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## Field-case simulation of CO<sub>2</sub>-plume migration using vertical-equilibrium models

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### Abstract

When injected in deep saline aquifers, CO<sub>2</sub> moves radially away from the injection well and progressively higher in the formation because of buoyancy forces. Analyses have shown that after the injection period, CO<sub>2</sub> will potentially migrate over several kilometers in the horizontal direction but only tens of meters in the vertical direction, limited by the aquifer caprock [1, 2]. Because of the large horizontal plume dimensions, three-dimensional numerical simulations of the plume migration over long periods of time are computationally intensive. Thus, to get results within a reasonable time frame, one is typically forced to use coarse meshes and long time steps which result in inaccurate results because of numerical errors in resolving the plume tip.

Given the large aspect ratio between the vertical and horizontal plume dimensions, it is reasonable to approximate the CO<sub>2</sub> migration using vertically averaged models. Such models can, in many cases, be more accurate than coarse three-dimensional computations. In particular, models based on vertical equilibrium (VE) [3] are attractive to simulate the long-term fate of CO<sub>2</sub> sequestered into deep saline aquifers. The reduced spatial dimensionality resulting from the vertical integration ensures that the computational performance of VE models exceeds the performance of standard three-dimensional models. Thus, VE models are suitable to study the long-time and large-scale behavior of plumes in real large-scale CO<sub>2</sub>-injection projects [4, 1, 2, 5]. We investigate the use of VE models to simulate CO<sub>2</sub> migration in a real large-scale field case based on data from the Sleipner site in the North Sea. We discuss the potential and limitations of VE models and show how VE models can be used to give reliable estimates of long-term CO<sub>2</sub> migration. In particular, we focus on a VE formulation that incorporates the aquifer geometry and heterogeneity, and that considers the effects of hydrodynamic and residual trapping. We compare the results of VE simulations with standard reservoir simulation tools on test cases and discuss their advantages and limitations and show how, provided that certain conditions are met, they can be used to give reliable estimates of long-term CO<sub>2</sub> migration.

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### 1. Introduction

Carbon capture and storage (CCS) is a promising technology for reducing CO<sub>2</sub> emissions to the atmosphere. To become an effective part of the solution to the climate problem, CCS technology will have to be applied at a very large scale to store a significant part of the increasing CO<sub>2</sub> emissions [6]. CO<sub>2</sub> injection into deep saline aquifers would provide large volumes to store CO<sub>2</sub>. Investigations of the risk of CO<sub>2</sub> leakage from the aquifers will require simulations that consider large temporal and spatial scales and because of the inherent uncertainty of geological characterizations, simulation of multiple realizations of a given storage scenario will be required for risk analysis. This is the main motivation for the development of fast simulation tools.

The CO<sub>2</sub>-brine system is simpler than the fluid system used in the oil industry, where black-oil or component-based formulations are standard. In particular, it is expected that at typical injection conditions, strong gravity segregation will occur over relatively short time-scales because of the large density differences between the resident brine and the injected supercritical CO<sub>2</sub>. This feature of the flow system can be used to develop fast simulation tools particularly tuned for simulating the long-term migration of the injected CO<sub>2</sub>.

Models based on a vertical equilibrium (VE) assumption have been used for long time to describe flow in porous media. Dupuit's approximation, which is commonly used in groundwater hydrology, is an example of this kind of models. In the oil industry, VE models were extended during the 50's and 60's to simulate two-phase and

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three-phase vertically segregated flows [7, 8, 9]. The interest in VE models diminished as computational resources increased. However, interface models for scenarios with strong gravity segregation (like steam injection) were also an active research area in the 80's and 90's [10, 11].

In recent years, there has been a renewed interest in VE methods as a means to simulate large-scale CO<sub>2</sub> migration, for which a sharp-interface assumption with vertical equilibrium may be reasonable. Many authors have developed analytical solutions to study different aspects of CO<sub>2</sub> injection, assuming rapid vertical segregation and vertical equilibrium [12, 4, 1, 13, 14, 15, 16]. In particular Gasda et al. [17], extended a VE formulation with sub-scale analytic functions and demonstrated the potential of using a VE formulation to speed up simulations of CO<sub>2</sub> migration. Numerical calculations using a VE formulation compared well with full 3D simulations in a recent benchmark study [18].

Herein, we investigate the use of VE models for a realistic large-field case based on data from the Sleipner site. Our calculations consider the effects of hydrodynamic and residual trapping. We discuss the potential and limitations of VE models and show how VE models can be combined with standard methods to give reliable results both for the plume development (injection stage) and plume migration (post injection). Particularly, we focus on a model that incorporates the aquifer geometry and heterogeneity in a flexible way that enables us to utilize 3D simulations whenever needed, for example, for the injection period in heterogeneous reservoirs. To investigate large-scale CO<sub>2</sub>-injection projects with realistic rock properties over long time periods, it is crucial to reduce the computational cost. VE models enables this by using analytical solutions to capture the vertical features in the flow system, thereby reducing the dimensionality of the problem. Achieving the same in a three dimensional simulation requires prohibitively high vertical resolution.

The main objective of this paper is to compare simulations of CO<sub>2</sub> migration in the Utsira formation in the North Sea using a standard three-dimensional reservoir simulator and two-dimensional VE formulations. To our knowledge, this is one of the first comparisons between full-3D and VE calculations for a real CO<sub>2</sub> injection site. Our aims are to demonstrate the benefits of using a VE model to simulate CO<sub>2</sub> migration in a realistic setting and to discuss how VE models can be used to develop fast techniques to simulate CO<sub>2</sub> injection at the basin scale.

## 2. Mathematical formulation

In this section we present a brief summary of the derivation of a vertical equilibrium formulation. A more thorough derivation can be found in [19]. First, we assume that CO<sub>2</sub> migration in saline aquifers can be modeled as a two-phase problem with brine and CO<sub>2</sub> as the wetting (*w*) and non-wetting (*n*) fluids, respectively. Furthermore, we consider the evolution of a CO<sub>2</sub> plume in an aquifer whose mean direction makes a constant dip angle  $\theta$  with the horizontal plane as shown in Figure 1. We start the derivation by writing a mass conservation

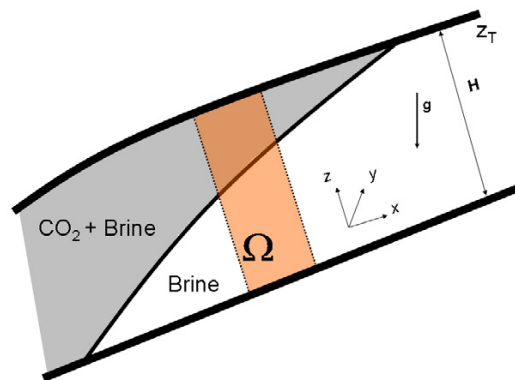


Figure 1: Schematic of the CO<sub>2</sub> plume and aquifer considered to derive a vertical equilibrium formulation for CO<sub>2</sub> migration.

equation for each fluid phase inside control volume  $\Omega = \Delta x \Delta y H$  to obtain

$$\frac{\partial}{\partial t} \int_{\Omega} \phi s_{\alpha} + \int_{\partial\Omega} \mathbf{f}_{\alpha} = \int_{\Omega} q_{\alpha}, \quad (1)$$

where  $s_{\alpha}$  is the core-scale saturation of phase  $\alpha$ ,  $\phi$  is the rock porosity,  $\mathbf{f}_{\alpha}$  are the fluid fluxes that pass through the control volume boundaries and  $q_{\alpha}$  represents source and/or sink terms. Taking the limit  $\Delta x, \Delta y \rightarrow 0$  and

assuming no flow perpendicular to the top and bottom of the aquifer, we obtain

$$\frac{\partial}{\partial t} \int_0^H \phi s_\alpha dz + \nabla_{\parallel} \cdot \int_0^H \mathbf{u}_\alpha^H dz = \int_0^H q_\alpha dz, \tag{2}$$

where  $\mathbf{u}_\alpha^H = (u_\alpha^x, u_\alpha^y)$  and  $\nabla_{\parallel} = (\partial/\partial x, \partial/\partial y)$  are two-dimensional vectors in the aquifer plane. The second term on the left hand side includes the vertical integral of the horizontal velocity of the fluid. Applying the generalized Darcy’s law we have that  $\mathbf{u}_\alpha^H = -k\lambda_\alpha (\nabla_{\parallel} p_\alpha - \rho_\alpha \mathbf{g}^H)$ , so that,

$$\int_0^H \mathbf{u}_\alpha^H dz = - \int_0^H k\lambda_\alpha (\nabla_{\parallel} p_\alpha - \rho_\alpha \mathbf{g}^H) dz. \tag{3}$$

Here  $k$  is the permeability of the medium,  $\lambda_\alpha$  and  $\rho_\alpha$  are the mobility and density of phase  $\alpha$ , respectively; and  $\mathbf{g}^H$  is the projection of gravity onto the aquifer plane. To evaluate (3), we assume that [3]: i) the velocity component perpendicular to the aquifer plane is very small, and ii) the fluid density in each phase is constant. Hence the fluids are in hydrostatic equilibrium in the vertical direction. Then, pressure in each fluid phase can be written in terms of the fluid pressure at the top of the aquifer and the elevation of the top of the aquifer ( $z_T$ ), i.e. we take the caprock surface as a datum level to measure fluid pressures. Then, the pressure gradient in the aquifer plane can be evaluated as,

$$\nabla_{\parallel} p_\alpha = \nabla_{\parallel} P_\alpha - g_z \rho_\alpha \nabla_{\parallel} z_T. \tag{4}$$

Next, we define the set of vertically integrated variables and parameters listed in Table 2. Substituting (4)

Table 1: Vertically-averaged variables and parameters.

Parameter	Expression	Parameter	Expression
Gravity	$\mathbf{G} = g_z \nabla_{\parallel} z_T + \mathbf{g}^H$	Velocities	$\mathbf{U}_\alpha = \frac{1}{H} \int_0^H \mathbf{u}_\alpha^H dz$
Porosity	$\Phi = \frac{1}{H} \int_0^H \phi dz$	Saturations	$S_\alpha = \frac{1}{\Phi H} \int_0^H \phi s_\alpha dz$
Permeability	$K = \frac{1}{H} \int_0^H k dz$	Pressures	$P_\alpha = p_\alpha(z_T)$
Mobilities	$\Lambda_\alpha = \frac{1}{KH} \int_0^H k \lambda_\alpha dz$	Sources/Sinks	$Q_\alpha = \frac{1}{H} \int_0^H q_\alpha dz$

into (3) and the vertically integrated parameters into (2), we obtain a mass conservation equation for the vertically integrated fluid saturations  $S_\alpha$ . Table 2 shows a comparison between the original 3D equations and their vertically integrated equivalents.

Table 2: Equations that define the full 3D and 2D vertical equilibrium (VE) models.

3D	2D
$\frac{\partial(\phi s_\alpha)}{\partial t} + \nabla \cdot \mathbf{u}_\alpha = q_\alpha$	$\Phi \frac{\partial S_\alpha}{\partial t} + \nabla_{\parallel} \cdot \mathbf{U}_\alpha = Q_\alpha$
$\mathbf{u}_\alpha = -k\lambda_\alpha (\nabla p_\alpha - \rho_\alpha \mathbf{g})$	$\mathbf{U}_\alpha = -K\Lambda_\alpha (\nabla_{\parallel} P_\alpha - \rho_\alpha \mathbf{G})$
$s_w + s_n = 1$	$S_w + S_n = 1$
$\lambda_\alpha = \lambda_\alpha(s_w)$	$\Lambda_\alpha = \Lambda_\alpha(S_w)$
$p_c = p_n - p_w = p_c(s_w)$	$P_c = P_n - P_w = P_c(S_w)$

The last step in the derivation of the vertically integrated model is to evaluate the vertically integrated mobilities ( $\Lambda_\alpha$ ) and capillary pressure ( $P_c$ ) as function of the vertically integrated saturations ( $S_\alpha$ ). Assuming hydrostatic pressure distribution, so that  $p_n(z) = P_n - \rho_n g_z(z_T - z)$  and  $p_w(z) = P_w - \rho_w g_z(z_T - z)$ , we have that by definition capillary pressure as function of elevation can be computed as [3],

$$p_c(z) = p_n(z) - p_w(z) = P_n - P_w - \Delta\rho g_z(z_T - z) \tag{5}$$

where the capillary pressure at the top of the aquifer is a function of the wetting saturation at  $z_T$ ,  $P_c = P_n - P_w = p_c(s_w(z_T))$ . Then, given the wetting saturation at the top of the aquifer,  $s_w^T = s_w(z_T)$ , we can get a reconstruction of the fine scale saturation as function of  $z$  evaluation the inverse function of  $p_c(z)$ , to obtain,

$$\hat{s}_\alpha(z) = p_c^{-1}(p_c(z; s_w^T)) \tag{6}$$

Notice that  $\hat{s}_w(z)$  is not the true fine scale saturation but the one by assuming hydrostatic fluid pressure distribution in the vertical direction. Now, the vertically integrated constitutive relations can be directly computed by evaluating,  $S_\alpha = S_\alpha(\hat{s}_\alpha(s))$ ,  $\Lambda_\alpha = \frac{1}{KH} \int_0^H k \lambda_\alpha(\hat{s}_w) dz$  and  $P_c = p_c(s_w^T)$ .

### 3. Numerical simulations

In this section we compare a 3D and a VE model to simulate CO<sub>2</sub> migration in the Utsira Sand aquifer, which is a major saline aquifer in the North Sea, into which CO<sub>2</sub> separated from gas extracted from the overlying Sleipner field has been injected at a rate of approximately 1 Mt/year since 1996 [20, 21]. The Utsira Sand extends for more than 400 km in north-south direction and between 50 and 100 km in the east-west axis, covering an area of approximately  $2.6 \cdot 10^4$  km<sup>2</sup> [21]. The geometry of the aquifer is irregular and complex. While the top surface is undulatory and varies smoothly in the depth range of 550-1500 m, the bottom is more complex with multiple domes of up to 100 m high and 1–2 km wide. The aquifer thickness ranges from 300 m near the CO<sub>2</sub> injection site to 200 m farther north (200 km from the injection site). The reservoir caprock is several hundred meters thick and comprises several units of low permeability materials (shales, glacio-marine clay, and glacial till) [21]. Geophysical logs indicate that the main reservoir has a proportion of clean sand between 0.7 and 1.0 with a small shale fraction composed by multiple thin (~1 m) layers that constitute vertical flow barriers. The interpretation of seismic surveys, performed periodically since the CO<sub>2</sub> injection started, indicate that such shale layers have a major impact on the CO<sub>2</sub> migration because a significant part of the rising CO<sub>2</sub> has been trapped underneath these low permeability layers forming multiple quasi-independent plumes [20, 22]. Analyses of core samples of the Utsira formation sand have estimated porosity values between 35 % and 40 % and permeability in the range 1000-3000 mD [21].

#### Model setup

Numerical simulations were performed using a preliminary numerical model setup by the Statoil R&D group [23] to study how CO<sub>2</sub> migrates once it reaches the upper-most sand layer. Thus, the model includes the section of the aquifer immediately underneath the caprock and above the upper most shale layer as shown in Figure 2. The domain covers an area of approximately 60 km<sup>2</sup> and has an average thickness of 25 m. The numerical grid includes 120,000 hexahedral cells with constant 50 m spacing in the horizontal directions and average 5 m spacing in the vertical direction. Estimated permeability values for the top sand layer and caprock are shown in Figure 2. In the model the horizontal components of the permeability tensor are assumed isotropic and vary between 1789 and 2018 mD, while the vertical component is assigned as equal to 1/10th of the horizontal value. Because of the relative low permeability of the caprock and the underlying shale relative to the main sand aquifer, they are modeled as impermeable boundaries. The porosity of the aquifer sand was set according to a linear correlation with the permeability and has a mean value equal to 0.36. The amount of CO<sub>2</sub> that reaches the top of the aquifer was simulated as a point source with specified injection rates that increase from 0 to  $5 \cdot 10^6$  m<sup>3</sup>/year during the first 32 years and then set to zero until the end of the simulation (132 years). The total amount of CO<sub>2</sub> injected is  $5.3 \cdot 10^6$  m<sup>3</sup> at reservoir conditions.

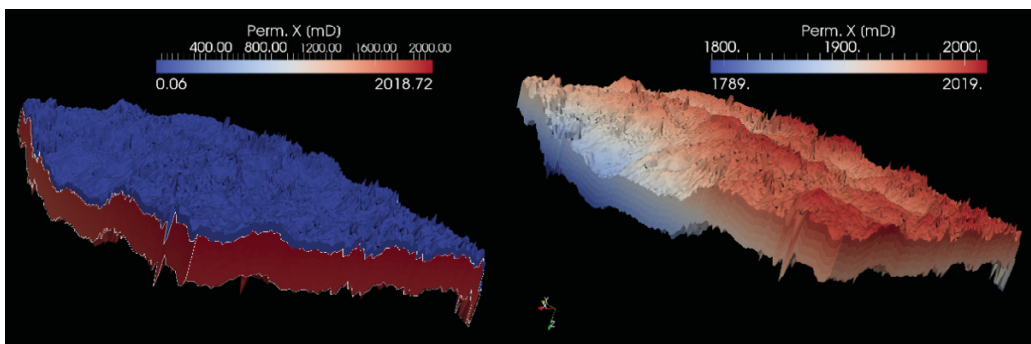


Figure 2: Estimated horizontal permeability for the upper 25 m of the Utsira Sand aquifer and lower 10 m of the caprock. There are large contrasts in permeability between the main aquifer and the caprock (left), but only moderated differences within the aquifer itself (right).

#### Simulation results

We present results of 3D and VE simulations carried out with the commercial ECLIPSE Reservoir simulator [24] and the VE module of the open-source Matlab Reservoir Simulation Toolbox (MRST) developed at SINTEF ICT and available at <http://www.sintef.no/Projectweb/MRST/>. In the following discussion we will refer to the different numerical solutions as ECLIPSE-3D, ECLIPSE-VE and MRST-VE. To test the sensitive of the 3D solution with respect to the vertical discretization, we run the ECLIPSE-3D simulations using the original grid (coarse) and a refined grid (fine) that has five times more horizontal layers than the original one. Capillary forces were not included in the simulations presented below, however, as explained above, they can be easily included in the VE formulation without introducing additional computational complexity [9, 25]. The 3D simulations

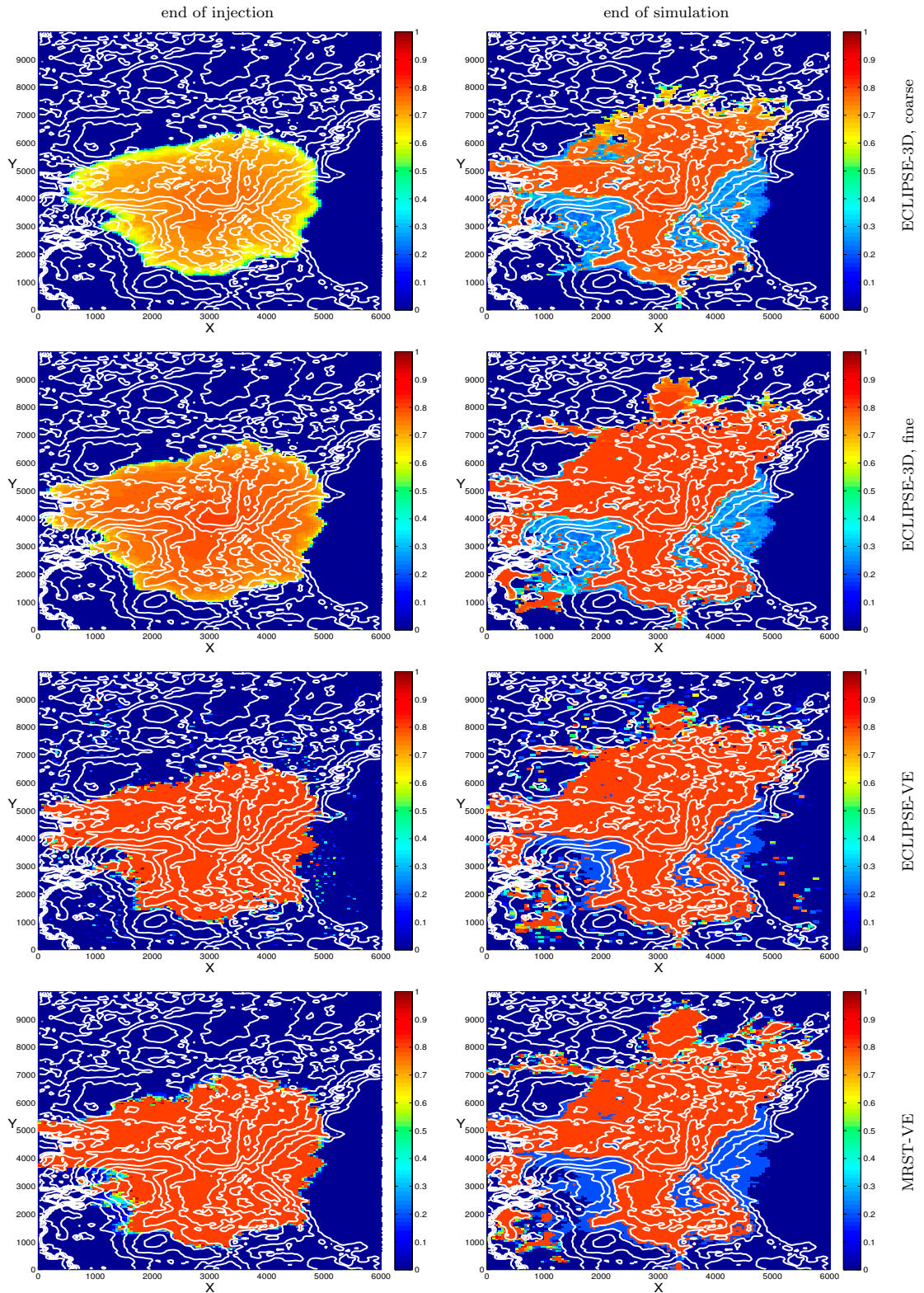


Figure 3: CO<sub>2</sub> saturation in the top cells at the end of injection (left column) and at the end of simulation (right column). Saturations computed with ECLIPSE-3D with coarse grid (first row), ECLIPSE-3D with fine grid (second row), ECLIPSE-VE (third row), and MRST-VE (fourth row). The white lines are contour lines of the height of the top of the aquifer with height distance 5 m.



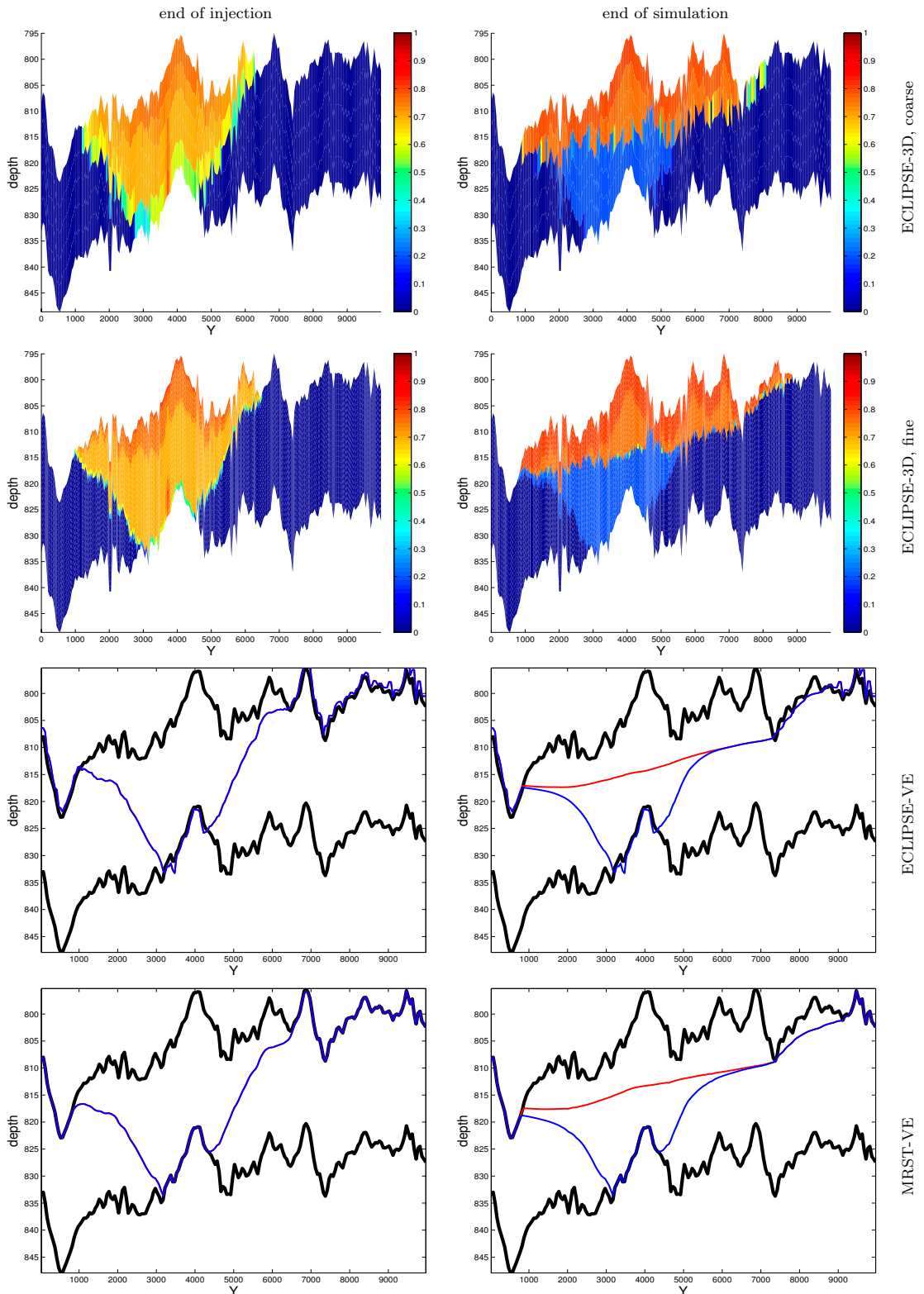


Figure 4: CO<sub>2</sub> saturation along vertical cross-section parallel to the x-axis that passes through injection point. Saturation profiles at the end of the injection period (left column) and at the end of simulation (right column). Saturations were computed with ECLIPSE-3D with coarse grid (first row), ECLIPSE-3D with fine grid (second row), ECLIPSE-VE (third row) and MRST-VE (fourth row) simulators. Blue and red lines in the last two rows show contours of trapped and mobile CO<sub>2</sub>, respectively; black lines show the position of the bottom and top of the aquifer at the center of the cell.

were performed using both a fully implicit and an implicit-pressure, explicit-saturation (IMPES) formulation. For the coarse grid, the implicit simulation took 14 hours while the IMPES simulation took 36 minutes. The fine-grid 3D simulation took 14 hours using the IMPES option. For ECLIPSE-VE, the fully implicit option was fastest and used 19 minutes, while the IMPES time-stepping scheme used 2 hours. MRST-VE is based on a sequential splitting approach and took 12 minutes.

Figure 3 shows CO<sub>2</sub> saturation in the top cells of the model at the end of injection (32 years) and end of the simulation (132 years). Overall there is a very good agreement between the solution computed with the ECLIPSE-3D simulator in a fine grid and the two VE solutions. The difference between the two ECLIPSE-3D simulations are due to numerical errors that diminish as the grid is refined in the vertical direction. In particular, the CO<sub>2</sub> plume simulated with the coarse grid moves slower than the one simulated with the fine grid. This observation is confirmed by Figure 4, which shows simulated CO<sub>2</sub> saturations in a vertical cross-section that passes through the injection point and is parallel to the x-axis. The difference in plume speed between the coarse and fine grids is caused by CO<sub>2</sub> moving more rapidly for higher saturation values. The large cell size of the coarse grid results in a large difference between the average of the nonlinear relative permeability functions and the relative permeability functions evaluated in the average saturation. The smaller size of the cells in the refined grid reduce this effect and the CO<sub>2</sub> plume expands faster. As the CO<sub>2</sub> plume moves away from the injection area following the top of the numerical domain, it becomes thinner and the numerical errors due to poor vertical discretization become more important. This source of error is absent in the VE models because the vertical geometry of the plume is implicitly accounted for.

Figure 4 also confirms that vertical segregation of CO<sub>2</sub> and brine occurs in relatively short time and that the system reaches vertical equilibrium even before the end of the injection period. Similar patterns were observed in several other cross-sections that are not shown here. If capillary forces were included, they would not change the time required to reach vertical equilibrium, but would introduce a capillary fringe. If the capillary fringe is smaller than the vertical resolution, the vertically-averaged model will still give a better description of the system than the 3D model. Introducing capillary forces in the vertically-averaged model for our homogeneous system, however introduces very little extra computational complexity. If capillary forces were included in the simulations discussed here, the thickness of the capillary fringe would be smaller than the vertical cell spacing, hence the VE models would also give a better representation of the system than the full 3D models.

#### 4. Conclusions

We have presented results of full 3D and 2D vertical-equilibrium simulations of the migration of CO<sub>2</sub> in a realistic model of a site where CO<sub>2</sub> has been stored for more than a decade. The analysis of these results demonstrates that for the specific case of CO<sub>2</sub> migration in the Utsira Sand aquifer, VE models provide solutions that are more accurate. The VE model is much faster than corresponding 3D simulations that resolve the same dynamics. VE models are also more accurate than 3D models when full local segregation is achieved, because the vertical extension of the CO<sub>2</sub> plume is implicitly included in the model so that the VE results are independent of the vertical resolution. This is particularly important for simulations of long-term migration of CO<sub>2</sub>, where the plume thins out as it moves farther from the injection site. The VE models have reduced dimensionality compared with full 3D models and also avoid thin cells, thereby gaining a computational advantage. In addition, VE models perform better because of the weaker coupling between the pressure and transport equations [26] which make them more suitable for sequential splitting approaches. Such splitting approaches can be troublesome in three-dimensional simulations of CO<sub>2</sub> migration because of the strong coupling between the pressure and saturation equations caused by gravity.

Based on the results discussed above, we recommend that more effort should go into developing more accurate and faster VE models for simulating CO<sub>2</sub> migration. Moreover, we anticipate that the renewed interest in vertical equilibrium models will result in the development of new simulators that would be able to represent more complex physical mechanisms that affect CO<sub>2</sub> migration such as capillary pressure and CO<sub>2</sub> dissolution into brine.

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