

Investigating the Impact of Caprock Morphology on CO₂ Plume Migration and Trapping Mechanisms Using the MRST-CO2lab and ECLIPSE-blackoil codes.

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Abstract

One of the possible options to mitigate the climate change is sequestering anthropogenic carbon in the deep saline aquifers. When injected in the formation, due to the difference in buoyancy forces between the gas and the brine, the free phase CO₂ is driven upwards and will eventually collect as a separate, thin layer beneath the caprock. Therefore, the structural geometry of this upper seal plays a significant role in the long-term CO₂ plume migration and trapping behaviour. In practice, at the kilometre scale, there are considerable topography changes, and the caprock structure is identified by domes and anticlines. Researchers primarily use 3D numerical simulators to study the long-term behaviour of the CO₂ plume. This study looks at the impact of the dipping and sinusoidal pattern between two strata on the storage process using a full 3D simulation as well as an upscaled model based on the vertical equilibrium (VE) assumption. The 3D simulation is performed using the ECLIPSE-blackoil and the MRST (MATLAB Reservoir Simulation Toolkit) is used for the VE approach. Under the VE assumption, the CO₂ plume flow in 3D can be approximated in terms of its thickness to obtain a 2D simulation model, which significantly decrease the computational cost and avoids the discretization error caused by limited vertical resolution in a 3D model. Over the time period simulated, our observations of lateral migration showed that the CO₂ and resident brine became quickly separated and formed two separate layers. To our knowledge, this is one of the first comparisons between the standard three-dimensional reservoir simulator and two-dimensional VE formulation for studying the impact of caprock morphology on CO₂ storage.

1. Introduction

Carbon capture and storage (CCS) is considered an important mitigation option in the context of reducing anthropogenic climate change. The principle is to capture the produced CO₂ from heavy industrial sources and securely store it into deep geological formations. Since the purpose is to permanently remove the stored CO₂ from the carbon cycle, it is therefore important to improve an understanding of the processes involved and develop confidence in its long-term carbon storage performance (Shariatipour, Pickup *et al.* 2014).

Typical aquifers are seen as thin, sometimes slightly tilted sheets, which extend to thousands of square kilometres. The injected supercritical CO₂ can be mobile and migrate long distances (potentially up to hundreds of kilometres) horizontally, while its vertical movement within the aquifer is just tens of metres, limited by the caprock (Shariatipour, Pickup *et al.* 2016). Moreover, under most relevant conditions, the density of the injected CO₂ is noticeably lower than the resident brine, which together with the disparity in lateral and vertical scales, results in a prompt vertical fluid segregation compared with the up-dip migration. In other words, while studying the plume migration from a long-term

perspective, we can assume that the fluids are fully segregated and are in vertical equilibrium (Nilsen, Lie *et al.* 2016a). In other words, we can ignore vertical flow, implying a static vertical pressure gradient which depends on the pore fluid specific gravity. (Bjørnarå, Mathias *et al.* 2014)

The VE model in MRST has been formulated with fully implicit solvers which are robust and more efficient and make it adaptable to the industry standards (Nilsen, Lie *et al.* 2016b). At timescales larger than the vertical segregation time, the VE assumption is approximately correct, making it suitable for large-scale, long-term simulations. It is worth to mention that VE-simulation does not necessarily introduce "more error" than a 3D simulation, but it introduces different types of errors. During the 3D simulation, a significant time was dedicated to solving the equations for the bottom layers which potentially have no CO₂ flowing in them, The VE approach reduces the dimension of the problem to 2D, which significantly reduces the computational cost, thus allowing the use of significantly higher lateral resolution, which increases the precision of the influence of caprock geometry. Analytical formulations are used to reconstruct the 3D solution from the upscaled 2D variables used in the VE formulation. While using the vertical equilibrium model, the CO₂ plume thickness is approximated to achieve a 2D depth-integrated simulation model. This assumption is common in several subdivisions of physics such as the Dupuit approximation, which states in an unconfined flat aquifer with a hydrostatic groundwater, the water flow is relative to the aquifer thickness (Bear 2013). Moreover, similar models were employed several decades earlier in the petroleum industry (Martin 1958, Coats, Nielsen *et al.* 1967, Martin 1968, Coats, Dempsey *et al.* 1971)

In the majority of the real storage cases, the CO₂ will be in a supercritical phase, which generally has a lower density than resident brine and consequently, tends to migrate upwards unless held back by different trapping mechanisms. The benchmark studies show that using modern methods in 3D numerical simulations is challenging and the important questions regarding the CO₂ sequestration cannot be predicted convincingly, even in a highly idealized problem (Nordbotten, Flemisch *et al.* 2012, Class, Ebigbo *et al.* 2009). Moreover, 3D simulators tend to underestimate the plume migration speed by more than 30% (Nilsen, Lie *et al.* 2016a), resulted by a remarkable difference in physical scales. While the lateral extension of the aquifer is typically measured in tens or hundreds of kilometres, the formation thickness is usually at the scale of tens to a few hundreds of meters. For long-term plume migration, the plume is dominated by gravity and capillary forces. The plume has already formed a thin layer caused by gravity segregation, which is relatively a short-term process. Therefore the important trapping and migration processes happen on a scale of a few metres or less, which highlights the importance of the high vertical resolution to capture the behaviour of the thin plume, while using a conventional 3D simulation (Vertical resolution does not have any impact on the VE simulations). Moreover, any resolution in the horizontal direction should be also high enough to resolve the unstable dynamics of convective dissolution.

Model information, especially the data representing the formation characteristics, always exhibit uncertainty in the 3D simulation of the CO₂ storage. The heterogeneity significantly changes the plume migration path regardless of the fluid driving force. Most of the aquifers in reality, such as Sleipner in the North Sea, have a complex layered structure, which due to the dearth of seismic information and the limited number of wells (i.e. observation), makes it impossible to achieve a detailed modelling of these structures. Therefore the geological models are fairly homogeneous and the plume migration on a long-term scale is mainly dominated by the caprock topography.

During this study, we have employed the MRST-CO2lab module (Bao, Lie *et al.* 2017) and the results are then compared with the ECLIPSE-blackoil simulator. The MRST (MATLAB Reservoir Simulation Toolkit) has been developed by the Computational Geoscience Group within the Department of Mathematics and Cybernetics at the division of SINTEF Digital. The CO2lab module of MRST contains a vertical equilibrium simulation model to facilitate the modelling of large-scale CO₂ migration. The implemented VE model in MRST includes the majority of the modelling features, and its effectiveness has been proven in previous studies (Nilsen, Herrera *et al.* 2011). The fact that the VE model has the same structure for multiphase fluid flow as traditional equations, makes it

possible to formulate them in a black-oil simulation framework. The goal is to show how VE and 3D simulation methods perform in models with various top surface morphologies.

2. Mathematical formulation

Here we present a brief comparison of mathematics beyond the VE and 3D simulations. Two components are present in basic modelling of CO₂ storage in aquifers, namely water (w) and gas (g). Mass conservation describes the flow dynamics,

$$\frac{\partial(\phi\rho_\alpha S_\alpha)}{\partial t} + \nabla \cdot \rho_\alpha u_\alpha = \rho_\alpha q_\alpha$$

where α denotes fluid phase (w or g), ϕ is porosity, ρ_α , S_α , u_α are fluid density, saturation and velocity, respectively, and q_α is the volumetric flux. Based on Darcy's equation the fluid velocity is,

$$u_\alpha = -k\lambda_\alpha(\nabla p_\alpha - \rho_\alpha g)$$

where k is the rock permeability, λ_α is fluid mobility, p_α is pressure and g is gravitational acceleration.

The governing equation in the vertical equilibrium method can be simply derived from the one presented earlier, by replacing all the parameter and variables with their vertically averaged counterparts. In order to make this discussion easier to follow, the equations represented here are based on the assumption that there is a sharp interface between the fluids, which is not necessarily the case in our simulation studies. The equation representing the conservation mass in VE models becomes,

$$\phi \frac{\partial h}{\partial t} + \nabla f(h) (u_t - k(\rho_w - \rho_g)\lambda_g(h)\lambda_w(H - h)g\nabla(z_t + h)) = q_g$$

where h represents the plume thickness, z_t is the depth of the top surface and u_t is the total volume flux which is given by Darcy's equation,

$$u_t = -k\lambda_t(h)(\nabla p_i - [\rho_w - (\rho_w - \rho_g)f_g(h)]g\nabla(z_t + h))$$

where p_i is the pressure at the interface of gas and water and f_g is the fractional flow function for gas phase which is given by, $f_g = \lambda_g/[\lambda_w(H - h) + \lambda_g(h)]$. It is worth to mention that the lambda used in the VE formulation are no longer the mobility used in the fine-scale formulation. This is an upscaled variables that is referred to as mobility for convenience, since it play a similar role in the upscaled equations (Nilsen, Krogstad, Andersen, Allen, & Lie, 2017).

3. Numerical simulations

3.1. Model setup:

In order to simulate the long-term behaviour of the CO₂ plume, a 15 (km)×15 (km)×0.1 (km) 3D closed boundary model has been considered. The contact boundary between the caprock and formation is based on four sinusoidal and two tangential functions in x and y-direction,

$$Z = A\sin(Bx) + A\sin(By) - R_x \sin(Cx) - R_y \sin(Cy) + x \tan(S_x) + y \tan(S_y) \text{ Eq.1}$$

where A, B and C are constant, R_x , R_y , S_x and S_y are variables which are unique for each case.

First two sinusoidal terms characterise the local domes which represent the structural traps (16 in total). The next two sinusoidal terms represent the small-scale topography variation on top of the caprock in both x and y directions, which in this paper we refer to a rugosity. It is worth mentioning that in the literature rugosity refers to a topography variation less than 10m; which is not evident in

seismic investigations but can be detected using LiDAR scanning of outcrops and geostatistical earth models (Pringle, Brunt *et al.* 2010, Jones, McCaffrey *et al.* 2009). As rugosity has a smaller wavelength than the structures representing the domes, C is considered to be much larger than B. The amplitude of rugosity in x and y directions which is represented by the R_x while R_y respectively, is one of the parameters in our sensitivity analysis. The next two terms provide the possibility of investigating a tilted aquifer, where S_x and S_y are the dip angles in the x or y directions, respectively. The base case model is flat, with no rugosity ($R_x = R_y = S_x = S_y = 0$). In order to analyse quantitatively how dipping and small scale structures affects the CO₂ storage process, 10 sets of geological models have been constructed using different rugosity and slope in the x and y directions. The amplitude of the dome is 40 m, having $R_{x,y} = 20$ adds a sinusoidal structure with an average amplitude of 20 m to the dome. Table 1 is a list of simulations parameters.

Table 1. List of simulation cases

Case #	R_x (m)	R_y (m)	S_x (rad)	S_y (rad)
1	0	0	0	$\pi/18$
2	0	0	$\pi/18$	0
3	0	20	0	$\pi/18$
4	0	20	$\pi/18$	$\pi/18$
5	20	0	0	0
6	20	0	$\pi/18$	0
7	20	0	$\pi/18$	$\pi/18$
8	20	20	0	$\pi/18$
9	20	20	$\pi/18$	0
10	20	20	$\pi/18$	$\pi/18$

Each of the geological models is then used as the basis for a simulation using MRST-VE and ECLIPSE-blackoil and their results are compared. CO₂ is injected through one centre injector for 10 years, followed by 1000 years of the post-injection period. The model is homogenous with a constant porosity and permeability throughout the reservoir. More information about the model is shown in Table 2.

Table 2. Model information

Parameter	Value
Reservoir Dimensions (NX×NY×NZ)	101×101×9
Rock compressibility (1/bars)	4.35 e-5
Water density at surface condition (kg/m ³)	1067.28
CO ₂ density at surface condition (kg/m ³)	1.87
Salinity (ppm)	150000
Residual water saturation (S_{rw})	0.27
Residual CO ₂ saturation (S_{rc})	0.20
Permeability (mD)	500
k_v/k_h	0.1
Porosity	0.2
Pressure at the 1500 m depth (bar)	147

3.2. Simulation results

The CO₂ plume saturation in the top cells of the two models (base case and case number 10) at the end of simulation is presented in Figure 1. Capillary forces are not considered in this study. The simulations in ECLIPSE and MRST have been performed using fully implicit formulations. Overall there is a good agreement between the results from the ECLIPSE blackoil simulator and vertical equilibrium in the MRST. The plume speed is seen to be higher in the VE model which could be partially due to the earlier segregation, and partially due to the numerical diffusion caused by limited vertical resolution in the 3D model. The other reason is that unless linear relative permeability curves are used, 3D simulators tend to underestimate the migration speed of gas plumes that are thin relative to the vertical resolution employed. This phenomena can be seen in Figure 1, resulting in lower residual trapping in the plume path.

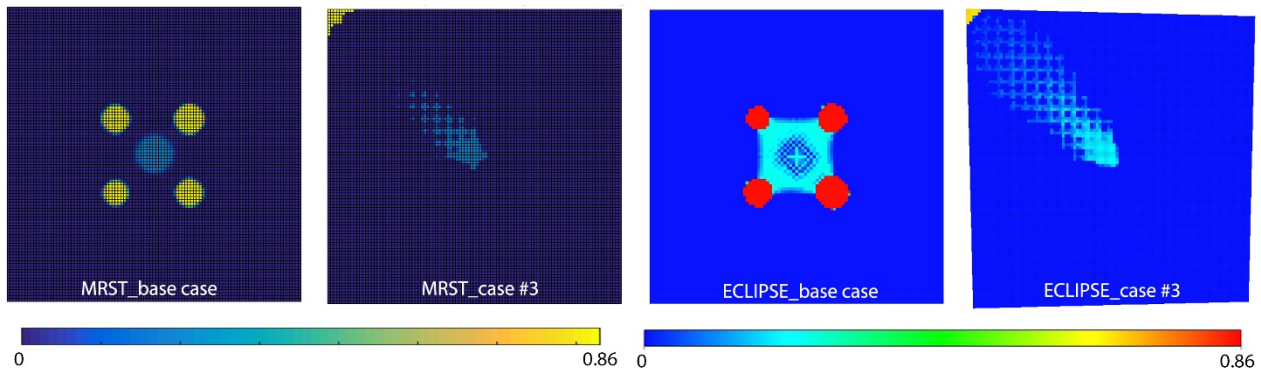


Figure 1. CO₂ saturation profile at the end of simulation in the base case and case number 10 in ECLIPSE and MRST.

The percentage of CO₂ dissolution for all the cases is presented in Figure 2. Here, we have investigated the amount of dissolved CO₂ at the end of injection (Figure 2a) and simulation (Figure 2b). The results indicate that there is a large discrepancy at early times, which is likely caused by the VE assumption not being approximately valid at this point. The figures clearly confirm this statement, as while there is a significant difference between the results of the two methods at the end of injection (Figure 2a), the results are more aligned at the end of the simulation. Moreover, the lower migration speed 3D simulation results in a higher contact time between the plume and brine which eventually increases the dissolution (Figure 2b).

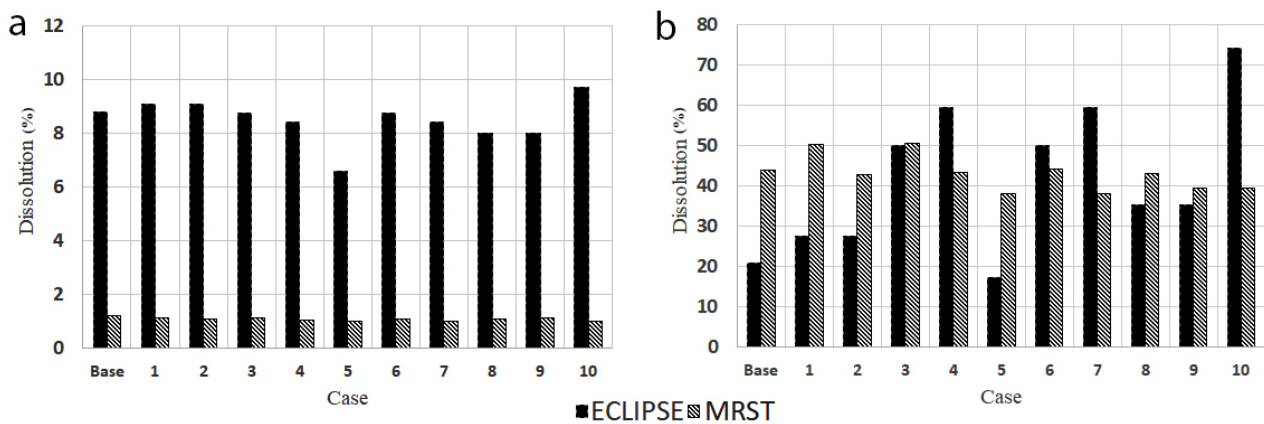


Figure 2. CO₂ dissolution in the aquifer (percentage), at the end of injection (a) and simulation (b) for all the cases.

In the cases in which the model is tilted in both x and y directions (4, 7 and 10), the dissolution calculated by ECLIPSE-blackoil is higher than the MRST. As mentioned earlier, in VE the plume migrates upwards more rapidly which decreases the interaction time with the resident brine and

therefore lowers the extent of dissolution. When the model is tilted from both sides, the resulted buoyancy force also accelerates the upward migration is reduced. In Case 3, where the plume migration path is perpendicular to the rugosity orientation, the plume speed is reduced and as a result, the interaction time between the CO₂ and brine increases, resulting in similar a dissolution in the VE and blackoil. The same statement is applicable to Case 6. Therefore, as far as the model is not tilted diagonally and the rugosity is perpendicular to the migration path, the amount of dissolution seen using both simulators is almost identical.

Due to the buoyancy force resulting from its lower density in comparison to the resident brine, the injected CO₂ spends the majority of the time beneath the caprock. Keeping all the parameters constant, except the caprock shape, it is possible to investigate the impact of the top morphology on the CO₂ storage process. Results show that adding a relatively small scale structural relief to the top surface of model decreases the dissolution (Case 5 vs base case), which is due to the plume being immobilized before it collects at the boundary resulting in less interaction with resident water. On the other hand, dissolution is seen to be higher in the tilted models (Cases 6 and 7 vs 5), due to the plume migrating farther to eventually dissolve in less saturated brines in zones far from the injection point.

The simulation time for each model is presented in Figure 3. As expected, the minimum computation time is for the base case and increased due to the additional complexity resulting from rugosity and slope. The MRST-VE tool has a lower computational cost and is almost three times faster than the ECLIPSE-blackoil simulator. This computationally lightweight approach enables a more extensive exploration of uncertainty.

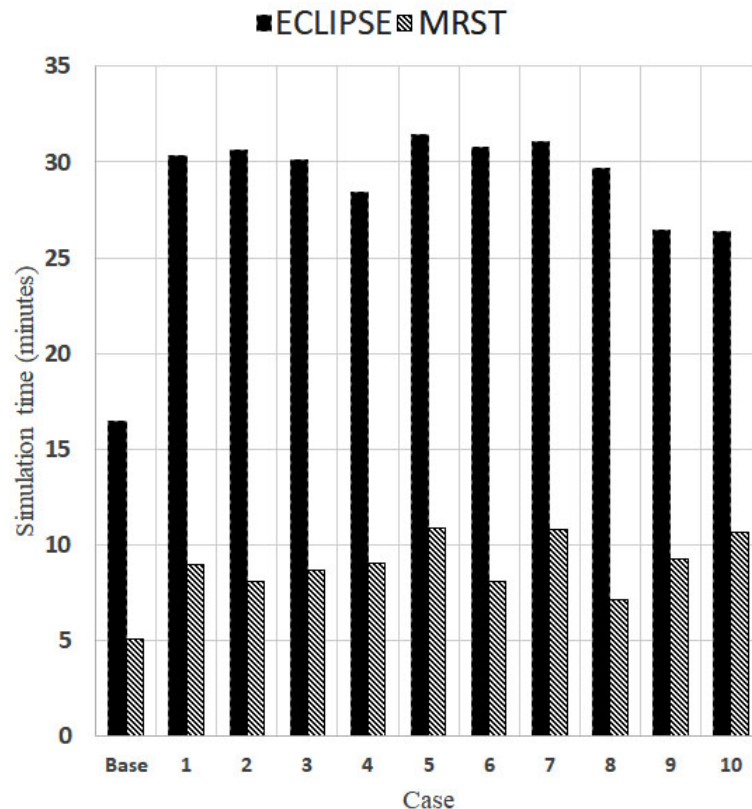


Figure 3. Simulation time for all the cases

4. Conclusion

The VE model is seen to be more appropriate in the long-term and the results show a good match between the final saturation profiles of the CO₂ plume in the two simulation methods. The computational cost for the MRST-VE model is significantly lower than ECLIPSE-blackoil one, which

provides the possibility of studying more complex models. The dissolution is seen to increase in tilted models while additional rugosity results in a lower dissolution.

The results indicate the feasibility of vertical equilibrium models for the simulation of CO₂ migration, and hopefully, this approach will be employed more in the future for the development of simulators. Possible future investigations would be to use the VE and compositional models in ECLIPSE to undertake a comprehensive study on the feasibility of VE module in MRST for simulating CO₂ storage process in the saline aquifers.

5. Acknowledgement

The authors would like to thank the Centre for Fluid and Complex Systems at Coventry University for providing financial support for this project. The authors also wish to thank Schlumberger for the use of the ECLIPSE software and SINTEF for the use of MRST. Special thanks also to Dr Odd Andersen and Dr Phil Costen for reviewing the paper and sharing their constructive comments with us.

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