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# Application of Vertically-Integrated Models with Subscale Vertical Dynamics to Field Sites for $CO_2$ Sequestration

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**Abstract**

To address the engineering questions on security issues of geological carbon sequestration (GCS), a broad range of computational models with different levels of complexity have been developed - from multiphase multicomponent fully coupled three-dimensional models to simplified analytical solutions. Within this wide range of models, a family of so-called vertical equilibrium (VE) models has been developed. These models assume that $CO_2$ and brine have segregated due to buoyancy and reached a hydrostatic pressure distribution in the vertical direction. Such VE models are computationally efficient due to the dimensional reduction in the vertical, and accurate as long as the VE assumption is satisfied. However, a study comparing results from a VE model to results from a full three-dimensional model found that there are realistic conditions for which the VE assumption is not justified, especially for geological formations that have low vertical permeability, on the order of 10 milliDarcy or lower [1].

In an attempt to overcome the VE limitation of the vertically-integrated models, a new type of vertically-integrated model which relaxes the VE assumption while still using a vertically-integrated framework has been developed [2]. The new vertically-integrated model is cast into a multiscale framework, where the coarse scale is the horizontal domain and the fine scale is the vertical domain corresponding to the thickness of a geologic formation. This type of model maintains much of the computational advantages of the VE models, while allowing a much wider range of problem to be modelled. In this paper, we extend the model in [2] to include horizontally layered geologic heterogeneities and develop a new dynamic reconstruction model, which we refer to as a “multi-layer dynamic

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reconstruction" model. The model in [2] is called "single-layer dynamic reconstruction" model to distinguish the modelling approaches. We apply both dynamic reconstruction models to field injection sites, including a hypothetical injection scenario into the Mount Simon formation in the Illinois Basin, USA and the well-known industrial-scale injection into the Utsira formation at the Sleipner site in Norway. The modelling results show that the multi-layer dynamic reconstruction model is capable of dealing with horizontally layered heterogeneities and gives results that agree reasonably well with results from the full multi-dimensional model, although in geologic layers with high permeability the reconstruction algorithm is not able to fully capture the horizontal driving forces due to buoyancy. This could be important over long time scales for highly permeable geologic layers. The single-layer dynamic reconstruction model was shown be to the right model choice for homogeneous formations with relatively low permeability where it takes a long time for $CO_2$ and brine to reach vertical equilibrium [2]. In this study, we found that for homogeneous formations with high permeability and steep capillary pressure curves, the single-layer dynamic reconstruction model gives results that are analogous to vertical equilibrium models, with the fast segregation dynamics requiring small time steps in the dynamic reconstruction algorithm. As such vertical equilibrium models are the appropriate choice for systems with high permeability, although we also note that the behaviour of the brine relative permeability curve at low brine saturations is an additional important consideration and must be included in the overall analysis.


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*Keywords:* $CO_2$ sequestration, vertically-integrated models, multiscale modeling, dynamic reconstruction,

## 1. Introduction

Geological carbon sequestration (GCS) is a promising strategy for mitigation of global warming by reducing carbon emissions from large stationary sources [3], such as coal-fired power plants. A range of engineering questions regarding the storage security of $CO_2$ has to be addressed for the GCS technology to be successful. One primary question is how $CO_2$ migrates in the subsurface. To answer this question, a broad range of mathematical models has been developed, spanning from the simple analytical solutions which impose vertical equilibrium, a sharp interface assumption, and strict geometric limits [4-9], to more general numerical vertical equilibrium models with subscale analytical solutions [10, 11], to full multidimensional models, such as [12-16]. More recently, a new type of vertically-integrated model called "dynamic reconstruction" has been developed [2]. In terms of model complexity, the dynamic reconstruction model provides an intermediate choice between conventional VE models and full multi-dimensional models. The dynamic reconstruction model relaxes the VE assumption by treating the vertical dynamics as a one-dimensional fine-scale problem and then, just like the conventional VE models, coupling the reconstruction with a set of vertically-integrated coarse-scale equations. Although heretofore limited to homogeneous geologic formations, this type of model extends the applicability of vertically-integrated models to problems for which the vertical dynamics of $CO_2$ and brine are important, while still maintaining much of the computational advantages of the VE models.

In this paper, we extend the dynamic reconstruction model of [2] to include horizontally layered heterogeneity, which is a typical type of heterogeneity encountered in GCS operations due to the geologic sedimentation history of many potential storage formations. We refer to the extended model as a multi-layer dynamic reconstruction model while the model in [2] is called single-layer dynamic reconstruction model. To investigate the applicability of both of these models, we selected two application test sites: the first one is the Mount Simon formation in the Illinois Basin, and the second one is the $9^{th}$ layer of the Utsira formation at the Sleipner site. Mount Simon is selected to test the appropriateness of the multi-layer dynamic reconstruction model for a field site with horizontally layered heterogeneities, while the Utsira formation allows us to investigate the appropriateness of the single-layer dynamic reconstruction model for high permeable homogeneous geologic formations.

We start with a brief review of the single-layer dynamic reconstruction model which was presented in detail in [2], and conceptually introduce the multi-layer dynamic reconstruction model. Then we show the model scenarios and simulation results for the two test cases. In the end, we summarize the paper and discuss the possible extensions and future directions.

## 2. Mathematical Model

We first conceptually review the single-layer dynamic reconstruction model, which was presented in detail in [2]. The single-layer dynamic reconstruction model relaxes the VE assumption, which is usually taken by the conventional VE models, and casts the governing equations into a multiscale framework to include the vertical dynamics as a fine-scale problem. The coarse scale is the horizontal domain, while the fine scale is the vertical domain which corresponds to the thickness of a geologic layer. As in the VE models, a vertically-integrated equation is solved for the pressure defined at the coarse scale. But, in contrast to VE models that solve a second vertically-integrated equation for the vertically-integrated phase saturation, followed by an analytical reconstruction of the pressure profiles in the vertical direction, the single-layer dynamic reconstruction model solves locally one-dimensional (vertical) two-phase flow equations to calculate the vertical transients of the fluid saturation profiles. This allows the vertical dynamics of $CO_2$ and brine to be modeled explicitly. In these locally one-dimensional equations, fine-scale horizontal fluxes are included as source and sinks. The horizontal fluxes are computed from the reconstructed vertical fine-scale pressure field, which is obtained from the coarse-scale pressure and the vertical structure of the fine-scale pressure from the previous time step. This type of dynamic reconstruction model extends the applicability of vertically-integrated models to problems where vertical dynamics of $CO_2$ and brine are important, while maintaining much of the computational advantages of the conventional vertically-integrated models.

The single-layer dynamic reconstruction model is limited to homogeneous geologic formations. In this paper, we extend the single-layer dynamic reconstruction model to a multi-layer model, which is capable of including horizontally layered heterogeneities. The essence of the multi-layer dynamic reconstruction model is the coupling scheme that couples different geologic layers on the coarse scale with a set of vertically-integrated equations, while within each of those layers, a dynamic reconstruction algorithm in direct analogy to [2] is used. The difference between the dynamic reconstruction algorithm used in the single-layer model and the multi-layer model lies in the pressure reconstruction. In a general form, the pressure reconstruction in the single-layer and the multi-layer model can both be written as

$$p_\alpha(x_1,x_2,x_3,t) = P_\alpha(x_1,x_2,t) + \pi_\alpha(x_1,x_2,x_3,t) \tag{1}$$

where $p_\alpha$ and $P_\alpha$ are the fine-scale and coarse-scale pressures of phase $\alpha$, respectively; $(x_1,x_2,x_3)$ denote the spatial coordinates of a point on the fine-scale; the fine-scale pressure $p_\alpha(x_1,x_2,x_3)$ is defined to be the pressure at $(x_1,x_2,x_3)$, while the coarse-scale pressure is usually taken to be the fine-scale pressure at a reference elevation. $\pi_\alpha$ defines the fine-scale reconstruction of the pressure field for phase $\alpha$ from the coarse-scale phase pressure.

In the single-layer algorithm a saturation weighted hydrostatic reconstruction is used [2]. In that case, if we take the brine phase as an example, the fine-scale pressure reconstruction is

$$\pi_b(x_1,x_2,x_3,t) = \int_{\xi_B}^{x_3}\left[\left(s_c\rho_c + s_b\rho_b\right)g + s_c\frac{\partial p^{cap}(s_b)}{\partial x_3}\right]\mathrm{d}x_3 \tag{2}$$

The multi-layer dynamic reconstruction model uses a different pressure reconstruction, where $\pi_\alpha$ is directly set to be zero. In other words, a constant pressure profile along vertical is set for each layer, that is

$$p_\alpha(x_1,x_2,x_3,t) = P_\alpha(x_1,x_2,t) \tag{3}$$

In both models, the reconstructed fine-scale pressure is only used to calculate the fine-scale horizontal fluxes, and is not directly used in the calculation of vertical fluxes. The vertical fluxes are calculated using a fractional flow equation where the vertical total flux is obtained based on mass conservation from the horizontal fluxes. Therefore, the suitability of the pressure reconstruction mainly depends on how well it captures the horizontal fluxes. In the early time or close to the injection point, $CO_2$ and brine have not segregated and the horizontal flow is mainly driven by injection. At later time or far away from the injection point, the segregation of $CO_2$ and brine takes place, and the horizontal flow is mainly driven the horizontal forces due to buoyancy. The pressure reconstruction in [2] was designed to be capable of capturing such an evolution of driving forces. The pressure reconstruction in the multi-layer dynamic reconstruction model approximates the horizontal pressure gradient to be the same along vertical, which is not able to model the horizontal driving forces due to buoyancy. We choose this reconstruction for the multi-layer model instead of the reconstruction of the single-layer model in equation (2), because equation (2) leads to numerical instability in the multi-layer model. The reconstruction we use for the multilayer dynamic reconstruction model is an appropriate approximation when the horizontal flow is mainly driven by injection, but it might induce significant errors when $CO_2$ and brine are segregated and the horizontal forces due to buoyancy become important. We continue to work on improvements to this reconstruction operator in the context of multi-layer domains.

The coupling between the layers in the multi-layer dynamic reconstruction model is done by formulating an effective (Darcy) flux equation based on the coarse-scale pressures from neighboring layers, with the coefficients (permeabilities and mobilities) obtained by averaging between the centers of the layers. This leads to a coupled system of equations containing all the layers in the multi-layer system on the coarse scale. The coarse-scale pressures are determined from that system of equations, and the vertical fluxes between the layers are estimated based on the coarse-scale pressures from the effective flux equation. Once the vertical fluxes between the layers are estimated, the saturation reconstruction for each layer is essentially the same as for the single-layer model except that the fluxes at the top and bottom of the layers are nonzero, although the top and bottom boundaries of the formation remain as no-flow boundaries.

## 3. Modeling of Injection at the Mount Simon Formation

For the purpose of illustrating the applicability of the two models, we simplify the physical system to a two-dimensional (2D) Cartesian slice, which has one vertical and one horizontal dimension. This setup corresponds to a cross-section of a formation that has an array of vertical injection wells, with the cross-section perpendicular to the line of the array. A similar setup was used in [17]. We use a full 2D simulator [18], which fully couples the horizontal and vertical dimensions with an IMPES-type method, to compare with the two dynamic reconstruction models.

### *3.1. Model Setup*

The Mount Simon Sandstone formation in the Illinois Basin is the primary storage target of the ADM-Decatur $CO_2$ storage project, which is a large-scale demonstration that aims to inject 1.1 Mt $CO_2$ into the Mount Simon Formation over a three-year period started from the year of 2011. The Mount Simon is assumed to be sealed at the top by the Eau Claire shale and at the bottom by crystalline rock. Within the formation, rock properties exhibit typical layered heterogeneity due to the depositional history. The Mount Simon formation was approximated as 24 geologic layers in a three-dimensional simulation using TOUGH2 by [19]. In this study, we take the geologic data from [19] and obtain a nine-layer system by combining some of the layers. For layers that consist of a number of sub-layers in [19], the porosity and horizontal permeability are assigned by arithmetic averaging, while the vertical permeability is obtained by harmonic averaging. The distribution of porosity and permeability along the vertical are shown in Figure 1. $CO_2$ is injected into the 74.1 m thick bottom layer. The injection rate is equivalent to an array of vertical injection wells that extends 1000-meter long with an injection rate of 2.0 Mt/year. The top and the bottom of the formation are taken to be no-flow boundaries. The density and viscosity of $CO_2$ and brine are 900 kg/m$^3$ and $4.25 \times 10^{-5}$ Pa s, and 1100 kg/m$^3$ and $3.0 \times 10^{-4}$ Pa s, respectively. For the relative permeability, we use Brooks-Corey curves with a pore size distribution parameter of 2.0. We have neglected the capillary pressure and residual saturation in this study for simplicity, although the multi-layer dynamic reconstruction model allows inclusion of them. In the simulation setup, by taking advantage of symmetry, we use a half domain and inject into the bottom left corner of the domain. On the right hand side of the domain, the boundary is set to have a hydrostatic pressure distribution of brine. The half-domain extends 5 km in the horizontal direction, and the thickness of the formation is 401 meters as shown in Figure 1. The numerical grid has $\Delta x = 25.0$ m and $\Delta z \approx 2.0$ m ($\Delta z$ is slightly different in each geologic layer but close to 2.0 m). Two scenarios are considered: the first one directly uses the data in Figure 1; the second one decreases both the vertical and horizontal permeability by a factor of 10.

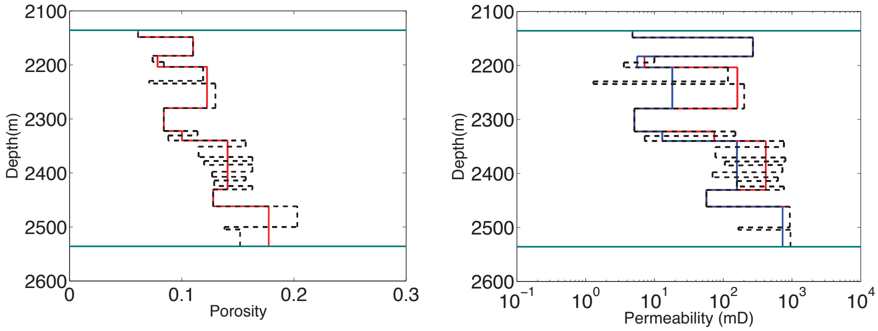


Fig. 1. Distribution of the geologic properties of the Mount Simon formation. The black dashed lines represent the geologic data from [19] which has 24 geologic layers. The red lines represent the nine-layer data used for this study, which is obtained by averaging from the 24 layers. In the permeability profile, the red lines and blue lines denote the horizontal and vertical averaged permeability, respectively.

### 3.2. Results

We present two sets of simulation comparisons for the Mount Simon formation. The first comparison uses the parameters in Figure 1 and the second one uses permeability decreased by a factor of 10 from Figure 1.

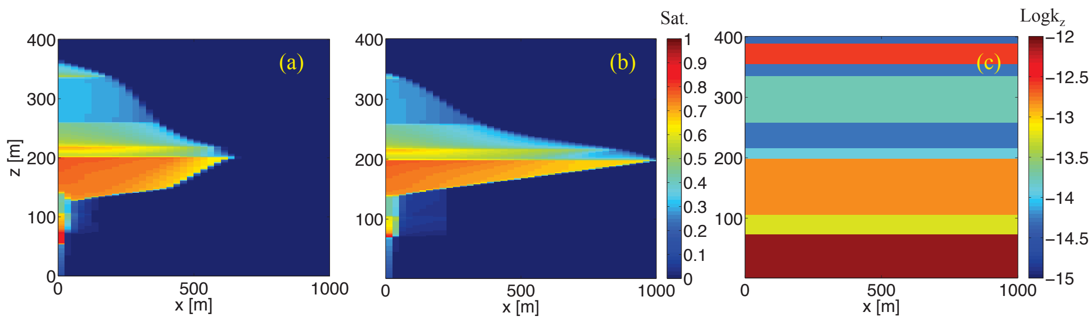


Fig. 2. $CO_2$ plume comparison for the multi-layer dynamic reconstruction model and the full 2D model, with parameters of the Mount Simon formation after 5 years of injection. Injection takes place on the left of the bottom layer that is 74.1 m thick. The color scale represents magnitude of $CO_2$ saturation in (a) and (b), while represents vertical permeability on the log scale in (c). (a) Multilayer dynamic reconstruction model; (b) Full 2D model; (c) Vertical permeability distribution on the log scale.

With the original parameters, we get $CO_2$ plume simulations from the multi-layer dynamic reconstruction model and the full 2D model as shown in Figure 2(a) and 2(b). Figure 2(c) illustrates the layered vertical permeability structure of the formation. The two models do not agree very well. The multi-layer dynamic reconstruction model tends to underestimate the $CO_2$ plume extent in the horizontal while overestimating the extent of vertical migration. Specifically, if we take the third layer from the bottom as an example, we can see that the $CO_2$ plume of the multi-layer model extends much less than the full 2D model in the horizontal. This deviation might reasonably be attributed to the pressure reconstruction in the multi-layer dynamic reconstruction model, which as was mentioned in the section 2, is not able to model the horizontal driving forces due to buoyancy. Therefore, it leads to significant errors when the horizontal driving forces due to buoyancy become important. To investigate the validity of this hypothesis, we use the same set of parameters but decrease the permeability by a factor of 10. In this case it can be expected that viscous forces due to injection are the dominant driving forces. Figure 3 shows that the two models have excellent agreement with the decreased permeability, which verifies that the pressure reconstruction of the multi-layer dynamic reconstruction model works very well when viscous force due to injection is the dominant horizontal driving force while buoyancy effects are negligible.

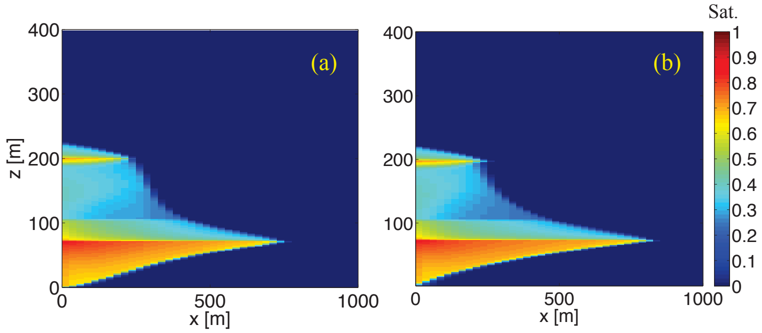


Fig. 3. $CO_2$ distribution for the multi-layer dynamic reconstruction model and the full 2D model after 5 years injection. The parameters are the same as in Figure 3 except with permeability decreased by a factor of 10. The color scale represents magnitude of $CO_2$ saturation. (a) Multi-layer dynamic reconstruction model; (b) Full 2D model.

## 4. Modeling of the 9th Layer of the Utsira Formation at Sleipner

In the Sleipner test case, we neglect the topography of the caprock and also simplify the physical system as a 2D domain with a point source at the left bottom corner, which corresponds a formation with a horizontal line source perpendicular to the cross-section. We compare the single-layer dynamic reconstruction model with a full 2D model and a VE model with capillary transition zone. In the following two subsections, details of the model setup and the modeling results are given.

### *4.1. Model Setup*

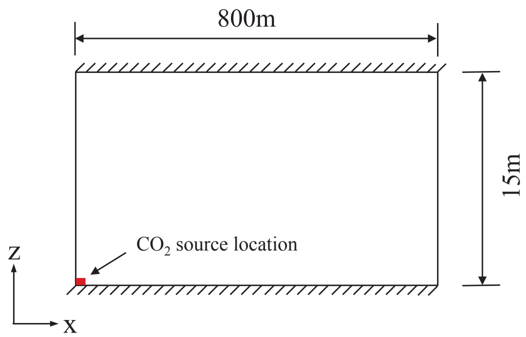


Fig. 4. Model setup for the single-layer dynamic reconstruction model based on the 9th layer of the Utsira formation.

The second model is based on the 9th layer of the Utsira Formation at the Sleipner site. The Utsira formation is known to be separated by thin lateral intra-sand shale layers, but those separated layers have relatively homogeneous geologic properties. In this study, we take the 9th layer that is above a thin shale layer and treat it as a homogeneous layer. This is to test if the single-layer dynamic reconstruction model is the appropriate model choice for a highly permeable formation. In the simulation, fluid properties are representative values of the Sleipner formation taken from [20, 21], density and viscosity of $CO_2$ and brine are 706 kg/m$^3$ and $5.77 \times 10^{-5}$ Pa s, and 1020 kg/m$^3$ and $6.9 \times 10^{-4}$ Pa s, respectively. Permeability of the formation is 2.0 Darcy with an anisotropy ratio of 0.28. Residual saturation is neglected, so the residual saturation is zero for both $CO_2$ and brine. For the relative permeability and the capillary pressure, we use Brooks-Corey curves with a pore size distribution parameter of 2.8 and an entry pressure of 2500 Pa. Similar to the setup for the Mount Simon model, we take a half domain and inject $CO_2$ from the bottom of the left hand side. The $CO_2$ in the 9th layer is believed to be leaked from the lower layers, therefore we put a point source of $CO_2$ at the bottom of the formation (the red block in Figure 4). The point source is equivalent to a 500-m long horizontal line source with a mass rate of 0.1418 Mt/year. The half-domain is 800 meters long and 15 meters thick. The top and bottom boundaries are set to be no-flow boundaries. The right hand side of the domain is set to have a hydrostatic pressure distribution for brine. The numerical grid has $\Delta x = 5.0$ m and $\Delta z = 0.125$ m and the injection is from the bottom two cells, that is the injection interval is 0.25 m thick.

*4.2. Results*

The 9th layer of the Utsira formation has relatively homogeneous and high permeability (on the order of Darcy). Because of its homogeneity, the 9th layer is a good demonstration case for the single-layer dynamic reconstruction model. We show $CO_2$ plume comparisons of the single-layer dynamic reconstruction model, the full 2D model and a VE model after 1 year of $CO_2$ migration into the 9th layer.

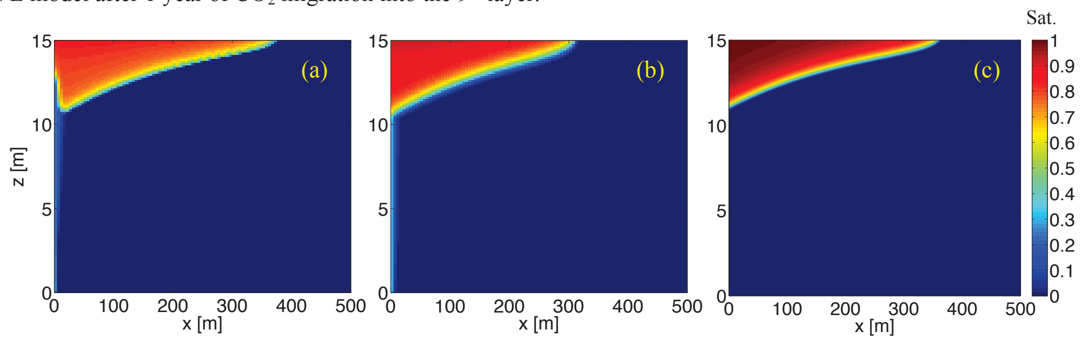


Fig. 5. $CO_2$ distribution comparison of the single-layer dynamic reconstruction model with the full 2D model and the VE model after 1 year of leakage into the formation. The color scale represents magnitude of $CO_2$ saturation. (a) Single-layer dynamic reconstruction model; (b) Full 2D model; (c) VE model

The plumes of the single-layer dynamic reconstruction and the full 2D model have close agreement, except in the region that is close to the $CO_2$ source location. This is because the pressure reconstruction equation (2) is not appropriate in the region where strong vertical flow is involved (which is directly above the leakage source), which also explains the slight overestimate of the $CO_2$ plume extent in the single-layer dynamic reconstruction model. The VE model overestimates the $CO_2$ plume extent as well. It should be noted that $CO_2$ and brine still have not fully segregated in both the single-layer dynamic reconstruction model and the full 2D model even with the fairly large vertical permeability of 0.56 Darcy. This is mainly because brine drainage becomes very slow due to the very small relative permeability over a substantial range of brine saturations that approach the residual saturation (in this study it is zero) from above. This also explains the differences with the VE model result which has high $CO_2$ saturations close to 1 in most of the plume and overestimates the $CO_2$ plume extent. The VE model directly neglects the slow brine drainage process and assumes that the drainage happens instantaneously, and this includes drainage through the range of very low (but nonzero) brine relative permeability values. This calls into question the meaning of residual saturation and the treatment of drainage processes that (mathematically) require thousands of years to occur. Despite the absence of the slow brine drainage process, results of the VE model overall have very good agreement with results of the full 2D model.

## 5. Summary and Discussion

A single-layer and a multi-layer dynamic reconstruction model have been tested with parameters based on actual injection sites, including the typical horizontally layered heterogeneous Mount Simon formation and the homogeneous highly permeable 9$^{th}$ layer of the Utsira formation at the Sleipner site. The test case of the Mount Simon formation shows that the multi-layer dynamic reconstruction model is able to predict $CO_2$ migration in a horizontally layered heterogeneous formation when the horizontal flow is dominated by viscous forces due to injection (e.g., low permeability). However, when some of the layers have relatively high permeability, which means the horizontal driving forces due to buoyancy could be dominant, results from the multilayer dynamic reconstruction model can deviate significantly from the results of the full 2D model. This is not surprising, because the pressure reconstruction of the multi-layer dynamic reconstruction model is not able to capture the buoyancy effect in the horizontal, which induces errors when the horizontal driving forces due to buoyancy become important. One possible strategy to improve the multi-layer model is to use different reconstruction algorithms for layers with different geologic properties (mainly permeability), and couple those layers using a coupling scheme similar to that in the current multi-layer model. The choice of reconstruction algorithms would then depend on whether buoyant forces or viscous forces are the dominant horizontal driving force. Improved pressure reconstruction algorithms continue to be a focus of our ongoing research.

The Sleipner test case shows that all three models give similar results, but the fast dynamics in the vertical requires small time steps in the models that include vertical dynamics, and the thin capillary transition zone requires fine vertical grid resolution. In this case the VE model becomes attractive in terms of both of these constraints, because it directly imposes a (vertical equilibrium) solution structure in the vertical and no vertical numerical grid resolution is required. Although the VE model is not able to capture the very slow drainage processes associated with the saturation region corresponding to very low brine relative permeability, it does not make a big difference in the $CO_2$ plume. Therefore, given the strong reduction of computational effort, for the geologic formations with high permeability and especially those with thin capillary transition zones, the VE model is recommended, even for early times.

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