structure and the initial filling is 100 % water. The structure is closed in top and bottom and kept open on the left side with a constant pressure of 100 bar. The injection pressure is 140 bar on the right hand side injection point in the middle of the block. As expected Calcite buffer the system, and even after 100 years most regions have pH above 5 except some regions close to the injection zone.
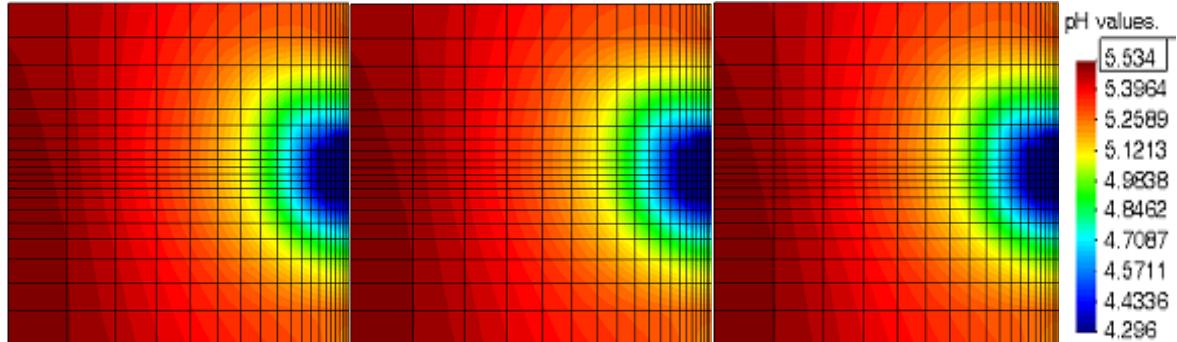
Fig. 1a   Fig.1b   Fig. 1c

Fig.1. Simulated results of pH values at the time points of 100 years after CO2 injected. From left porosities are 0.1, 0.2 and 0.3 respectively. The mineral compositions are the same in all simulations, 0.97 volume fraction of calcite, and 0.03 volume fraction of quartz.
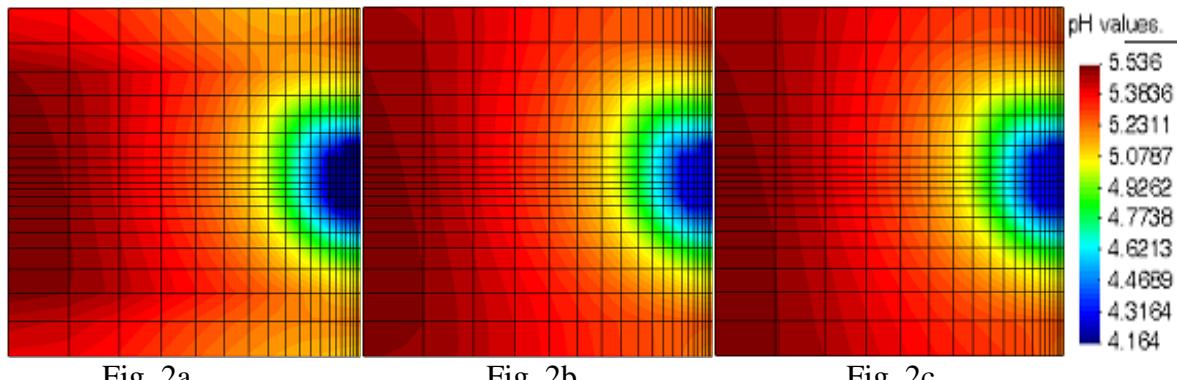

Fig. 2a   Fig. 2b   Fig. 2c

Fig.2. Simulated results of pH values at the time points of 100 years after CO2 injected. From left calcite percentages are 0.1, 0.5, and 0.97 respectively. The porosities are the same, 0.1.

Estimated fluxes and gas pressures after 100 years of injection are plotted in fig. 3a and fig. 3b respectively. The estimated principal stresses in xx and yy directions are plotted in figures 4a and 4b respectively. Positive direction for x is towards right and positive direction for y is upwards. Negative values for stress mean net stress opposite to these directions. The conditions for fracturing is based on a comparison between Terzaghi effective stress (stress in a particular direction plus local pressure in the same direction) and the tensile strength (breakdown stress). Properties of different Calcite will vary somewhat and we have not succeeded in finding any values for tensile strength which could be used. It is expected to be lower than ultimate strength, for which values of around 3 MPa is reported different places. This type of geomechanical analyses will be the same when considering geomechanical stability for necessary injection pressure and pressure needed for hydraulic fracturing in order to increase injectivity in formations with low permeability. Comparing the xx stress from (4a) and the overpressures which can be estimated from the local pressures (3b) there are some regions close to the border to the left which would involve fracturing. As expected from this horizontally directed flow example, with very little buyoncy due to no initial vertical pressure difference these are no geomechanical issues in the vertical direction, as can be seen from fig. (3b) and fig. (4).
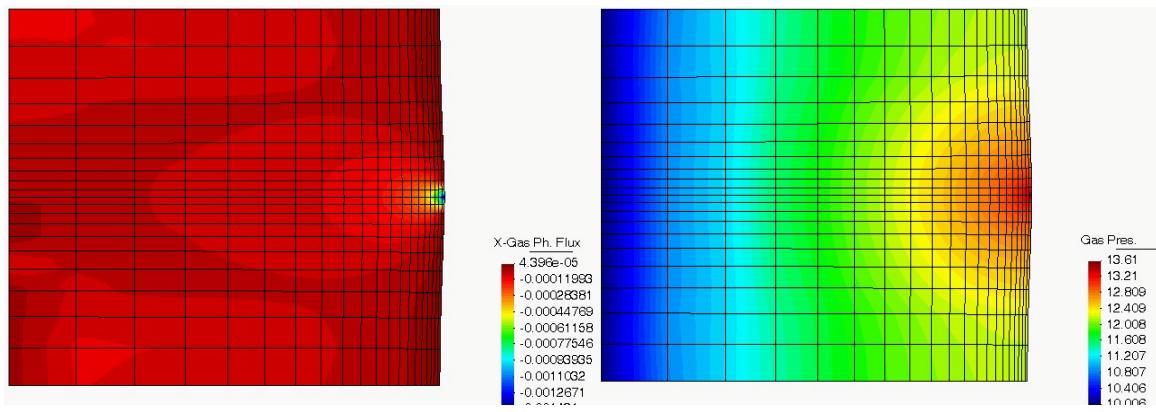
(3a)   (3b)

Fig. 3 Estimated gas flux in the x-direction in kg/s (3a) and gas pressure in MPa (3b) at 100 years
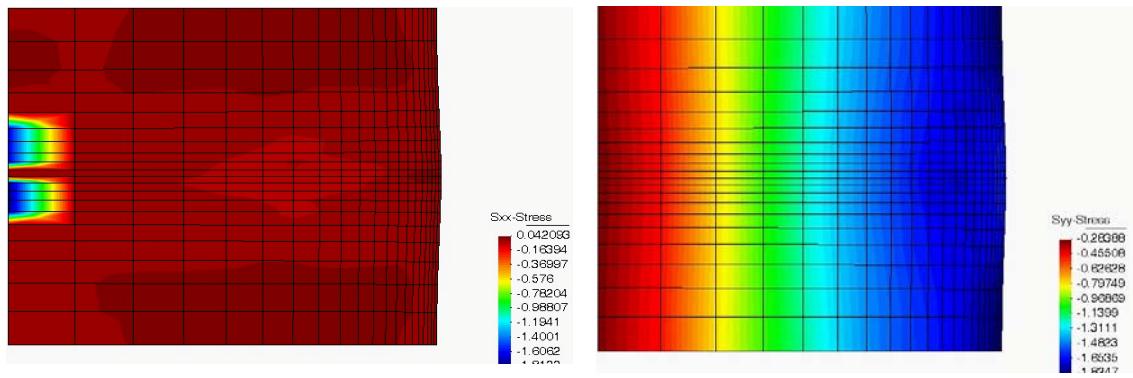
(4a)   (4b)

Fig. 4 Estimated stress distribution in xx (4a) and yy (4b) directions after 100 years of injection

5. Conclusion

A new reservoir storage simulator for CO_2 have been developed on the RetrasoCodeBright platform by inclusion of non-ideal gas description using an equation of state for calculation of gas solubility and incorporation of realistic fluid densities as function of local pressures and temperatures. The simulator contains state of the art geochemical descriptions and a great advantage is the implicit geomechanical module which enable simultaneous analyses of possible geomechanical implications for every time step and every region of the reservoir in consideration. Numerical algorithms have also been modified so as to ensure converged solutions for the high pressures relevant for storage of CO_2. A simple test case has been used to illustrate numerical solutions from the new CO_2 simulator.

6. Acknowledgements

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