Improved Newton Raphson Method – An Effective Tool in Solving Flow-Mechanic-Chemistry Equations of CO2 Storage in Saline Aquifers

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Abstract: - The geological storage of CO_2 in saline aquifers is believed to be one of the most promising ways to reduce the concentration of this greenhouse gas in the atmosphere. But the specific high pressure and temperature conditions at CO2 injection induces numerical challenges in solving the coupled flow, geo-mechanical, chemical dynamic equations when traditional Newton Raphson iteration method is adopted to solve these equations iteratively. Newton-Raphson method is highly efficient in the convergence speed. However, traditional Newton-Raphson method can tend to diverge due to a number of causes. The first problem is related to the need for good initial guesses. Unsuitable initial values will often redirect the iteration towards non-convergent solutions. make Another problem is that the system itself is not "well-behaviored", which means that the independent variables that need to be solved may be vibrating, or one or some of the variables are changing extremely fast. Reactive flow simulations in porous medium, with implicit geo-mechanical analysis, are very complex problems which suffer from both of these divergence problems. Here we present an improved Newton-Raphson method by adding an easily found optimum relaxation factor, which can guarantee that the solutions of the equations can be successfully found even when the conditions are extreme. The method is both effective and practical. In this paper we demonstrate the application of this mathematical tool in simulating CO2 storage in saline aquifers with code RCB (RetrasoCodeBright).

Key-Words: - Newton-Raphson method, Optimum relaxation factor, CO2 storage, Geomechanics, Geochemistry, Saline aquifer.

1 Introductions

1.1 Geological sequestration of CO2 in saline aquifers

The geological storage of greenhouse gas in deep saline aquifers can be one of the most promising options to reduce emissions of CO2 to the atmosphere. Besides natural effects of water vapour, CO2 is the major greenhouse effect contributor in the atmosphere [1]. 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 CO2 storage. Several CO2 storage projects are at present active, i.e. the SACS project [2] initiated 1998 in North Sea Utsira Formation reservoirs; the CO_2SINK project started in April 2004 at Ketzin in Germany have demonstrated the big potential of saline aquifers for long term CO2 deposits [3]. Additional projects for geological CO2 storage are planned for the near future.

To study the migration, transformation and to predict the ultimate long term fate of CO_2 injected we need to relate to modeling tool. Experiments and pilot plants, as well as real injection sites, can only be traced and monitored for a very limited number of years. These modeling tools have to incorporate all relevant chemical species of significance. Groundwater compositions and detailed mineral characterization is desirable for proper analyses. And since ions are transported with the "bulk" flow, as well as internally in each volumetric block by diffusion it is necessary to couple the implications of chemical reactions to multi-phase models for flow of brine, CO2 and transport of solutes in liquid by means of advection and diffusion. A common concern is whether the reservoir will be mechanically stable over the long time scales in consideration. Erosion of minerals in low pH zones may lead to collapse. Precipitation of minerals in other zones will change flow patterns and local pressures and also need to be clarified in terms of potential geo-mechanical consequences. From a geo-mechanical point of view the challenges ranges from fairly rigid problems over

to highly non-rigid geomechanical behavior, as is to be expected during outdrying and potential embrittlement of shale and clay in the cap rock zones.

In this work we focus on some typical numerical challenges which are encountered when solving the coupled dynamic equations related to simulations of reactive transport with implicit geo-mechanical analysis. We use simplified model reservoir systems so as to better be able to isolate and illustrate some critical aspects related to the numerical methods.

1.2 Numerical modeling code RCB

Several numerical codes for modeling reactive transport related to storage of CO2 in aquifers have been presented in recent years. Different perspectives from researchers, specific geological situations in the reservoirs, and different numerical algorithms distinguish the different codes. Most available codes for reactive transport related to CO2 storage are based on finite volume algorithms and if they have geo-mechanical couplings this is often as an explicit coupling to the reactive transport code. One limitation of this approach is that it may not capture appropriately the geo-mechanical issues which may happen rapidly. Another limitation is that most of these approaches have built in a finite element library which is needed for the communication with the geo-mechanical analysis but other than that the transfer of information between the reactive transport simulator and the geo-mechanical analyses may be too limited for non-linear geo-mechanical problems. Newton Raphson iteration method is the classical adopted approach for solving this kind of complicated coupled non-linear equations due to its high efficient convergence speed, if the solution converges.

To develop a new modeling code that fits for more common situations, the project “Observing the effect of long term CO2 storage in saline aquifers” is carried out in Department of Physics and Technology in University of Bergen. And as the centre of the project, code RCB (RetrasoCodeBright) has been chosen to be 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). Retraso (REactive TRAnsport of SOlutes) is a code for solving two-dimensional reactive transport problems (Saaltink et al., 1997).

Relative to many other available reservoir modeling tools, the implicit algorithm for the geomechanical analysis is a distinction which makes this code attractive as a basis for development of a state of the art simulator for CO2 storage scenarios. RCB code contains many significant features [4,5]. It is developed on

2 Working principles and problem in the original RCB code

2.1 Working principles

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 [4,5]. Both parts will be sequentially finished calculating in one time step. All the solutions from last time step will be the corresponding parameters sent to the iteration of next time step. A schematic flowsheet is illustrated in figure 1.

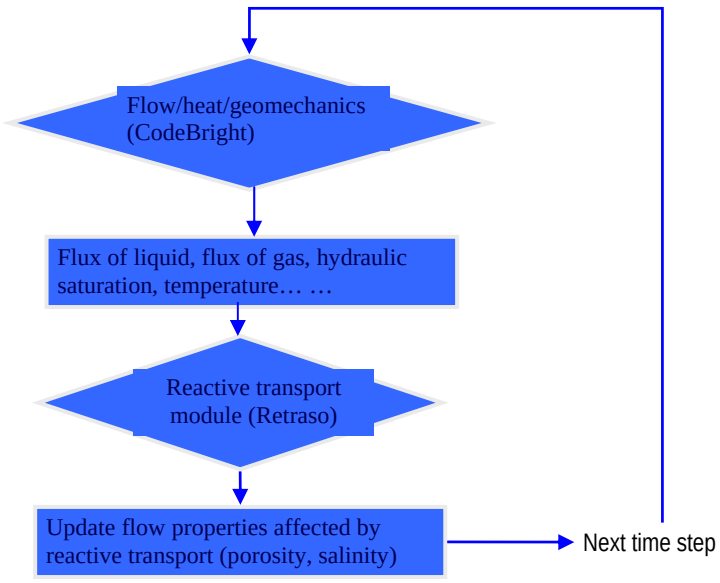


Fig. 1 RCB solves the integrated equations sequentially in one time step.

In flow/geomechanics part the mathematical equations for the system are highly non-linear and they will be solved numerically [6]. 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 Newton-Raphson method is adopted for an iterative scheme [6, 7].

In reactive transport part the numerical

scheme is similar with flow/geomechanics part. The chemical reactions which are being modeled are also solved using a Newton-Raphson approach.

The original RetrasoCodebright was written for ideal gas and had to be corrected for realistic fluid behavior. All density dependent terms concerning the CO2 phase have been corrected using a compressibility factor derived from an equation of state [8].

$$PV = ZnRT \qquad (1)$$

where Z is the compressibility factor, n is number of moles, P is pressure, V is volume, T is temperature and R is the universal gas constant (8.3143 J/moles K).

The corresponding correction of solubility of CO2 [9] follows well-known thermodynamic principles and through the use of the fugacity coefficient derived from the same equation of state (pure CO2 is assumed here) we arrive at Henry's law in the form of equation (2) below.

$$x_{co2}^{b} = \frac{P\phi}{H_{co2}} \exp\left\{ \frac{\overline{v}^{\infty}}{RT}(1-P) \right\} \qquad (2)$$

where ϕ is the fugacity coefficient for CO2 estimated from the SRK equation of state, H_{co2} is the Henrys law coefficient for CO2, P is pressure (bar), T is temperature (K), R is the gas constant, and $\overline{v}^{\infty}$ is the partial molar volume of CO2 at infinite dilution.

2.2 The divergence problem

Due to the implicit couplings between geo-mechanics and fluid flow we have chosen RCB as a platform for simulations of CO2 storage scenarios in saline aquifers. But unfortunately the original RCB code can not be used directly for our purpose. One of the reasons is that numerical solutions does not converge in the Newton-Raphson iteration scheme if CO2 injection pressure is higher than around 55 bar. In typical injection scenarios CO2 is injected at super-critical fluid conditions. For the Utsira case the injection pressure is close to 120 bar [2].

The divergence problem happens twice sequentially in RCB code. Actually the extreme high injecting pressure makes gas pressure, liquid pressure, and mechanical deformation etc. change extremely fast or unpredictable especially in the vicinity around the injection areas. Newton method fails first in CodeBright part, and then it fails again in Retraso part.

3 Improved Newton-Raphson method

3.1 General conventional Newton-Raphson method

In the context of this paper we only give a brief summary of the Newton-Raphson method [10]. This iterative method is used to determine the zero of a function. The finite element method leads to solve the equation:

$$[S(X)] \bullet X - Q = 0 \qquad (3)$$

where S is the global finite element matrix, X is the vector of nodal potentials in a finite element grid and Q is the forcing function vector.

If $R(X)$ is the nodal residual vector of equation (1) for a given X :

$$R(X) = S(X) \bullet X - Q \qquad (4)$$

Solving equation (1) is the same determining the zero of the function $R(X)$, that is to say finding the nodal potential vector X which satisfies:

$$R(X) = 0 \qquad (5)$$

It should be recalled that R and X are N -component vectors, N being the number of unknowns of the discretized problem.

R is a nonlinear function of X . If X^P is the current solution at the P -th step of iterative scheme, the solution at the next step is given by:

$$R(X^{P+1}) = R(X^P) + [\frac{\partial R^T}{\partial X}]^P \bullet (X^{P+1} - X^P) = 0 \qquad (6)$$

The matrix $[\frac{\partial R^T}{\partial X}]$, which is evaluated at each iteration, is called the Jacobin matrix. At each step the following linear problem is solved:

$$X^{P+1} - X^P = -([\frac{\partial R^T}{\partial X}]^{-1})^P \bullet R(X^P) \qquad (7)$$

Convergence is considered to have been achieved when the relative norm of the potential correction vector:

$$\Delta X^P = X^{P+1} - X^P \qquad (8)$$

is zero within a pre-specified tolerance [10].

3.2 Newton-Raphson scheme in CodeBright

Conventional Newton method is applied in CodeBright. When nonlinear hydro- mechanics system is analyzed using the conventional Newton-Raphson method, the iterative process often fails to provide convergent solutions [11,12]. This is the reason that RCB diverges for CO2 injection pressures higher than 55 bar.

The governing equations for non-isothermal multiphase flow of liquid and gas through porous deformable saline media are well established and the papers by Olivella et.al. [6, 7] and references therein may serve as examples of relevant literature in the filed. Variables and corresponding equations are listed in table 1.

n	**e name**	**e**
um of stresses	ments	
of liquid mass	ressure	
of gas mass	sure	
ce of internal energy	ture	

Table1. Equations and variables

After the spatial discretization of the partial differential equations, the residuals that are obtained can be written (for one finite element) as:

$$\begin{pmatrix} r_u \\ r_{Pl} \\ r_{Pg} \\ r_T \end{pmatrix} = \frac{d}{dt}\begin{pmatrix} d_u \\ d_{Pl} \\ d_{Pg} \\ d_T \end{pmatrix} + \begin{pmatrix} a_u \\ a_{Pl} \\ a_{Pg} \\ a_T \end{pmatrix} + \begin{pmatrix} b_u \\ b_{Pl} \\ b_{Pg} \\ b_T \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (9)$$

where **r** are the residuals, *d***d**/*dt* are the storage or accumulation terms, **a** are the conductance terms, and **b** are the sink/source terms and boundary conditions. After time discretization a more compact form can read as:

$$r\left(X^{k+1}\right) = \frac{d^{k+1} - d^k}{\Delta t^k} + A\left(X^{k+\varepsilon}\right)X^{k+\theta} + b\left(X^{k+\theta}\right) = 0 \quad (10)$$

where k is the time step index, : $\mathbf{X}=[(ux,uy,uz,Pl,Pg,T)_{(1)}, \ldots, (ux,uy,uz,Pl,Pg,T)_{(n)}]$, is the vector of unknowns (i.e. a maximum of seven degrees of freedom per node), **A** represents the conductance matrix. The Newton-Raphson scheme of solution for this non-linear system of AE's is:

$$\frac{\partial r\left(X^{k+1}\right)}{\partial X^{k+1}}\left(X^{k+1,l+1} - X^{k+1,l}\right) = -R\left(X^{k+1,l}\right) \quad (11)$$

where l indicates iteration. In the present approach, the standard Galerkin method is used with some variations in order to facilitate computations.

3.3 Improved Newton-Raphson method in code RCB

We rewrite equation (5) by introducing a relaxation factor α to improve Newton method in the case of scalar potential, as the following:

$$X_{new}^{P+1} = X^P + \alpha \bullet (X^{P+1} - X^P) \quad (12)$$

where P is the iteration number, α is between 0 and 1. If α is equal to 1, it is the conventional Newton method.

α is not unique. Commonly if the relaxation factor α which minimizes the total square residual for the Galerkin method is introduced at each step of the nonlinear iteration, convergent solution can be always obtained [11]. Therefore we call it as the optimum relaxation factor, marked as α_m . However usually it is very expensive in CPU time in determining α_m , because a large number of repeating calculations of square residual is required.

Fujiwara at al. [11] proposed a very efficient algorithm to quickly determine the optimal scalar magnetostatic vector potential to improve Newton-Raphson method. This algorithm is also suitable for improving the iterative processes in the CodeBright part as well as in the subsequent Retraso part.

Here we briefly describe the algorithm. We define the objective function W [13] which is the total square residual of the Galerkin method as follows:

$$W^{(k+1)} = \sum_{i=1}^{nu}\left\{G_i^{(k+1)}\right\}^2 \quad (13)$$

where k is the iteration step, nu is the number of unknown variables. The relaxation factor is determined so that the objective functions $W^{(k+1)}$ at the (k+1)-th step of the nonlinear iteration is less than $W^{(k)}$ at the previous step k as follows:

$$W^{(k+1)} < W^{(k)} \quad (14)$$

The relaxation factor which satisfies (12) is searched iteratively for by using the following equation:

$$\alpha^{(k)} = 1/2^n \qquad (n = 0,1,...,i) \qquad (15)$$

When (14) is satisfied, the iterative searching process stops, and the calculation of (15) changing n is determined at $n = i$. This robust method ensures not only that the optimal factor can be determined but also that it can be determined by a significantly less time consuming approach.

4 A 2D hydro-mechanical-chemical example

This example illustrates a simple 2D saline aquifer with CO2 injection case.

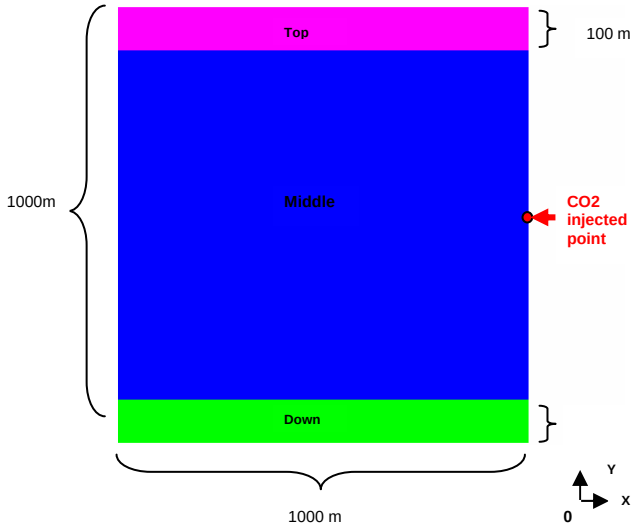


Fig.2 Geometry of the 2D reservoir and the CO2 injecting point

The geometry of this 2D domain is a 1000 m x 1000 m square. There are two different kinds of geological structures in the whole domain as illustrated with two different colors. The pink zone (Top) and green zone (Down) has the same geological structure. And the blue zone (Middle) has different geological structure. Each of "Top" and "Down" zones is a 1000m x 100m rectangular; while the blue zone is a 1000m x 800m rectangular. CO2 is injected into the middle point of the right boundary.

Initially, there is fine grained sand of pure calcite and its saturate solution in the "Middle" zone. In "Top" and "Down" zones, there are fine grained sand of 3% calcite and 97% quartz. The CO2 injecting pressure is 120 bar. Temperature does not change in the whole process. It is kept 25 Celsius in the whole area from the injection started.

The initial liquid pressure and gas pressure in the 2D reservoir are respectively 50 bar and 30 bar. Except the boundary on the left side, neither liquid nor gas can infiltrate through other boundaries. Except the boundary on the right side, every boundary has displacements restriction. It is assumed that there are no initial displacements and no initial stress in the whole area.

5 Results and discussions

The simulation results for hydraulic, mechanic movements and chemical transport in the 2D saline aquifer processed by improved RCB code can be visualized in GiD window [14]. Information about quite a few geomechanical and geochemical features can be got to know from this visual window. Here different evolution time points have been chosen at which some important features describing the changing in geometry, liquid and gas transport are illustrated for comparison for that CO2 is treated as ideal gas and a real fluid with gas density correction and CO2 solubility correction. They are liquid phase flux, pH value, porosity and stress.

Simulated results for the liquid flux 420 days after start of injection is plotted in fig.3. pH values after 13 days, 116 days and 420 days are plotted in figures 4, 5 and 6 respectively. Porosity and stress after 420 days are plotted in figures 7 and 8 respectively

5.1 Liquid phase flux

Example of simulated results for liquid phase flux is illustrated in fig. 3. Since the driving forces for flow is defined pressure differences we do not expect dramatic changes between ideal gas and realistic CO2 description for the liquid flux.

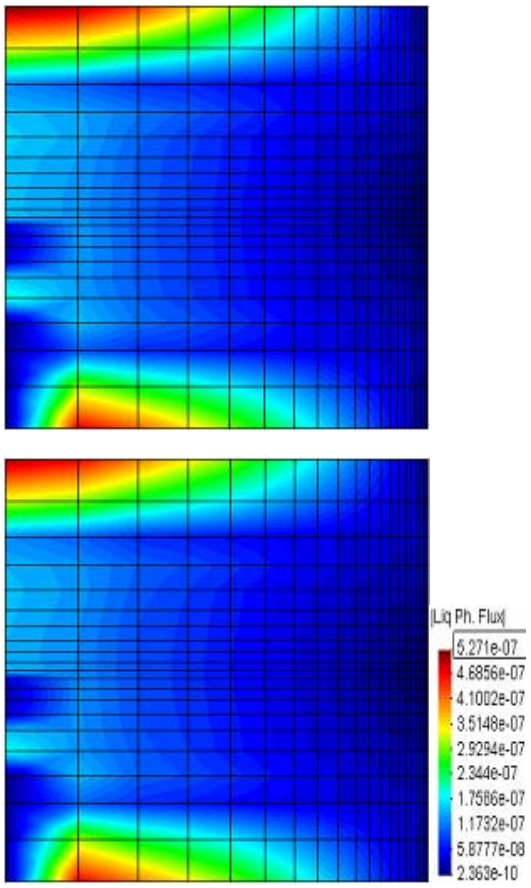


Fig.3 Plotted simulated results of liquid phase flux (m/s) at the time points of 420 days after CO2 injected. CO2 treated as ideal gas (top) and CO2 treated as real fluid (bottom).

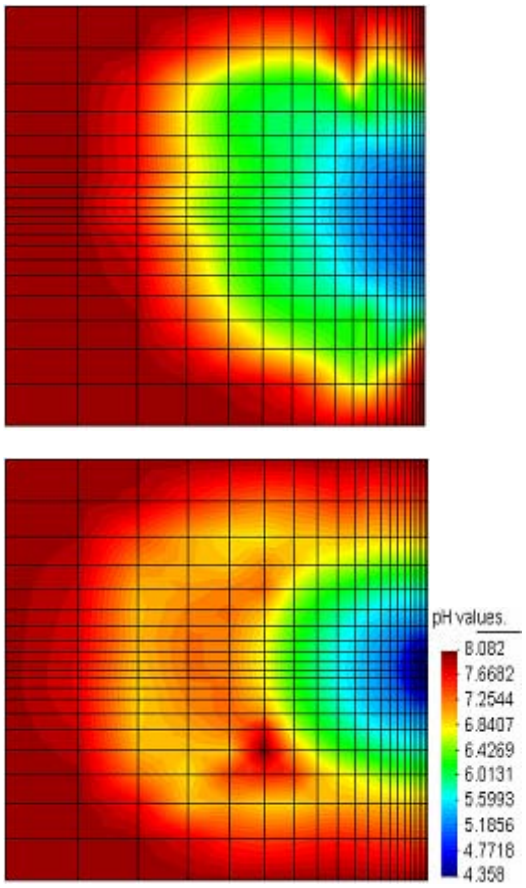
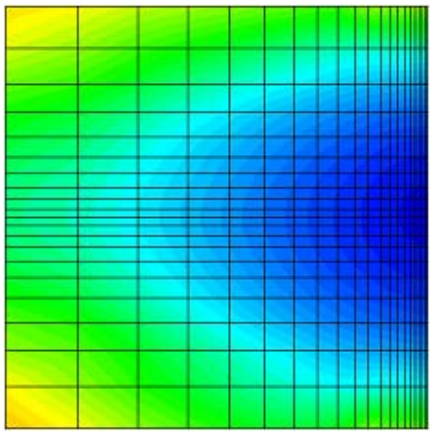


Fig.4 Plotted simulated results of pH values at the time points of 13 days after CO2 injected. CO2 treated as ideal gas (top) and CO2 treated as real fluid (bottom).

5.2 pH value

The difference in the pH between ideal gas description and real gas description is essentially in the fugacity coefficient which would imply that less CO2 is dissolved because the fugacity coefficient is less than unity in these conditions. This then also implies that the buffering effect due to calcite dissolution will be smaller in this case and larger regions of lower pH might be the case for the realistic fluid description versus the ideal gas description. On the other hand the mass of gas transport trough the reservoir will be larger for the realistic case versus the ideal gas and the total combination of these effects is what shows up in figures 4 – 6.



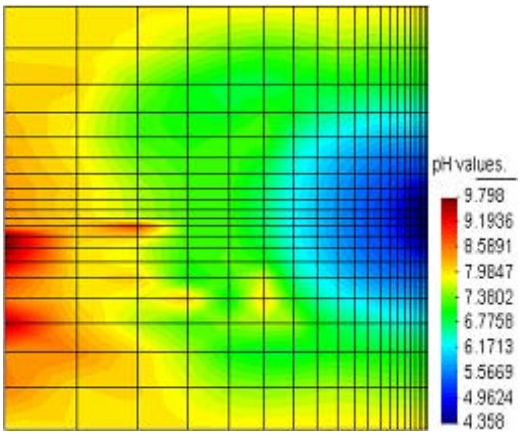


Fig.5 Plotted simulated results of pH values at the time points of 116 days after CO2 injected. CO2 treated as ideal gas (top) and CO2 treated as real fluid (bottom).

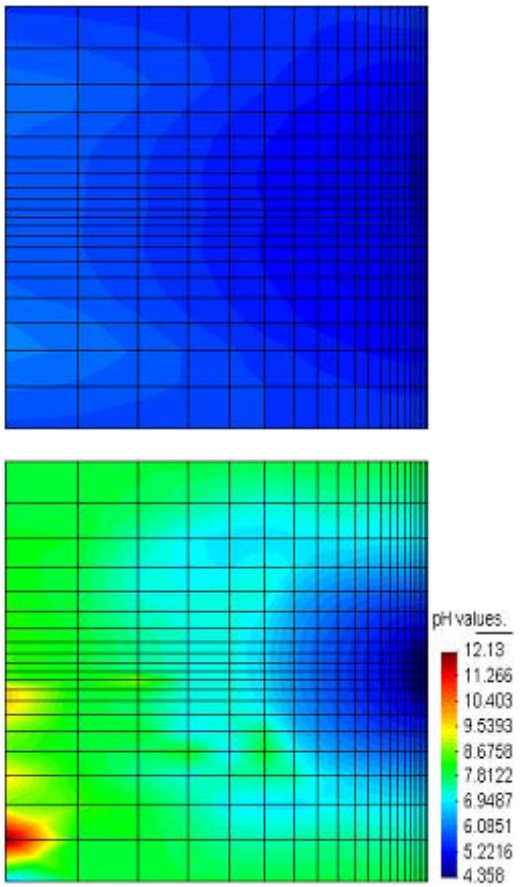


Fig.6 Plotted simulated results of pH values at the time points of 420 days after CO2 injected. CO2 treated as ideal gas (top) and CO2 treated as real fluid (bottom).

5.3 Porosity

For the limited times in consideration here the Calcite dissolution buffering still limits the erosion and the porositu changes are fairly limited, as illustrated in fig. 7 below.

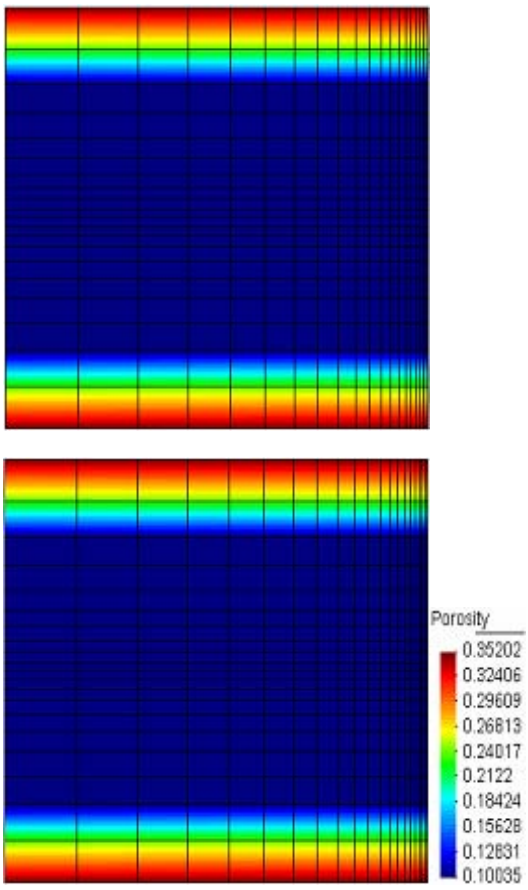


Fig.7 Plotted simulated results of porosity at the time points of 420 days after CO2 injected. CO2 treated as ideal gas (top) and CO2 treated as real fluid (bottom).

5.4 Stress

The estimated stress is plotted in fig. 8 and clearly shows the difference between the realistic description and the ideal gas case. In the ideal gas case there are some scattered regions close to the injection zone with fairly high stress. The realistic fluid description also shows a slightly enhanced stress level close to the injection zone but significantly less pronounced.

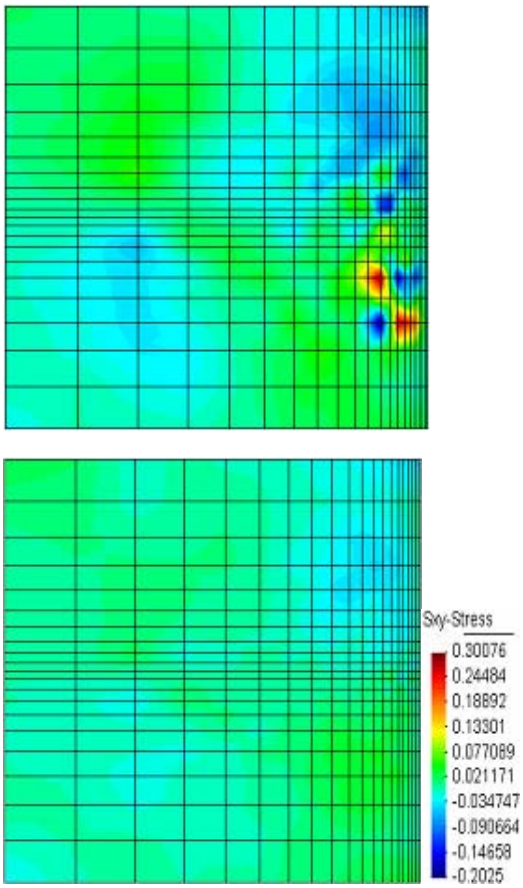


Fig. 8 Plotted simulated results of stress (MPa) at the time points of 420 days after CO2 injected. CO2 treated as ideal gas (top) and CO2 treated as real fluid (bottom).

By adjusting the time reduction factor in Newton-Raphson iteration process according to every different physical and chemical change in CO2 fluid condition and specific geology, the solution can be found without any divergent problem. And the simulation time is quite acceptable for us. It takes about 20 hours for improved code RCB to do the simulation for 100 years on the example above.

6 Conclusions

We have extended an ideal gas reservoir simulator into a realistic fluid simulator for CO2 reservoir storage simulations. In addition to the corrections for non-ideal gas in all density dependent terms as well as terms which depends on the fugacity of the fluid we have modified the algorithms for iterations in the module that solves for flow and geo-mechanics as well as the subsequent module for the reactive transport calculations.

By adjusting the time reduction factor in Newton-Raphson iteration process according to every different physical and chemical change in CO2 fluid condition and specific geology numerical solutions are achieved without any divergence problem. Simulation times are acceptable compared to final volume codes for simulations of CO2 storage scenarios.

Dissolution of calcite carbonate, the rapidly dissolving mineral, in the low pH regions leads to a buffering effect due to released carbonate ions that shifts the dissolution reactions towards less dissolved CO2. But the ions are transported with the reservoir fluid flow and the question is the balance between the buffering and the erosion due to dissolved carbonates and ion transport away from the vicinity of the injection region. As expected the differences between the ideal gas approximation and the realistic fluid description is significant. Within the simulated period the effects on porosity and stress is very limited but the ideal gas case appear to result in some regions close to the injection zone with relatively high stress compared to the realistic fluid case.

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