

Robust simulation of sharp-interface models for fast estimation of CO₂ trapping capacity in large-scale aquifer systems

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Abstract Modeling geological carbon storage represents a new and substantial challenge for the subsurface geosciences. To increase understanding and make good engineering decisions, containment processes and large-scale storage operations must be simulated in a thousand-year perspective. Large differences in spatial and temporal scales make it prohibitively expensive to compute the fate of injected CO₂ using traditional 3D simulators. Instead, accurate forecast can be computed using simplified models that are adapted to the specific setting of the buoyancy-driven migration of the light fluid phase. This paper presents a family of vertically integrated models for studying the combined large-scale and long-term effects of structural, residual, and solubility trapping of CO₂. The models are based on an assumption of a sharp interface separating CO₂ and brine and can provide a detailed inventory of the injected CO₂ volumes over periods of thousands of years within reasonable computational time. To be compatible with simulation tools used in industry, the models are formulated in a black-oil framework. The models are implemented in MRST-co2lab, which is an open community

software developed especially to study and optimize large-scale, long-term geological storage of CO₂. The resulting simulators are fully implicit and handle input from standard geomodeling tools.

Keywords CO₂ storage · Vertical equilibrium · Compressibility · Dissolution

1 Introduction

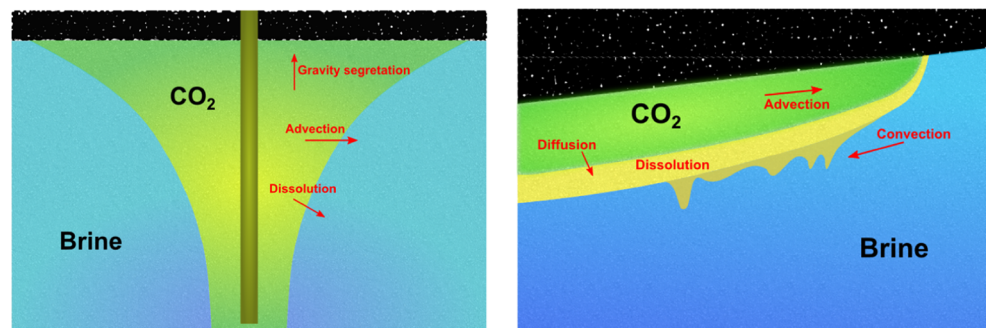
Dipping saline aquifers comprise the largest volumes available for large-scale storage of CO₂. To accurately estimate the storage capacity of an open aquifer, one must determine the maximum amount of CO₂ that can be injected and how far and how fast the injected plume will migrate throughout the aquifer. The injection and migration processes are governed by delicate balances of various physical mechanisms (see Fig. 1) which may change with time and spatial location. Resolving these processes is a challenging multiscale problem that involves a large disparity in spatial and temporal scales. CO₂ is very mobile and can travel large distances, but the flow is usually confined to thin layers underneath a sealing caprock or other low-permeable vertical barriers. A typical saline aquifer considered for CO₂ storage can be viewed as a thin, slightly inclined sheet that spans thousands of square kilometers. This, in combination with differences in density between the supercritical CO₂ plume and the resident brine, means that the vertical fluid segregation will be almost instantaneous compared with the up-dip migration. The tendency of forming a relative flat fluid interface is an effect of the pressure distribution, which in turn depends strongly on the flow in the vertical direction, particularly near the interface. The vertical fluid distribution must also be accurately represented to avoid introducing large errors

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Fig. 1 Illustration of injection and trapping of CO₂ under a sealing caprock. The plots show forces active during the injection (left) and migration phase (right)



in the forecast of the updip migration. (For nonlinear relative permeabilities, a large error will result from replacing the average of the mobility by the mobility of the average phase distribution). The thin plume and sharp transition between CO₂ and brine means that high vertical resolution is required to compute the vertical phase distribution. High grid resolution is also needed in the lateral direction to resolve the unstable dynamics of convective dissolution, which retards and limits the plume migration and to account for small undulations in the caprock topography, that may both retard the migration of the plume and divert its path. In other words, simulating likely outcomes over a period of thousands of years is in most cases computationally intractable with conventional 3D reservoir simulators.

This is clearly demonstrated in the recent Stuttgart benchmark [1], in which a variety of commercial simulators and research codes were used by leading academic and industry experts to solve three model problems. Despite a large computational effort and significant work spent in eliminating differences in input data, the reported results are striking in their disparity, particularly for the study of how a supercritical CO₂ plume forms and migrates upward in a small region of the Johansen formation [2, 3] from the Norwegian North Sea. At the end of simulation, the reported results show almost no consensus in the simulated shapes of the CO₂ plume.

In our opinion, there is an urgent need to advance state-of-the-art in numerical simulation to improve the assessment of storage capacity, facilitate approval of specific storage projects, and help realize the storage potential both globally and locally on the Norwegian Continental Shelf. In terms of modeling, efforts are needed along several parallel paths. First, one must continue to develop reliable numerical methods that model fundamental flow physics accurately and correctly. Second, these methods must be combined in robust numerical formulations that account for varying degrees of coupling between the different physical effects that drive or influence CO₂ migration. These numerical formulations need to be sufficiently flexible so that one in a simple and case-dependent manner can combine the flow equations with thermal, geomechanical, and geochemical

effects. Finally, the formulations must be implemented as trustworthy software that enables transparent comparisons of models, methods, and simulated outcomes.

We believe that the only way these challenges can be tackled is through collaboration, development, and extensive use of community software. To contribute to this and to accelerate transfer of knowledge developed in academic research projects to end-users in industry and the public sector, we have started developing a community software called MRST-co2lab [4–8] implemented on top of the open-source Matlab Reservoir Simulation Toolbox (MRST) [9–12]. Both MRST and its CO₂ module can be freely downloaded and used under the GNU General Public License v3.0. The software offers reliable modeling of realistic storage scenarios, enables interactive experimentation with various model assumptions like boundary conditions, fluid models and parameters, injection points and rates, amount of subscale trapping, and so on, and simplifies the development, implementation, and comparison of new models and computational methods. The software offers a hierarchy of models and tools of increasing computational complexity [7, 8], as well as a set of tutorials and examples that demonstrate and highlight how these tools can be applied to study fundamental flow physics as well as descriptions of realistic storage scenarios based on public data sets of the Johansen formation [2, 3], the Sleipner injection [13], and saline aquifers from the Norwegian Continental Shelf [14].

Herein, we present a family of vertically-integrated models for studying the combined large-scale and long-term effects of structural, residual, and solubility trapping to provide detailed inventories of injected CO₂ volumes over periods of thousands of years. All models are based on the assumption of vertical equilibrium (VE) with a sharp interface that separates the injected CO₂ from the resident brine. Apart from the open-source implementation, the novelty of our work lies in a flexible and robust formulation that unifies work from the early period of reservoir simulation [15–18], when practical numerical aspects were primarily in focus, with recent extensions of the VE framework [19] that focus more on physical effects related to

large-scale CO₂ injection. The validity of the simplifying assumptions underlying VE models has been studied both with respect to spatial [20] and temporal [21] scales, and the utility of VE models is thoroughly discussed in, e.g., [22, 23]. Early studies focused on VE models with a sharp-interface assumption [24–26], and models that only account for the basic effects of buoyant migration were successfully used to simulate long-term migration in the Utsira [27] and Johansen [28] aquifers. Later, the class of VE models has been extended to incorporate most of the flow effects that are pertinent to large-scale migration, including compressibility [29], convective dissolution [30, 31], capillary fringe [32], small-scale caprock topography variations [33–35], various hysteretic effects [36–38], multiple geological layers [39, 40], and heat transfer [41]. In particular, several studies show that vertical equilibrium simulations compare well with 3D simulators on case studies of the Johansen aquifer [42] and the 9th layer of the Sleipner injection [27, 43]. The assumption of vertical equilibrium not only reduces the number of spatial dimensions, and hence the number of grid cells, but will also reduce the coupling between pressure and fluid transport and improve the characteristic time constants of the problem [42]. As a result, VE simulations will typically be orders of magnitude faster and consume significantly less memory than conventional 3D simulators. In [23, 43], the authors report a simulation of CO₂ migration under the caprock at Sleipner, for which a VE simulator running for a few minutes on a single core produced forecasts with similar accuracy as a 3D simulation with TOUGH2 running for several hours on one hundred cores.

To develop our numerical framework, we first discuss modeling of various physical mechanisms including compressibility and retardation effects from subscale trapping. We then show how a general class of VE models can be recast as standard black-oil models using the traditional concept of pseudo-functions [44–47] and discuss the inclusion of dynamic dissolution effects. In particular, we point out in detail the approximations and numerical considerations needed to obtain flexible and efficient numerical formulations that resolve the main physical effect well within the accuracy normally available from input data. The overall formulation is implemented as an extension of existing black-oil solvers in MRST [12], which in turn have been implemented using automatic differentiation and hence enable simple computation of gradients and parameter sensitivities, e.g., through an adjoint formulation. This enables the users to easily perform sensitivity studies or formulate efficient strategies for rigorous mathematical optimization of large-scale injection strategies [6, 7, 48, 49]. In [50], we discuss how the framework can be extended to account for smooth transitions (capillary fringe) between pure CO₂ and brine. We also show how inclusion of more advanced flow physics naturally leads to pressure-dependence and

hysteretic effects in the vertically-integrated relative permeabilities and capillary pressure and suggest implementation choices we think are important to make flexible and efficient VE simulators.

Whereas the focus of the present paper is on reduced models, the functionality provided by MRST-co2lab also includes other computational tools for analysis of CO₂ storage. In [5], we discuss tools for fast and interactive estimation of structural trapping and potential migration paths under the assumption that CO₂ is injected at an infinitesimal rate. These tools do not account for temporal aspects, but will nevertheless reveal important information such as accessible structural traps, spill points and migration paths, good injection locations, points where the CO₂ may leak out through open boundaries, etc. In [6–8], we outline how the various tools can be combined to create a flexible tool chain for estimating storage capacities and studying injection scenarios. In particular, we study and optimize strategies for injecting hundreds of megatonnes of CO₂ into various saline aquifers in the Norwegian North Sea using data sets from the recent CO₂ Storage Atlas [14]. Finally, we mention that MRST-co2lab also contains conventional 3D simulation capabilities and that work is in progress to include additional physics such as thermal, geochemical, and geomechanical effects.

Complete MATLAB scripts containing all the statements necessary to reproduce the figures presented in this paper can be downloaded as part of the 2015b release of MRST-co2lab.

2 Trapping mechanisms

With a sharp-interface VE model, it is simple to make accurate inventories of carbon trapping for specific scenarios, detailing how injected CO₂ volumes are separated into parts that can be considered safely contained and parts that may potentially leak back to the surface. The general trend is that CO₂ becomes more securely trapped with time as a result of trapping processes taking place at different rates that vary from days to years to thousands of years.

When CO₂ is injected into a deep subsurface rock formation, it forms a separate mobile, typically dense phase (the CO₂ plume) that invades the medium and displaces other liquids present in the pore space (typically: brine). The CO₂ phase is almost always less dense than the resident fluids and will therefore rise upwards and hence be replaced by other fluids. However, as the volume fraction of the CO₂ phase falls below a certain level, CO₂ becomes trapped in the pore space between rock grains by capillary pressure from the other fluids and stops flowing. This is referred to as *residual trapping* and the corresponding volumes of CO₂ are denoted '*residual*' in the inventory. At any point,

the inventory of the plume is therefore subdivided into two categories: ‘*residual (plume)*’ refers to the fraction of the CO₂ column that will eventually stay behind in a residually trapped state when the plume leaves its current position, whereas ‘*movable (plume)*’ is the remaining part that is free to migrate away from the current position.

In most relevant scenarios, CO₂ is injected under a sealing rock in which the capillary pressure inside pore throats is greater than the buoyancy pressure of the CO₂. The top seal will prevent the direct upward movement of the plume and if the seal is sloping, the CO₂ will form a thin layer underneath that slowly migrates in the upslope direction until it encounters a structural trap, i.e., a fold in the top surface inside which the CO₂ will accumulate. Once inside a trap, the CO₂ will remain *structurally trapped* unless the height of the plume creates a capillary pressure that enables the CO₂ to enter the seal. The structurally trapped volumes are therefore divided into two similar categories: ‘*residual (traps)*’ will remain immobile and never leak, while ‘*movable (traps)*’ could in principle escape through a crack in the top seal. Once a trap is filled, the CO₂ will spill over and continue migrating upward. CO₂ can also be trapped in *stratigraphic traps* because of changes in rock type within the storage layer, but this mechanism is not represented in VE models.

The remaining trapping mechanisms are *solubility and mineral trapping*. Over time, CO₂ will dissolve in the resident fluids. Brine containing dissolved CO₂ is slightly denser than the surrounding fluids and will sink to the bottom of the rock formation, thereby trapping CO₂ more

securely. This enables a mixing process that increasingly disperses CO₂ into brine over time. The dissolved CO₂ forms a weak carbonic acid that may react with the reservoir rock to form and precipitate carbonate minerals that bind CO₂ permanently to the rock. This process may be rapid or very slow and is not accounted for herein.

To summarize, the ‘dissolved’, ‘residual (traps)’, and ‘residual’ volumes are safely stored unless changes occur in the aquifer that alter the residual saturation of CO₂ or cause the CO₂ to effervesce from the formation water (think of the fizz when you open a bottle of carbonated water). The ‘movable (traps)’ volumes are immobilized and will be safely stored unless the structural traps contain leakage points. The remaining volumes will continue to migrate in the upslope direction, the ‘residual (plume)’ volumes will eventually remain as residually trapped and only the ‘movable (plume)’ volumes may leak if not trapped by another trapping mechanism at a later time. If the aquifer model has open boundaries, some of the injected CO₂ may also leave the computational domain during the simulation and these volumes will, in lack of a better word, be referred to as ‘*leaked*’. We emphasize that this does not mean that the corresponding CO₂ has leaked back to the atmosphere; in most cases, it will continue to migrate inside another rock volume that is outside the simulation model. In the inventory in Fig. 2, the various categories of CO₂ volumes have been stacked according to increasing risk of leakage, from dissolved CO₂ (dark green color) to volumes that are still movable (yellow/orange) or have already left the simulated domain (red).

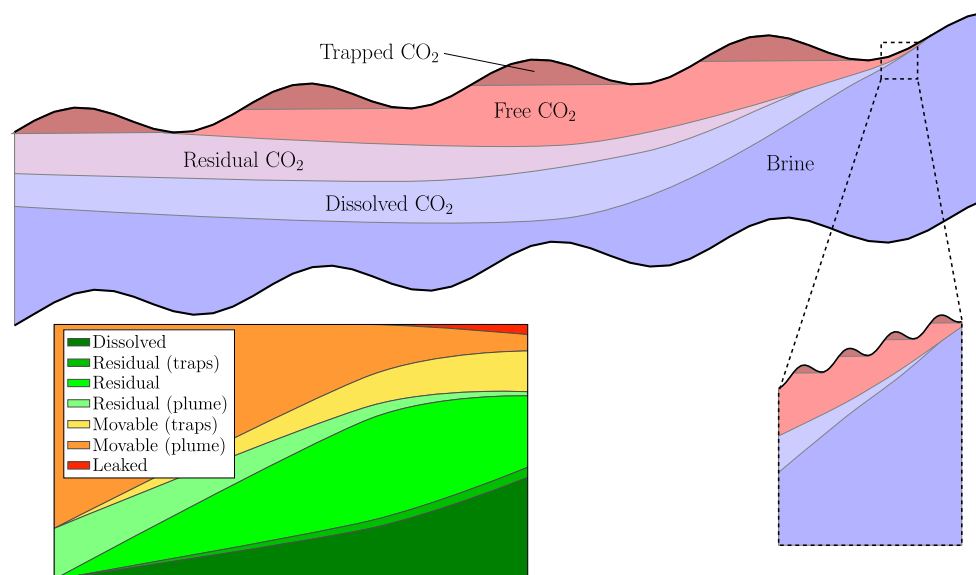


Fig. 2 Schematic of a vertical section of an aquifer showing the different forms in which the injected CO₂ can be present during migration. The *right inlet* shows small-scale undulations in the top surface which typically will not be resolved in a large-scale model. The *left*

inlet shows a detailed inventory of various categories of trapped CO₂, stacked in terms of increasing leakage risk, as function of time from the end of injection

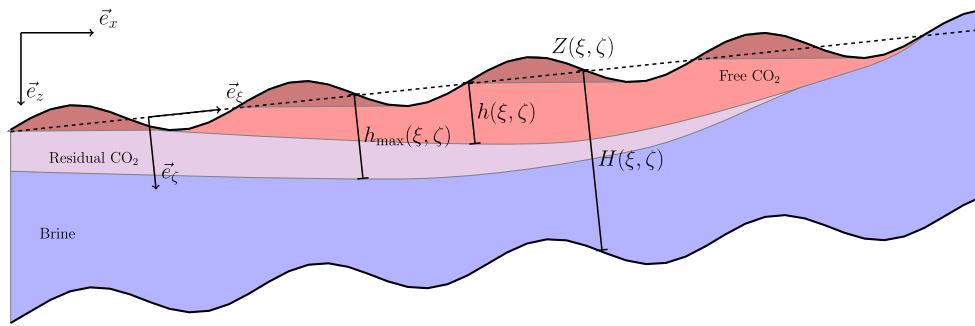


Fig. 3 Schematic of the fluid distribution and the coordinate systems used to derive the basic vertical-equilibrium model. Here, $h(\xi, \eta)$ is the interface between CO₂ and brine, and h_{\max} represents the historical maximum value of h for a given location. The dashed line indicates

assumed mean direction of flow within the aquifer (which is here illustrated as *straight*, but is allowed to be *slightly curved* in the general case)

3 Derivation of the basic VE model

Let brine and CO₂ be wetting and non-wetting fluids, respectively, and assume incompressible rock and fluids, no capillary forces, and impermeable top and bottom of the aquifer. Then, mass conservation and Darcy’s law read:

$$\frac{\partial}{\partial t}(\phi s_\alpha) + \nabla \cdot \vec{v}_\alpha = q_\alpha, \tag{1}$$

$$\vec{v}_\alpha = -\mathbf{k}\lambda_\alpha(\nabla p - \rho_\alpha \vec{g}). \tag{2}$$

Here, ϕ denotes porosity, \mathbf{k} permeability, p pressure, and \vec{g} the gravity vector, whereas s_α , λ_α , and q_α denote saturation, mobility, and volumetric source for phase $\alpha = \{w, n\}$.

We introduce a curvilinear coordinate system $(\vec{e}_\xi, \vec{e}_\eta, \vec{e}_\zeta)$ whose orientation is defined to align closely with the global system $(\vec{e}_x, \vec{e}_y, \vec{e}_z)$, but be slightly tilted so that \vec{e}_ζ locally is perpendicular to the main flow direction (disregarding small and medium-scale oscillations). The tilt only depends on ξ and η , is assumed to vary smoothly and at all points remain modest (a few degrees). We further write $\vec{g} = \vec{g}_\parallel + g_\zeta \vec{e}_\zeta$ and $\nabla = \nabla_\parallel + \vec{e}_\zeta \partial_\zeta$, where \parallel refers to the $(\vec{e}_\xi, \vec{e}_\eta)$ components of a vector/operator. In the new coordinate system, the aquifer is described by the top surface $Z(\xi, \eta)$ and its thickness $H(\xi, \eta)$ in the ζ -direction, see Fig. 3. Capital letters are used for quantities in the upscaled model.

Integrating (1) from top to bottom of the aquifer, neglecting distortions from the curvilinear nature of the coordinate system,¹ we obtain:

$$\frac{\partial}{\partial t} \left[\int_Z^{Z+H} S_\alpha \phi d\zeta \right] + \nabla_\parallel \cdot \left[\int_Z^{Z+H} \vec{v}_\alpha d\zeta \right] = \int_Z^{Z+H} q_\alpha d\zeta. \tag{3}$$

By design of the coordinate system, the flow along \vec{e}_ζ will take place very rapidly compared with the migration in the $(\vec{e}_\xi, \vec{e}_\eta)$ direction. Hence, we assume hydrostatic equilibrium in the \vec{e}_ζ direction. Since capillary pressure is neglected, CO₂ and brine will at equilibrium be separated by

a sharp interface located a distance $h(\xi, \eta)$ from the caprock along \vec{e}_ζ . Setting the pressure datum P_Z at the top surface, the pressure at a given depth ζ is determined by

$$p(\zeta) = \begin{cases} P_Z + \rho_n g_\zeta (\zeta - Z), & Z \leq \zeta \leq Z + h, \\ P_Z + \rho_n g_\zeta h + \rho_w g_\zeta (\zeta - Z - h), & Z + h \leq \zeta \leq Z + H. \end{cases} \tag{4}$$

Figure 3 shows how each vertical column is divided into three regions:

- The CO₂ plume between Z and $Z + h$ with residual brine saturation $s_{w,r}$, CO₂ saturation $1 - s_{w,r}$, and CO₂ mobility $\lambda_{n,e} = \lambda_n(1 - s_{w,r})$.
- The residual region between h and h_{\max} with CO₂ saturation $s_{n,r}$, brine saturation $1 - s_{n,r}$, and brine mobility $\lambda_{w,e} = \lambda_w(1 - s_{n,r})$.
- The region below h_{\max} filled by brine.

We hence define vertically-averaged quantities:

$$\mathbf{K} = \frac{1}{H} \int_Z^{Z+H} \mathbf{k}_\parallel d\zeta, \tag{5}$$

$$\Lambda_n(h) = \frac{1}{H} \left[\int_Z^{Z+h} \lambda_{n,e} \mathbf{k}_\parallel d\zeta \right] \mathbf{K}^{-1} \tag{6}$$

$$\Lambda_w(h, h_{\max}) = \frac{1}{H} \left[\int_{Z+h}^{Z+h_{\max}} \lambda_{w,e} \mathbf{k}_\parallel d\zeta + \int_{Z+h_{\max}}^{Z+H} \lambda_w(1) \mathbf{k}_\parallel d\zeta \right] \mathbf{K}^{-1} \tag{7}$$

Combining these expressions with Darcy’s law (2) and setting $\Delta\rho = \rho_w - \rho_n$, we obtain vertically-integrated fluxes:

$$\vec{V}_n = -H \Lambda_n \mathbf{K} [\nabla_\parallel (P_Z - \rho_n g_\zeta Z) - \rho_n \vec{g}_\parallel], \tag{8}$$

$$\vec{V}_w = -H \Lambda_w \mathbf{K} [\nabla_\parallel (P_Z - \rho_w g_\zeta Z) - g_\zeta \Delta\rho \nabla_\parallel h - \rho_w \vec{g}_\parallel]. \tag{9}$$

To develop the usual fractional-flow formulation, we introduce total velocity $\vec{V} = \vec{V}_n + \vec{V}_w$, assume that \mathbf{K} and

¹A detailed explanation of the approximations related to the curvilinear system is provided in Appendix A.

Λ_α commute (\mathbf{K} isotropic or \mathbf{k}_\parallel constant in ζ), and sum (3) over phases. After some manipulations, we obtain a pressure equation:

$$\nabla_\parallel \cdot \vec{V} = Q, \quad \vec{V} = -H \Lambda \mathbf{K} [\nabla_\parallel P_z - (\rho_n \mathbf{F}_n + \rho_w \mathbf{F}_w)(\vec{g}_\parallel + g_\zeta \nabla_\parallel Z) - \mathbf{F}_w g_\zeta \Delta \rho \nabla_\parallel h], \quad (10)$$

where $\Lambda(h, h_{\max}) = \Lambda_w(h, h_{\max}) + \Lambda_n(h)$ and $\mathbf{F}_\alpha(h, h_{\max}) = \Lambda_\alpha \Lambda^{-1}$, and a transport equation:

$$\frac{\partial}{\partial t} \Phi + \nabla_\parallel [\mathbf{F}_n \vec{V} + \Delta \rho \mathbf{K} \Lambda_w \mathbf{F}_n [\vec{g}_\parallel + g_\zeta \nabla_\parallel (Z + h)]] = Q_n, \quad (11)$$

where $\Phi(h, \xi, \eta) = \int_Z^{Z+h} \phi(1 - s_{w,r}) d\zeta$ and $Q_n = \int_Z^{Z+h} q_n d\zeta$. This is the so-called h -formulation of the VE model. If ϕ and \mathbf{K} are constant in the ζ -direction, we get the following upscaled porosity and relative mobilities:

$$\Phi(h) = \phi(1 - s_{w,r})h + \phi s_{n,r}(h_{\max} - h), \quad \Lambda_n(h) = h \lambda_{n,e},$$

$$\Lambda_w(h, h_{\max}) = (h_{\max} - h)\lambda_{w,e} + (H - h_{\max})\lambda_w(1).$$

To simplify implementation and avoid having to treat the curvilinear grid explicitly, we express the transport equation in terms of global coordinates by writing $\vec{g}_\parallel + g_\zeta \nabla_\parallel (Z + h) = |g| \nabla_\parallel z_n$, where z_n is the true vertical position of the CO₂-brine interface, and approximating ∇_\parallel by ∇_{xy} to obtain:

$$\frac{\partial}{\partial t} \Phi(h, x, y) + \nabla_{xy} [\mathbf{F}_n \vec{V} + \Delta \rho \mathbf{K} \Lambda_w \mathbf{F}_n [|g| \nabla_{xy} (Z + h)]] = Q_n. \quad (12)$$

As an additional approximation, we consider h to be measured along \vec{e}_z . Errors associated with the transformation of the grid and the transport equation are discussed in more detail in Appendix A.

In the absence of viscous forces, the stationary state of the system is given by the balance between gravity and the ‘capillary pressure’ $\nabla_{xy} h$. Writing the transport equation in physical coordinates honors explicitly the condition from the underlying 3D model that a horizontal interface is a stationary state.

Example 1 Consider a simple 1D model with a sealing caprock given by

$$z_t = D - L_1 \sin\left(\frac{x}{L_1}\right) \tan \theta + A \sin\left(\frac{2\pi x}{L_2}\right), \quad (13)$$

where D is maximum depth, $\theta = 0.03$ is the initial tilt angel, $L_1 = 20$ km is the characteristic length of the antiformal structure, and $L_2 = 0.3$ km is the wave-length L_2 of the small-scale structures; see Fig. 4. For the amplitude, we use either $A = 0$ or $A = 2$ m. The density of CO₂ is assumed to follow a model taken from [51] with a temperature variation given by

$$T = zK_T + T_s, \quad K_T = 30\text{K/km}, \quad T_s = 286\text{K}. \quad (14)$$

Given a hydrostatic pressure computed from a constant brine density of 1100 kg/m³, there will be different regimes of density variation depending on the depth of the aquifer as shown in Fig. 4. Here, we set $D = 2300$ m, at which the variation in density is relatively small. (The temperature varies from 335 to 357 K). In all calculations, we use isotropic permeability of 1 Darcy and constant porosity of 0.2. The brine and rock volumes are considered to be linear functions of pressure, with respective coefficients $4.3 \cdot 10^{-5} \text{ bar}^{-1}$ and $1.0 \cdot 10^{-5} \text{ bar}^{-1}$, based on a reference pressure of 100 bar. The storage scenario consists of 50 years of injection at an annual rate of $760 \cdot 10^6$ kg/year. The model is discretized with 1000 uniform grid cells, and we use uniform time steps of 2 years during the injection period and 20 years during the subsequent 2000 year migration period.

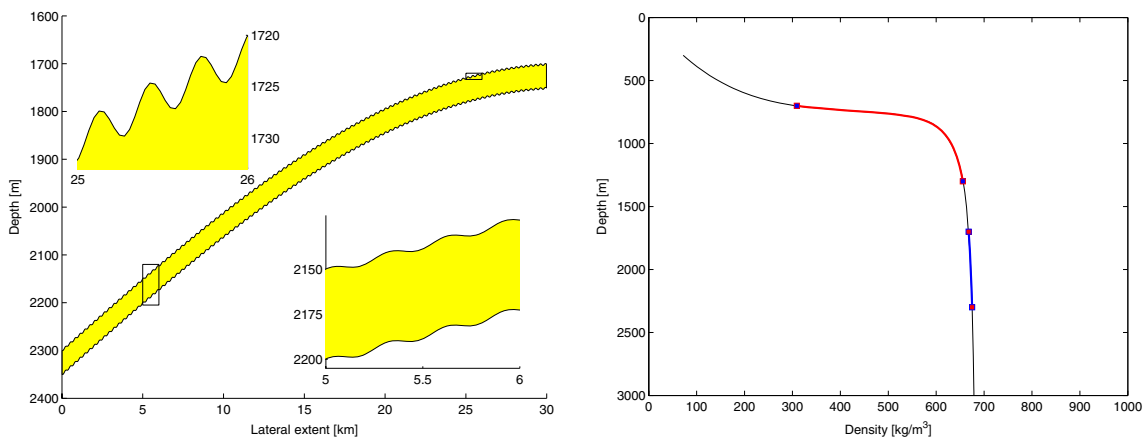


Fig. 4 Left: the geometry of Example 1. Right: the density of CO₂ given hydrostatic pressure; the blue line represents a deep model with $D = 2300$ m and the red line corresponds to a model with $D = 1300$. (From showAquiferModel.m and showDensityVariation.m)

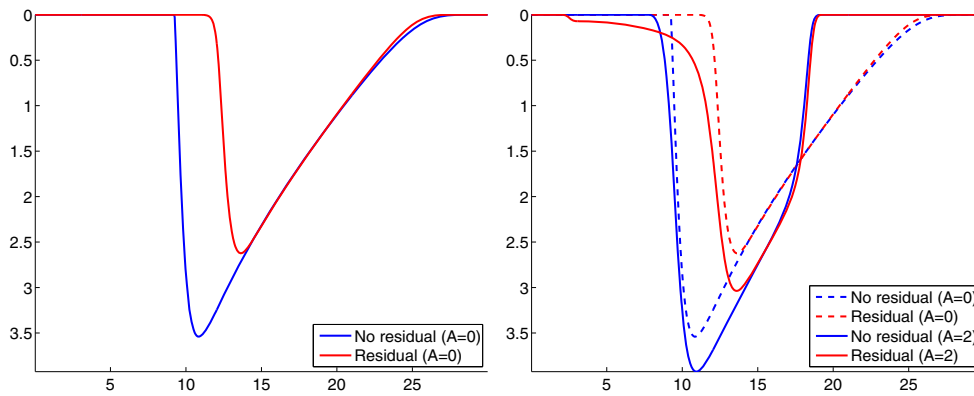


Fig. 5 Thickness of the CO₂ plume simulated by sharp-interface models for the 1D sloping aquifer in Example 1 after approximately 700 years. The *left plot* shows the effect of extending the basic model (*blue line*) with residual trapping (*red line*) for a surface without small-scale structures. In the *right plot*, these two outcomes

(shown as *dashed lines*) are compared with calculations that also include small-scale undulations; in the plot, the solutions are averaged over a region that is larger than the small-scale undulations. (From residualExample.m)

In its simplest form, the VE model describes a plume that continues to migrate upward until it either reaches the top of the formation, or until all of the CO₂ has become trapped in geometric structures in the caprock. If nonzero residual saturation is introduced, the migrating plume will leave behind a trail of residually trapped CO₂. As a result, the tail of the plume will move faster than the tip, which means that CO₂ injected into an infinite aquifer without structural traps will only spread a finite distance, see [52]. The left plot of Fig. 5 compares plume thickness computed with and without residual trapping after 700 years.

The presence of small-scale variation (rugosity) in the top seal will generally lead to trapping of small amounts of CO₂, thereby retarding the migration of the plume [33]. This, in turn, changes the solution to also include a shock at the front of the plume, as seen in the left plot of Fig. 5 and in more detail for the case with no residual trapping in Fig. 6. In Section 4.1, we will develop effective relative-permeability models that capture the retardation effect caused by caprock rugosity.

The four simulations were performed using a general-purpose, fully-implicit black-oil solver from MRST [12]; more details will be given in the next section. Computational costs are reported in Table 1. With residual trapping and rugosity, the prescribed 20-year time step is straddling the stability limit and hence the nonlinear solver was forced to halve many of the time steps, which explains the significant increase in CPU time. On the other hand, the relatively high computational cost is a MATLAB artifact that poorly reflects the efficiency of the underlying algorithm: With only 1000 cells in the model, the computational overhead induced by the combination of MATLAB and automatic differentiation is significant. In these particular runs, only 3 % of the total CPU time was spent solving linear systems. This is a known issue with MRST, which is significantly diminished if one goes to models with more unknowns.

Finally, we compare the simulation outcome of the VE model with that of a full 3D model for the case with smooth caprock ($A = 0$). The 3D model has a vertical resolution of 30 cells, with progressively thinner cells towards

Fig. 6 Sharp-interface simulation of the 1D aquifer with small-scale undulations in the top surface. The thin oscillatory *black line* is the thickness of the CO₂ plume after approximately 700 years and the *thick line* is the average. The *upper inlet* shows a magnification of the *red square*, while the *lower inlet* shows the corresponding vertical fluid distribution in the real coordinate system. (From residualExample.m)

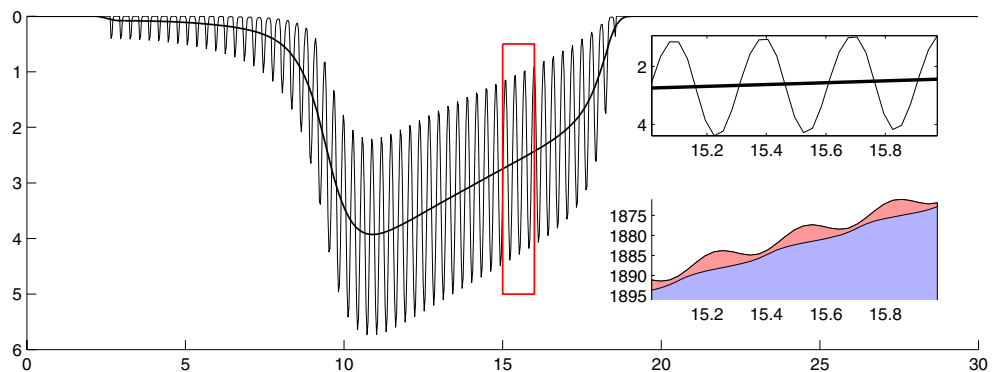


Table 1 Computational cost for the simulations in for Example 1 observed using MRST 2015a with MATLAB R2014a on an Intel Xeon 3.47 GHz CPU

	No residual	Residual
Smooth caprock	42 s	63 s
Caprock with rugosity	64 s	172 s

the top of the aquifer to better resolve the shape of the plume. The lateral resolution is 200 cells for both models. We use linear relative permeabilities and zero capillary pressure. As we can see from the left plot in Fig. 7, there is an almost perfect match between the models without residual saturation, except that plume in the 3D simulation has a characteristic staircase shape that will be present in all 3D simulations unless the width of the capillary fringe exceeds the height of the grid blocks. When residual saturation is included, the match between models still remains close. The required computational times to simulate 2000 years of migration using our laptop (Core i7-4500U processor, 8 GB RAM) for the VE simulations without/with residual saturations were 64 and 66 s, respectively. For the corresponding 3D simulations, the runtimes were 673 and 1005 s. We emphasize, however, that neither the VE nor the 3D simulation codes have been optimized for speed.

The simple aquifer geometry introduced above will be used repeatedly throughout the paper as a means to illustrate and discuss how including additional physical mechanisms affects the plume migration. In the next example, we consider a scenario with a touch of more geological realism.

Example 2 The Pliocenesand model from the CO₂ Storage Atlas [53] consist of 13,484 active cells and describes

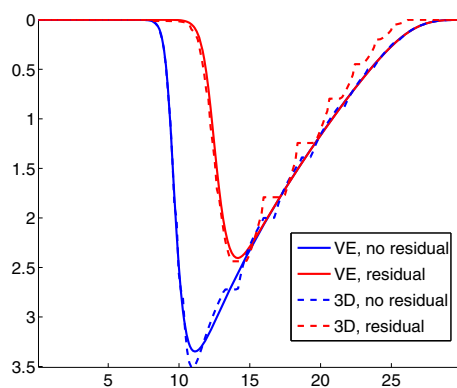
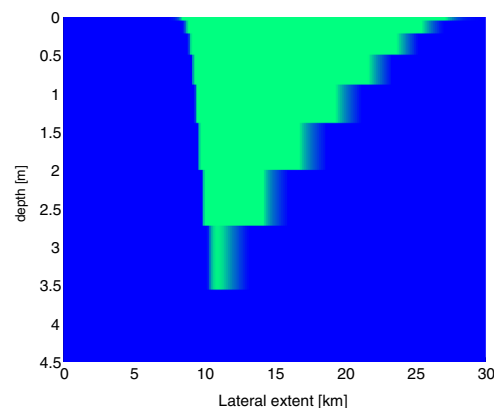


Fig. 7 Comparison between the VE models and corresponding full 3D models for the 1D sloping aquifer in Example 1 after approximately 700 years. The *left plot* compares the plume thicknesses resulting from VE and 3D simulations with (*red*) and without (*blue*) residual trapping included. The *right plot* illustrates the upper 4.5 m of the aquifer

a ridge ending in a large plain. The actual sand body lies too shallow to be a candidate for CO₂ storage, but the model can be used as a test case if we increase its burial depth to, e.g., a thousand meters. The top surface has almost no fine-scale structure and thus allows for a very low percentage (0.02 %) of structural trapping compared to the overall volume of the whole sand body. To store CO₂, one should therefore primarily consider residual and solubility trapping. We set the pressure to 100 bar at the top point and assume a homogeneous porosity of 25 % and a homogeneous, isotropic permeability of 1200 mD. Ten mega-tonnes of CO₂ are injected annually for 50 years from a single injection point halfway down the slope. Brine has constant density 975.86 kg/m³, viscosity 0.3086 cP, residual saturation equal 0.1, and an end-point mobility of 0.2142. The CO₂ phase has constant density 686.54 kg/m³, viscosity 0.056641 cP, residual saturation 0.2, and an end-point mobility of 0.85. In the simulation, we use time steps of 2 years during injection and 10 years afterward.

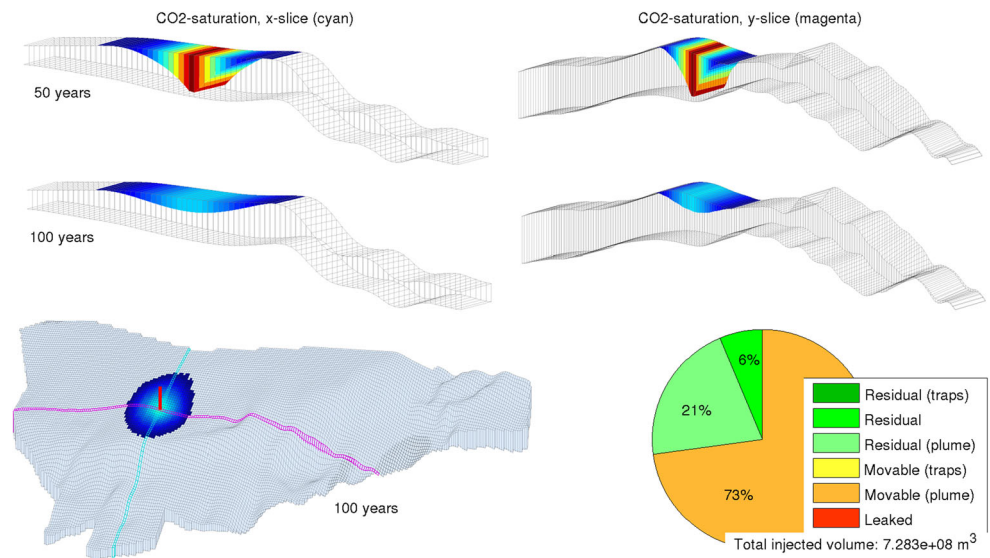
The injected CO₂ plume moves upward towards the plain, leaving behind a trail of residually trapped CO₂. Figure 8 shows the CO₂ plume at the end of injection and after 100 years along with an instantaneous volumetric inventory. From the pie chart, we see that 6 % of the injected CO₂ has been residually trapped after 100 years, while the remaining volume is still inside the plume. However, a significant fraction of the plume volume (20 % of the injected volume) will eventually remain as residually trapped when the plume leaves its current position.

After 500–600 years, the tip of the plume has crossed the upper plain and reached the open boundary. The amount that leaks will roughly be proportional to the square of the plume thickness. Since the tip of the plume is very thin and the caprock is almost horizontal, the leakage is insignificant



3D model (flattened, for presentational clarity) and the CO₂ saturation after approximately 700 years for the case without residual trapping. The complete phase segregation is evident, and we also see how the vertical grid discretization is related to the ‘staircase’ shaped curves shown on the *left plot*

Fig. 8 Injection into the Pliocenesand aquifer from a single injection point. The plots show fluid distribution at the end of the injection and after 50 years of migration, as well as an inventory of the trapping observed after 100 years. (From firstPlioExample.m)



at first and only visually noticeable in the CO₂ inventory in Fig. 9 after another 200–300 years. At the end of simulation, only 3 % has left our computational domain, and the mobile CO₂ has reached a region with a very low sloping angle and is thus almost immobilized.

Figure 10 reports CPU time per step in a sequentially implicit simulator that utilizes a standard two-point pressure solver and a fully-implicit transport solver from the `incomp` module of MRST [10] and a fully-implicit black-oil solver based on automatic differentiation [12]. Both simulators have time-step control and will, if necessary, reduce the time steps to ensure convergence. During the injection period, the flow is dominated by the ‘advective’ $\mathbf{F}_n \vec{V}$ term in Eq. 12 resulting from heightened pressure in the near-well region, and the sequentially implicit solver is significantly more efficient, partially because of the significant overhead in the black-oil solver as discussed in Example 1. During the first 600 years after injection ceases, the migration is dominated by the hyperbolic $\nabla_{xy}Z$ term in

Eq. 12, and the two simulators are equally efficient. After this point, the parabolic $\nabla_{xy}h$ term, which here plays the role of capillary forces in a conventional flow model, gradually becomes more important. The influence of the parabolic transport terms is more difficult to resolve in a sequential formulation and hence we see a gradual increase in the CPU time of each transport step. After 1260–1280 years, most of the mobile plume has reached the flat plane, and the plume is approaching a steady state. The dynamics of this state is governed mainly by the coupling of the gravitational $\nabla_{xy}Z$ and the parabolic $\nabla_{xy}h$ term and the effects of these terms in the pressure equation. These forces seek to enforce a flat interface between the CO₂ plume and the underlying brine. Operator-splitting methods, and in particular methods based on a total velocity formulation, are not suited for cases with such strong coupling between pressure and transport. In our case, the transport solver has to aggressively cut the time steps, which results in a dramatic increase in the CPU time. The fully-implicit formulation, on the other hand, is robust

Fig. 9 Detailed inventory of the CO₂ trapping process in the Pliocenesand formation over a period of 1500 years. (From firstPlioExample.m)

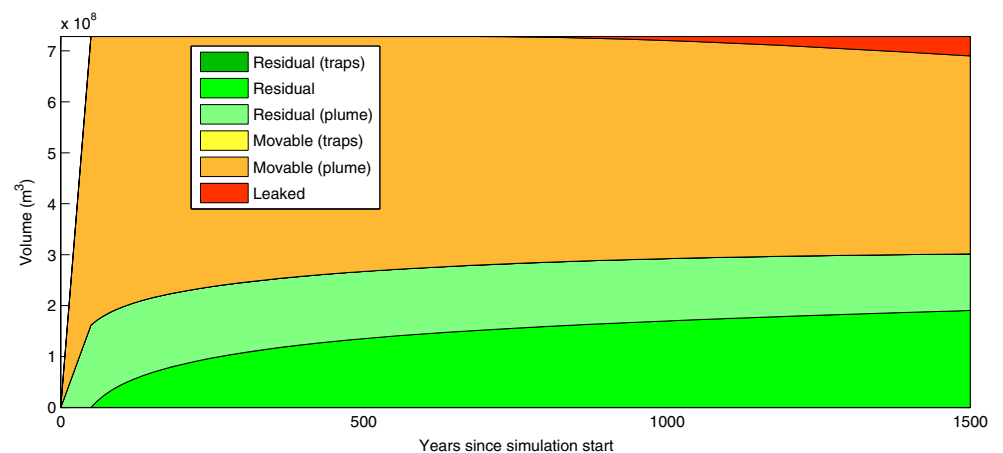
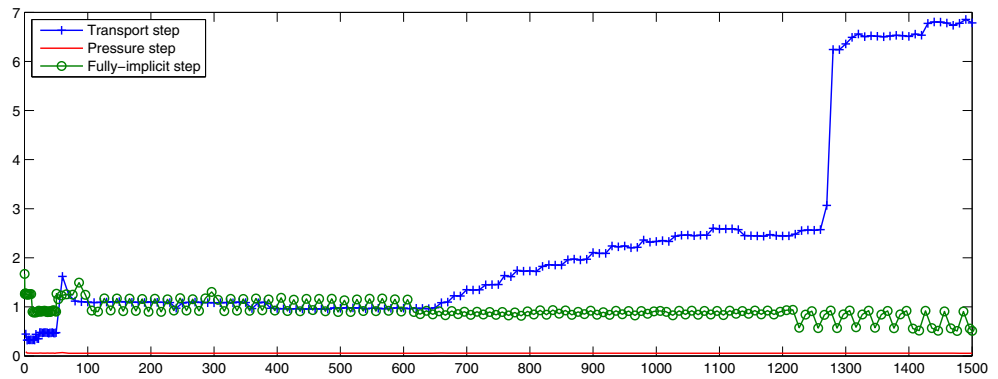


Fig. 10 CPU times in seconds for each step in a sequentially implicit simulation and in a fully-implicit, black-oil type simulation of the Pliocenesand injection measured for MRST 2015a with MATLAB R2014a on an Intel Xeon 3.47 GHz CPU



with respect to changing force balances and can, in particular, accurately resolve the near steady-state towards the end of the simulation.

As an alternative to using h as the primary unknown, one can use the fractional content $S = h/H$ of CO_2 in the vertical column to derive the so-called S -formulation having equations that look like standard pressure and transport equations known from the petroleum literature with S playing the role of saturation. In the rest of the section, we will detail the derivation for vertically homogeneous rock properties ϕ and \mathbf{k} . By integration over the column, it is easy to show that:

$$\begin{aligned} S(h, h_{\max}) &= \frac{h(1-s_{w,r})+(h_{\max}-h)s_{n,r}}{H}, \\ S_{\max}(h_{\max}) &= \frac{h_{\max}(1-s_{w,r})}{H}. \end{aligned} \tag{15}$$

where we recall that $s_{w,r}$ and $s_{n,r}$ are constants. Inversely, h can be written in terms of S and S_{\max} :

$$\begin{aligned} h(S, S_{\max}) &= H \frac{S(1-s_{w,r})-S_{\max}s_{n,r}}{(1-s_{w,r})(1-s_{w,r}-s_{n,r})}, \\ h_{\max}(S_{\max}) &= \frac{HS_{\max}}{1-s_{w,r}}. \end{aligned} \tag{16}$$

To obtain a set of standard transport equations formulated in S , we transform our coordinate system so that $Z \equiv 0$ and then write:

$$\begin{aligned} \Lambda_n(S, S_{\max}) &= \frac{1}{H} \left[\int_0^h \lambda_{n,e} \mathbf{k}_{\parallel} d\zeta \right] \mathbf{K}^{-1} = \frac{h(S, S_{\max})}{H} \lambda_{n,e} \\ \Lambda_w(S, S_{\max}) &= \frac{1}{H} \left[\int_h^{h_{\max}} \lambda_{w,e} \mathbf{k}_{\parallel} d\zeta + \int_{h_{\max}}^H \lambda_w(1) \mathbf{k}_{\parallel} d\zeta \right] \mathbf{K}^{-1} \\ &= \frac{h_{\max}(S_{\max})-h(S, S_{\max})}{H} \lambda_{w,e} + \frac{H-h_{\max}(S_{\max})}{H} \lambda_w(1) \end{aligned}$$

where the last equality sign in each equation assumes vertically constant rock properties. This formulation is easy to implement in a standard reservoir simulator; all one has to do is to replace the evaluation of mobility and capillary pressure functions by special functions that compute vertically integrated quantities. Likewise, the S -formulation is a more natural starting point when extending the vertical equilibrium model to black-oil type models or including physical effects like compressibility and hysteresis. A more detailed discussion of hysteresis is given in [50].

4 Extending with more flow physics

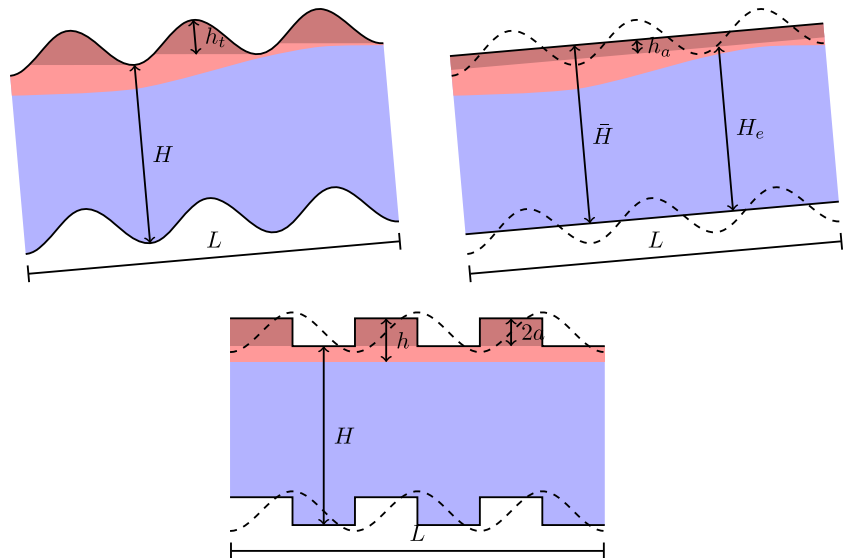
In this section, we present a general formulation that includes residual trapping, compressibility, dissolution, and resulting hysteresis effects. Apart from capillary fringe, which is discussed in [50], our models incorporate the physical effects discussed by Gasda et al. [30], but the formulation and notation will follow that of standard black-oil models used in the petroleum industry (see Appendix B) to make similarities and differences with models implemented in standard simulators as clear as possible.

The effects discussed in this section can be divided in two categories. The first category consists of capillary and hysteretic effects, which change effective mobilities and capillary pressures, and whose upscaled effect can be derived from considering one vertical column at a time. In Example 1, we also saw how small amounts of CO_2 trapped inside small-scale undulations in the top surface may retard the plume migration, which will in turn lead to hysteretic effects and changes in the effective mobility. Retardation phenomena of this form can therefore also be included in the first category. The second category includes compressibility, which affects the form of the mass balance equations and dissolution that also changes the number of unknowns and equations.

4.1 Sub-scale caprock variations

In potential CO_2 storage sites, the top surface that separates the permeable aquifer from the overlying caprock will have natural variability that spans several length scales. Whereas the characteristic dip angle caused by regional uplift may be constant for hundreds of kilometers, the topography on a kilometer scale will be more varied and contain different types of antiform structures (domes, anticlines, traps, etc) that can be identified from seismic surveys. In [33], it was demonstrated that various kinds of roughness straddling the scale of seismic resolution will impact the plume and potentially cause significant retardation in its updig migration. On an even smaller scale, the top surface is

Fig. 11 Upscaling of small-scale caprock undulations. *Upper left:* the representative volume to upscaled, where h_i is the height of the CO₂ column inside the sub-scale traps. *Upper right:* the sub-scale undulations have been replaced by a flat accretion layer inside which CO₂ is immobile, giving an aquifer with a reduced effective height H_e . *Lower:* sub-scale undulations are assumed to be step functions of amplitude a and the dip angle is disregarded to simplify the analytic calculation of upscaled relative permeability



characterized by submeter fluctuations that can only be observed in outcrop studies. Effective models that capture sub-scale roughness and rugosity effects [34, 35] are generally needed to study realistic migration scenarios, because even though VE models are highly efficient, they cannot resolve all relevant structural features in large-scale formations. Here, we briefly review such effective models based on analytical and numerical upscaling techniques for the case without residual trapping in 1D. Figure 11 shows a schematic of our conceptual setup.

In the simplest approach to upscaling, we assume that caprock undulations create a volume in which CO₂ becomes trapped and cannot flow. This volume is represented as a layer of zero horizontal permeability (accretion layer), whose thickness is constant over the averaging length $h_a = \frac{1}{L} \int_0^L h_i(x) dx$, see Fig. 11 for notation. Introducing the accretion layer reduces the effective height that is accessible to fluid flow to $H_e = \bar{H} - h_a$, where \bar{H} is the mean aquifer thickness over the length scale L . This model cannot distinguish the effect of different caprock topographies that give the same trapped volumes.

To capture the effect of sub-scale undulations more accurately, we average the depth-integrated rock and rock-fluid properties in the horizontal direction. For permeability, we use a simple homogeneous-equation approach for a periodic medium [54], resulting in an effective permeability $\bar{K} = [(\bar{H}/L) \int_0^L (KH)^{-1} dx]^{-1}$. For the relative mobilities, we use a steady-state method that assumes periodicity in the lateral direction (inflow across the left boundary equals outflow across the right boundary) and computes average relative permeabilities as function of volume-averaged saturations values \bar{S} . We start by observing that the total velocity is zero after injection has ceased. To obtain a steady-state

solution that corresponds to a given average saturation \bar{S}^i inside our averaging volume, we can therefore solve

$$\phi \partial_t s^i + \nabla \left[\mathbf{k} \frac{\lambda_w \lambda_n}{\lambda_w + \lambda_n} (\Delta \rho \vec{g} + \nabla p_c) \right] = 0, \quad s^i(\vec{x}, 0) = \bar{S}^i, \tag{17}$$

until steady state subject to periodic conditions in the x -direction and no flow across the top and bottom surfaces. For each steady-state solution $s^i(\vec{x})$, we reconstruct phase pressures from

$$\nabla \vec{v}_\alpha^i = 0, \quad \vec{v}_\alpha^i = -\mathbf{k} \lambda_\alpha(s_\alpha^i) \nabla [p_\alpha^i - \rho_\alpha \vec{g}] \tag{18}$$

subject to a pressure drop Δp in the x -direction and no flow across the top and bottom surfaces. This gives averaged phase fluxes F_α , which can be combined with the upscaled Darcy’s law for each phase, $F_\alpha = -\bar{H} \bar{K} \bar{\Lambda}_\alpha \Delta p / L$, to derive values for $\bar{\Lambda}_\alpha$. By repeating this procedure for an increasing sequence of saturation values, we can compute a set of averaged mobilities $\bar{\Lambda}_\alpha$ as function of \bar{S} or an equivalent average plume height \bar{h} .

Analytical expressions can be defined if we make further simplifying assumptions [34]. First, we can approximate the fine-scale undulations by a geometric form defined relative to a top surface that is flat on the averaging scale; see the lower plot in Fig. 11. With a sharp interface assumption, it then follows that

$$\bar{\Lambda}_n = \left[\frac{\bar{H} \bar{K}}{L} \int_0^L \frac{1}{h K \lambda_{n,e}} dx \right]^{-1}, \tag{19}$$

$$\bar{\Lambda}_w = \left[\frac{\bar{H} \bar{K}}{L} \int_0^L \frac{1}{(H-h) K \lambda_w(1)} dx \right]^{-1}.$$

Second, for small pressure gradients and an averaging scale much smaller than the total domain, we assume that the CO₂–brine interface is flat on the fine scale so that $h(x)$

is a simple function of the function describing the surface topography and Eq. 19 can be computed analytically. From the form of Eq. 19, we also see that $\bar{\Lambda}_n = 0$ if $h(x) = 0$ at some point, and hence, CO₂ will only be able to flow if the interface with brine lies deeper than the lowest point in the local topography.

Example 3 To compare the simple accretion layer model with effective models obtained by assuming sinusoidal or square undulations, we revisit the 1D aquifer from Example 1. In the true model, we set $A = 2$ and use the different upscaled relative permeabilities to compute approximate solutions for the model geometry without undulations ($A = 0$). Because the large-scale structure of the aquifer is the left half of an antiform, the thickness of the CO₂ layer that will be trapped inside small-scale undulations can simply be computed as $h_t(x) = \max_{r \geq x} z_t(r) - z_t(x)$. Then, the resulting function $h_t(x)$ is averaged over a length scale $L \gg L_2$ to obtain

$$a(x) = \left[\int_{-L/2}^{L/2} h_t(x+r)w(r) dr \right] / \left[\int_{-L/2}^{L/2} w(r) dr \right],$$

where w is a standard Gaussian mollifier function. Figure 12 illustrates the different steps of this estimation process.

Figure 13 compares the true plume depth with approximate solutions obtained by the accretion-layer model and the two analytical approaches. One might have expected that the model based on sinusoidal substructure would be closest to the fine-scale simulation, but by a coincidence, the simple accretion-layer model is most accurate. The plot to the right in Fig. 13 compares the relative permeabilities of the three effective models with the numerically upscaled relative permeability sampled at three different dip angles $\theta = 0, 0.0162$, and 0.03 that correspond to the angle at the top, midway and at the deepest point of the actual formation, respectively. The plot shows that when the height of the tip of the plume is in the range 2–4, the relative permeability

of the accretion-layer model is much closer to those of the numerically upscaled models, and this model will therefore give the best match for the front shock speed. The accretion curve is significantly different from the numerically upscaled curves for $\theta < 0.03$, and hence, this model cannot be expected to provide a good approximation towards the top of the antiform. We also note that whereas the trailing rarefaction wave seen in the fine-scale solution can be explained by the convex shape of the numerically upscaled relative permeability, it cannot be predicted by the concave curves of the ‘sinus’ and ‘square’ effective models. Better coarse-scale simulation can be obtained by introducing effective models that depend on both the local trapping volume and the local dip angle. In 2D, this would immediately involve tensorial relative-permeability effects.

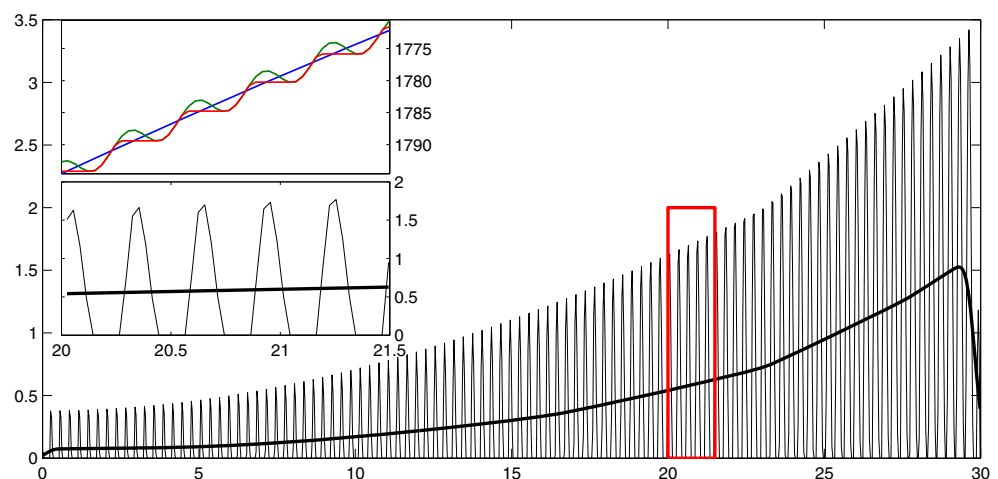
4.2 Compressibility and dissolution

In this section, we extend the basic VE model to compressible flow including dissolution of CO₂ into brine and write the resulting model as a set of two-dimensional, two-phase, black-oil equations. We start by writing the upscaled Darcy’s law for each phase as,

$$\begin{aligned} \bar{v}_w &= -\lambda_w(p_w, s_w, s_{\max})[\nabla p_w - g\rho_w(p_w, c)\nabla Z], \\ \bar{v}_n &= -\lambda_n(p_n, s_n, s_{\max})[\nabla p_n - g\rho_n(p_n)\nabla Z]. \end{aligned} \quad (20)$$

Here, lower-case symbols have been used to emphasize the similarity with the standard black-oil model and will henceforth represent upscaled quantities unless specified otherwise. The water phase is assumed to consist of brine containing a concentration c of dissolved CO₂, while hysteretic effects are modeled by tracking the maximal saturation s_{\max} , as defined in Eq. 15. The viscosities, relative permeabilities, and densities all depend on pressure, but are assumed to be constant within the vertical column of the underlying 3D model. Unlike in Section 3, we now operate with distinct phase pressures p_α , which are evaluated at the

Fig. 12 Estimation of the parameter characterizing sub-scale undulations. The *thin line* is the local trap height $h_t(x)$ and the *thick line* is the averaged height $a(x)$. The *lower inlet* shows a zoom of $h_t(x)$ and $a(x)$ inside the *red square*. The *upper inlet* zooms in on the top surface (green), the spill-point level of the local traps (red), and the top surface for the model without small-scale undulations (blue). (From `upscaleRelPerms.m` and `showUpscaledRelperms.m`)



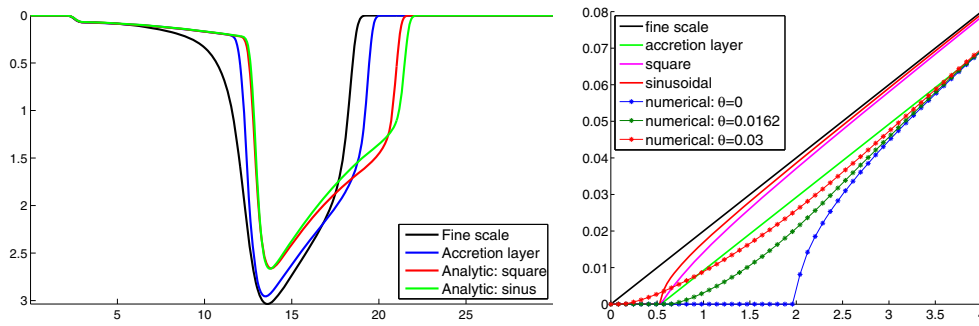


Fig. 13 Upscaling of sub-scale caprock topography. *Left*: The fine-scale solution compared with approximate solutions computed using an accretion-layer model and two analytical models that assume sinusoidal and square sub-scale undulations, respectively. *Right*: The corresponding upscaled relative permeabilities shown as functions of

h and sampled at $x = 20$ km. In addition, *lines with markers* show effective relative permeabilities obtained by direct numerical upscaling of the 1D aquifer model for three different dip angles θ . (From `upscalingExample.m` and `showUpscaleRelPerms.m`)

top surface. In other words, p_α refers to pressures defined in cells of the 2D surface grid that follows the caprock topography and should not be confused with pressures inside cells of a 3D volumetric model. If $p_{\alpha,i}$ represents the fine-scale phase pressures at the CO_2 -brine interface, it follows by assuming hydrostatic conditions that

$$\begin{aligned} p_w &= p_{w,i} - g\rho_w h, \\ p_n &= p_{n,i} - g\rho_n h, \\ p_c &= p_n - p_w = p_e + g\Delta\rho h \end{aligned} \tag{21}$$

Here, $p_e = p_{n,i} - p_{w,i}$ is the fine-scale entry pressure, whereas p_c can be understood as an upscaled ‘capillary pressure’. Because h can be obtained from the upscaled saturation by Eq. 16, the relation between the phase pressures can be written as a function of saturation and pressure:

$$p_w = p_n - p_c(p, s_n, s_{\max}) \tag{22}$$

In a standard black-oil model, p_c is usually a function of s_n and s_{\max} only. To evaluate densities, we introduce the (reciprocal) formation-volume factors b_α for each phase, which relate the densities at reservoir conditions to the densities $\rho_{\alpha,s}$ at surface conditions

$$\begin{aligned} \rho_w(p, c) &= (\rho_{w,s} + c\rho_{n,s}) b_w(p, c), \\ \rho_n(p) &= \rho_{n,s} b_n(p). \end{aligned} \tag{23}$$

Next, the conservation of CO_2 , water, and dissolved CO_2 is written as

$$\begin{aligned} \frac{\partial}{\partial t} [\phi b_n s_n + \phi c b_w (1 - s_n)] + \nabla \cdot [b_n \vec{v}_n + c b_w \vec{v}_w] &= q_n, \\ \frac{\partial}{\partial t} [\phi b_w (1 - s_n)] + \nabla \cdot (b_w \vec{v}_w) &= q_w, \\ \frac{\partial}{\partial t} [\phi c b_w (1 - s_n)] + \nabla \cdot (c b_w \vec{v}_w) &= q_{n,\text{dis}}. \end{aligned} \tag{24}$$

The effect of dissolution on long-term CO_2 storage has been widely discussed, and in particular, the possibility of enhanced dissolution because of convective mixing [55–57]. For an overview of this topic see [58]. The studies are predominantly theoretical and carried out for homogeneous

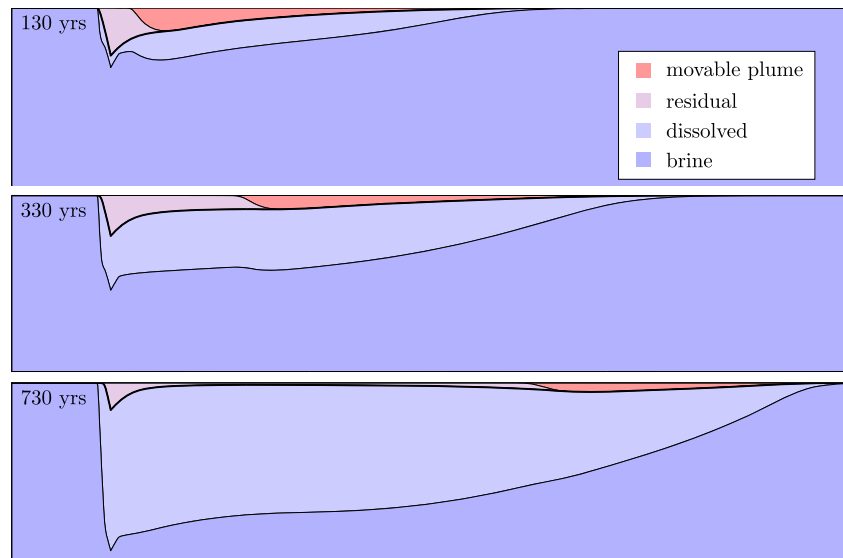
systems or idealized heterogeneous cases, see [59]. For real cases, the only data on dissolution rates is an estimated upper limit of 1.8 % per year for the Sleipner injection [60]. This estimate is consistent with a later study based on inversion of gravimetric data [61]. For convective mixing in porous media, one can only find indirect evidence of dissolution for analogous problems like salt dissolution, [62, 63]. Even for convection of heat, the few conclusive measurements are of convection induced purely by heating from below, see [64, 65] for reviews.

Despite the uncertainty that surrounds dissolution, we have included this effect in our models to be able to illustrate how dissolution may potentially affect the long-term fate of injected CO_2 . For a standard black-oil type of equation, the dissolution of gas is assumed to be instantaneous as long as the fluid phase is undersaturated. That is, the concentration c corresponds to the solution gas/oil ratio r_s used for petroleum systems. To mimic this type of model, we drop the last conservation law in Eq. 24 and set $c = c_{\max}$ and $s_{\max}(t) = \max_{\tau \leq t} s_n(\tau)$ wherever $s_n > 0$. We refer to this as the *instantaneous dissolution model*. Compared with the general black-oil formulation in Appendix B, this would be a model in which brine is given the role of the oleic phase and the supercritical CO_2 is given the role of the gaseous phase.

More accurate modeling of dissolution will introduce two main changes compared with traditional black-oil models: (i) dissolution is rate limited and (ii) dissolution affects the hysteresis variable,² i.e., s_{\max} or h_{\max} which tracks the maximum height at which CO_2 exists. The CO_2 will dissolve into brine from the layer of residual CO_2 saturation

²Here, hysteresis refers to the vertically-integrated equations and should not be confused with path-dependence between different imbibition and drainage curves in the fine-scale relative permeability and capillary functions, which is discussed in more detail in [36–38, 50]. Because of the sharp-interface assumption, only the end states of the bounding curves enter the equations.

Fig. 14 Evolution of the CO₂ distribution for $D = 1300$ m, $A = 0$, residual saturation, and rate-dependent dissolution. (From `dissolutionExample.m`)



that separates the brine phase from the free CO₂ plume, or directly from the plume when no such layer is present (i.e., when $s_{\max} = s_n$). In MRST-co2lab, the corresponding dissolution rate is modeled as

$$q_{n,\text{dis}} = \begin{cases} C\phi, & \text{if } s_{\max} > 0 \text{ and } c < c_{\max}, \\ 0, & \text{otherwise.} \end{cases} \quad (25)$$

The dynamics of the maximal saturation s_{\max} used to model hysteresis is represented using two different equations. The first equation describes how dissolution of CO₂ that is residually trapped below the free plume causes s_{\max} to decay

$$\frac{\partial b_n s_{\max}}{\partial t} = -q_{n,\text{dis}}, \text{ if } s_{\max} > s_n, \quad (26)$$

whereas the second equation states that s_{\max} increases with s_n in regions where CO₂ is invading or stagnant,

$$\frac{\partial s_{\max}}{\partial t} = \frac{\partial s_n}{\partial t}, \text{ if } s_{\max} = s_n. \quad (27)$$

Note that s_{\max} can never be less than s_n by definition. We call this the *rate-dependent dissolution model*.

Example 4 To include compressibility effects, we move our 1D aquifer to a depth between 1300 and 850 m. Figure 14 shows the evolution of the CO₂ plume for the case with rate-dependent dissolution and a top surface without small-scale undulations. Figure 15 illustrates how small-scale caprock undulations can effect the plume dynamics. In the top plot, we see how the interplay between undulations and tilt angle gives areas with very thin plume. To resolve these variations in an upscale sense, the effective relative permeability curves discussed in Example 3 obviously should be spatially dependent. In the bottom plot, we see that the residually trapped CO₂ is converted to dissolved CO₂

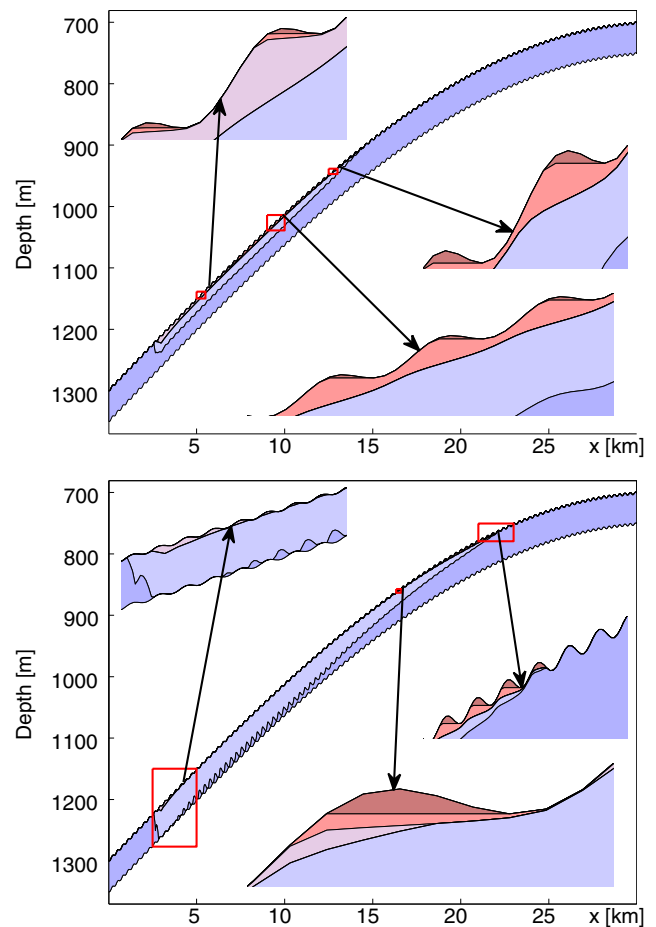
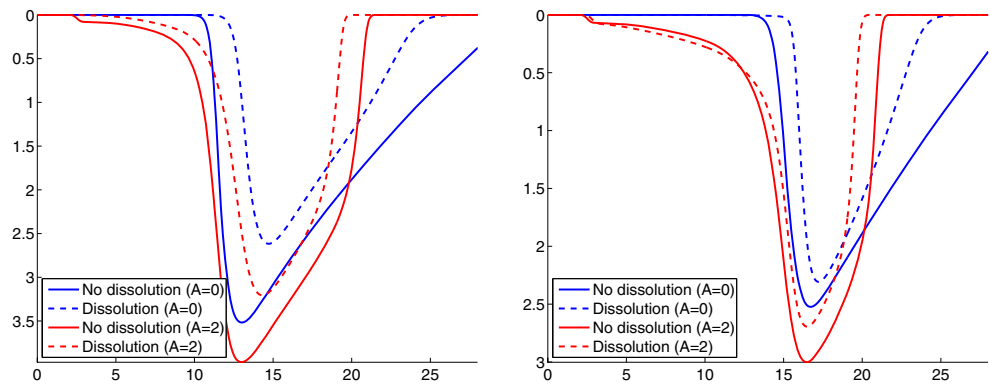


Fig. 15 The CO₂ distribution in global coordinates after 330 years (*top*) and after 930 years (*bottom*) for the case with compressibility, residual saturation, and rate-dependent dissolution. (From `dissolutionExample.m`)

Fig. 16 The flowing CO₂ phase 900 years after the injection has stopped. *Dashed/solid lines* denote models with/without rate-dependent dissolution, whereas *red/blue colors* signify cases with/without small-scale caprock undulations. The residual saturation is $s_{w,r} = 0$ to the left and $s_{w,r} = 0.2$ to the right. (From `dissolutionExample.m`)



except near the well, whereas near the tip of the plume, most of the CO₂ is trapped inside the small-scale undulations. Finally, Fig. 16 compares the flowing CO₂ computed by different VE models and shows how small-scale undulations retard the plume migration, whereas residual trapping and dissolution both reduce the thickness of the plume; dissolution also reduces the thickness of the layer of residual CO₂.

In the next example, we will compare the instantaneous and rate-dependent dissolution models on the Pliocenesand model.

Example 5 The Pliocenesand formation introduced in Example 2 is assumed to have a burial depth of at least 1200 m and a rock compressibility of 10^{-5} bar^{-1} . An annual amount of 5 Mt/year is injected over 50 years from a single injection well located at model coordinates (485, 6647) km. Both brine and CO₂ are compressible: brine has constant compressibility equal $4.3 \cdot 10^{-5} \text{ bar}^{-1}$, whereas the density of the CO₂ follows the Span & Wagner PVT model [51] as computed by the open-source `coolprop` package [66] with surface density equal 760 kg/m³. The dissolution process is assumed to either be non-existent, instantaneous, or follow (25) with $C = 0.05 \text{ m/year}$ and $c_{\text{max}} = 0.03$. This gives is a value which is in the range estimated in the literature [55, 56, 67]. Figure 17 illustrates how one

can conceptually think of the fluid distributions in the three resulting sharp-interface models.

Figure 18 shows two snapshots of the evolution of the CO₂ plume along with detailed carbon inventories resulting from the three different simulation models. Several interesting effects can be observed: Without dissolution, the plume will leave behind a relatively large amount of residual CO₂ as it propagates in the upslope direction. After approximately 750 years, the tip of the plume has reached the outskirts of the flat plain (seen to the left in the two snapshots) and starts to exit the simulated domain through the open boundary. After 3000 years, 24 % of the injected CO₂ has left the formation, 20 % is still free to move, while the remaining 56 % can be considered safely stored. With instantaneous dissolution, on the other hand, a large fraction of the injected CO₂ will be dissolved and this will retard the plume migration so that the tip of the plume does not reach the open boundaries within the simulation period. After 3000 years, 99.6 % of the injected CO₂ can be considered safely stored. With rate-dependent resolution, the retardation effect is much less than with instantaneous dissolution and the tip of the plume therefore reaches the outer boundary after approximately 1500 years and starts to leak. By comparing the two upper plots, we also see that the gradual dissolution causes the extent of the residual CO₂ to retract during the 500 year period between the snapshots. After 3000 years, 78 % of the injected CO₂ is dissolved, 6 % is

Fig. 17 Conceptual fluid distribution in the three different sharp-interface models used to study the effects of dissolution on the Pliocenesand formation. (In reality, the CO₂-saturated brine will be denser than the resident brine and hence sink to the bottom)

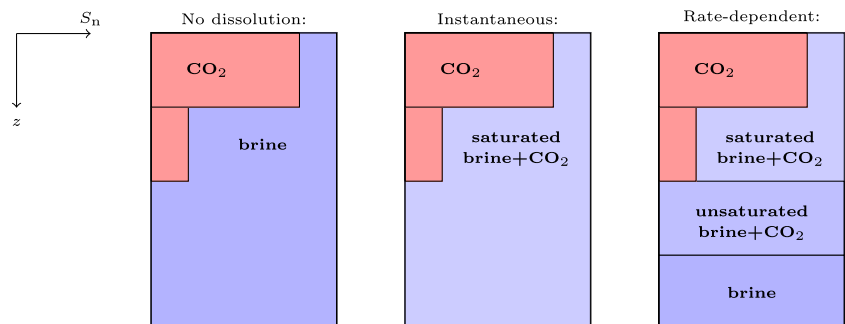
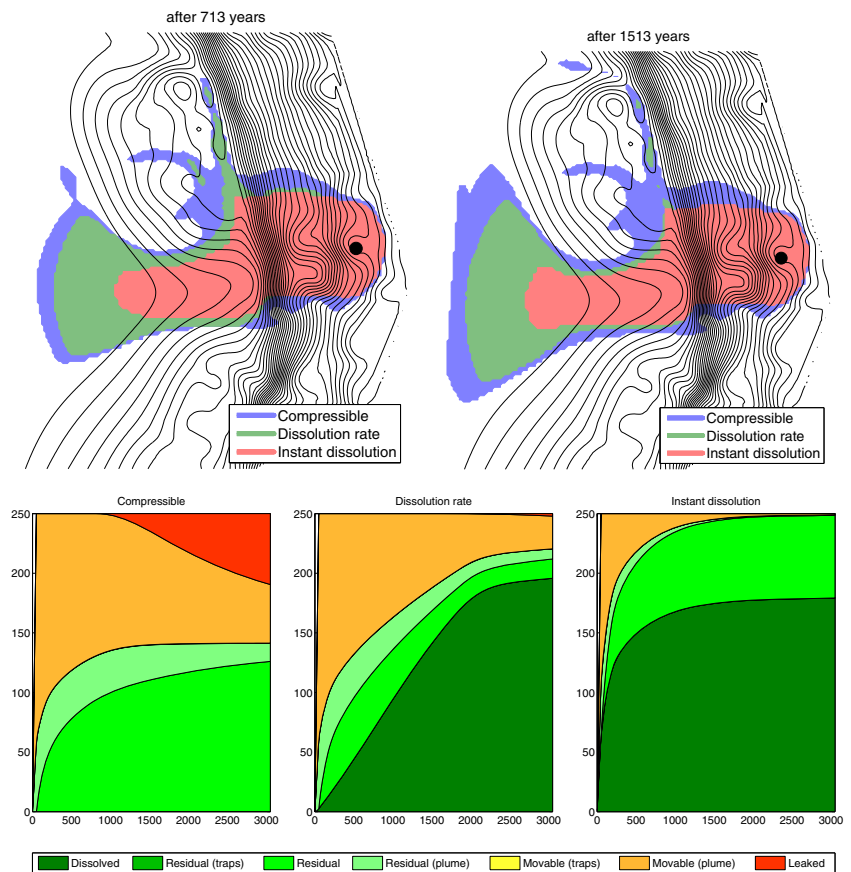


Fig. 18 Modeling the effects of dissolution on the CO₂ migration for a single injection point in the Pliocenesand formation. The *upper plots* show the extent of the residual CO₂ at two different instances in time computed by models without dissolution, with instantaneous dissolution and with rate-dependent dissolution. The *lower plots* show the corresponding carbon inventories (in units mega-tonnes and years since injection started). (From `secondPlioExample.m` and `showSecondPlioExample.m`)



residually trapped, 0.8 % has leaked, and 11 % is still free to move. The total CPU times for the three simulations are 189, 425 and 1118 s, respectively, on an Intel Xeon 3.47 GHz CPU. For the rate-dependent simulation, a large number of time-step cuts contribute to the high computational cost.

Finally, we remark that we have so far not considered lateral transport of CO₂ dissolved in brine induced by density differences. To model this effect, one has to introduce different velocities for water with CO₂ and water without CO₂. Our models did not include this effect since it is approximately one thousand times slower than the movement of the CO₂ plume: a factor one hundred is caused by less density difference with water, and a factor ten can be attributed to the larger viscosity compared to CO₂. However, transport of dissolved CO₂ may be important from a numerical point-of-view because without this effect there is no physical diffusion to smooth out and stabilize the concentration c . Making the other approximation based on putting the denser CO₂-rich water just below the CO₂ plume, which is the mental picture made when introducing convection-enhanced dissolution, will lead to a negative diffusion term that may amplify oscillations.

5 Choice of numerical methods

The VE models discussed above have the same structure as traditional equations for multiphase flow in porous media. The dominant discretization within reservoir simulation is the fully-implicit method with phase-based upstream-mobility weighting and two-point flux approximation. Alternatively, one can use the implicit pressure, explicit saturation (IMPES) method, in which the time step is limited by the CFL restriction on the explicit saturation update, or a sequential splitting that combines a pressure solver with an appropriate explicit or (semi-)implicit saturation solver. Several commercial simulators have vertical-equilibrium options that work with both fully-implicit and sequential solvers (see, e.g., [27, 68]). This option has been added both to improve computational performance and numerical accuracy for thin and/or well-segregated reservoirs. However, none of these simulators can incorporate all the model features discussed herein. Conversely, most research codes used in the literature to study CO₂ migration are based on a simple IMPES or sequential-splitting method and are not publicly available. In particular, the VESA code [26], which to the best of our knowledge is the most general

code reported in the literature, uses a nonstandard non-conservative version of IMPES, but nevertheless seems to work rather well.

We have previously used sequential splitting methods for the simplified incompressible models discussed in Section 3, and this choice has proved to be both efficient and robust in the sense that these methods produce stable solutions [27, 33]. In [42], we also pointed out that the coupling between pressure and transport tends to be weak for migration-type scenarios formulated in a VE framework compared to a standard 3D simulation. Also, for more complex models, our experience is that the combination of stable splitting methods (e.g., as discussed in [69]) with explicit and highly parallel transport solvers [70, 71] will efficiently resolve the primary flow effects for a range of relevant resolutions. This approach is particularly efficient for rectilinear grids with coarse resolutions like seen in the CO₂ Storage Atlas of the Norwegian Continental Shelf [14].

On the other hand, sequential and explicit methods have limitations on fine grids and for almost stationary states. In particular, the gravity effect that creates a flat CO₂ interface (e.g., inside a structural trap) turns up as a second-order term in the transport equation, similar to how capillary forces appear in traditional reservoir simulation. As a result, the transport equation will have a strong parabolic character and will be more tightly coupled to the pressure equations. It is well known within the reservoir simulation community that spatially-dependent and strong capillary pressure is best simulated using fully-implicit methods, since a tight coupling of pressure and transport will reduce the stability and put severe restrictions on the time step of IMPES and other sequential-splitting methods. Implicit methods can also be preferable during the injection stage since they have the ability to take long time steps. An example of such behavior was illustrated in Fig. 10.

For all these reasons, MRST-co2lab offers two different types of solvers: (i) sequential-splitting methods with explicit or implicit transport solvers to provide efficient solution of the basic model discussed in Section 3, and (ii) fully-implicit solvers for VE formulations that can easily handle steady-states and incorporate more physical flow effects like compressibility, hysteresis, and dissolution as discussed in Section 4. To the best of our knowledge, fully-implicit VE solvers that include all the main trapping mechanisms have not been reported previously in the literature. We believe that such solvers are particularly important to efficiently and robustly resolve the important stationary states of flat CO₂ interfaces. The fully-implicit solvers in MRST-co2lab are implemented using automatic differentiation [12], which makes it straightforward to compute gradients from adjoint equations. Having gradients is important to determine parameter sensitivities or if one wants to

use rigorous mathematical optimization methods to propose plausible injection points and strategies.

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Appendix A: change of coordinate systems

In Section 3, we derived a transport equation on the form

$$\frac{\partial}{\partial t} \Phi(h) + \nabla_{\parallel} \left[\mathbf{F}_n(h) \vec{V} + \mathbf{G}_n(h) [\vec{g}_{\parallel} + g_{\zeta} \nabla_{\parallel} (Z + h)] \right] = Q_n,$$

which involves operators ∇_{\parallel} that are defined relative to a rotated coordinate system that locally aligns with the top surface of the aquifer. The disadvantage of operating in this curvilinear coordinate system is that it is difficult to calculate volumes and that the absolute height of the CO₂ surface will depend on geometric interpretations. The latter is a disadvantage since a stationary state without driving forces, which in physical space is a horizontal interface between CO₂ and brine, will generally not correspond to a constant value of $h(\xi, \eta)$. Hence, it is more complicated to derive numerical schemes that honor this important physical property exactly. In our implementation, we have therefore chosen to work with transport equations formulated directly in the original physical coordinate system. This will potentially introduce two errors.

The first error is associated with the approximation $\nabla_{\parallel} \approx \nabla_{xy}$, which results in an error of the order θ^2 . However, for the important stationary case, we have equilibrium in all directions so the VE assumption will in fact be exact in the new coordinate system. Also, for plumes of significant thickness, the interface between CO₂ and water will be near horizontal and assuming equilibrium in the vertical direction will be an approximation that is at least as good as assuming equilibrium in the direction perpendicular to the top surface.

The second error comes from a change of geometry in our interpretation of the physical quantities. In the original formulation, the height h is defined relative to the vector \vec{e}_{ζ} , which is constant if we use a coordinate system aligned with the mean dip angle and variable if we use a curvilinear coordinate system that follows the top surface. When working in the physical coordinates, the height value will

be interpreted in the z -direction. Hence, we will calculate the volume of CO_2 by $h_z A_{xy}$ and interpret all lengths as measured in the xy plane, see Fig. 19. For a planar surface, we have that $A_{xy} = A_{\xi\eta} \cos \theta$ and $h_\zeta = h_z \cos \theta$, from which it follows that the volume is preserved. For a curved surface, the volume attached to each surface patch will generally be a function for which the side faces are not fully aligned with \vec{e}_ζ . Replacing this by a cuboid aligned with the physical coordinates will introduce an error. The bottom plot in Fig. 19 illustrates this; here, the column is a trapezoid with sides that deviate an angle $\theta_{12} = \frac{1}{2}(\theta_1 - \theta_2)$ and $\theta_{23} = \frac{1}{2}(\theta_2 - \theta_3)$, respectively, from being a rectangular. By replacing this trapezoid by a rectangular with the same base and height, we make the following error per unit distance

$$\begin{aligned} \frac{\Delta V}{\Delta x} &= \frac{1}{2} \frac{h^2}{\Delta x} [\tan \theta_{12} + \tan \theta_{23}] \\ &= \frac{1}{2} \frac{h^2}{\Delta x} \left[\tan\left(\frac{1}{2}(\theta_1 - \theta_2)\right) + \tan\left(\frac{1}{2}(\theta_2 - \theta_3)\right) \right] \\ &\approx \frac{1}{2} \frac{h^2}{\Delta x} \left[\frac{1}{2}(\theta_1 - \theta_2) + \frac{1}{2}(\theta_2 - \theta_3) \right] \\ &= \frac{1}{2} h^2 \frac{\theta_1 - \theta_3}{2\Delta x} \approx -\frac{1}{2} h^2 \frac{\partial \theta}{\partial x}. \end{aligned}$$

In other words, we get an error depending on the second derivative of the top surface. The approximation we have adopted is valid for small tilt angles and small curvature. It greatly simplifies the numerical code and processing of

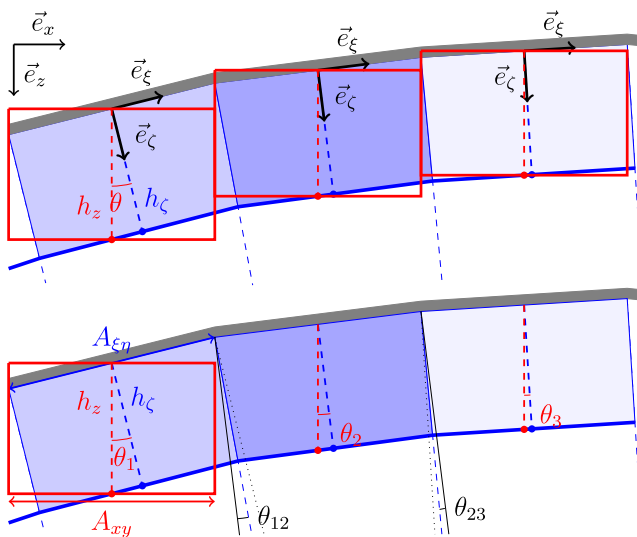


Fig. 19 Approximation of the column geometry for a plume (thick blue line) under a sloping caprock (thick gray line). The depth of the plume is defined pointwise for each ξ in the direction of the vector \vec{e}_ζ . For a discrete grid model, this gives volumes as shown by the blue boxes that can be associated with the centroids of the surface grid. To simplify the calculation, we reinterpret this volume as being along vertical pillars along \vec{e}_z , as shown by the red boxes. (The aspect ratios in the figures are greatly exaggerated for illustration purposes; typical θ values are a few degrees)

the grid since there is no need to introduce the local coordinate system. For realistic models, the spatial dimensions are generally working in our favor: grid cells will typically have lengths of the order 100–1000 m, the total height of an aquifer will at most be a few hundred meters, and the mean dip angle up to a few degrees.

In the derivation of the equations, we have integrated the permeability and porosity in the ζ -direction. In the cases where heterogeneity in the vertical direction is considered, we integrate in the z -direction or more precisely in the direction of the grid column in the case of corner-point grids and assume that the main flow will take place in the xy direction. Alternatively, we could integrate vertically at the start, assuming hydrostatic distribution in the vertical direction. This, however, introduces an error proportional to $\theta|v|$, where $|v|$ is the Darcy flow velocity. The end result of the derivation will be the same as we use, but the derivation will indicate a larger error of order $\mathcal{O}(\theta)$. For gravity driven flow, $|v|$ is of order $\mathcal{O}(\theta)$, which means that the pressure reconstruction is of order $\mathcal{O}(\theta^2)$. In addition, the pressure reconstruction is only used inside derivatives, and hence the error in the flux depends on the derivative of θ for constant $|v|$. This derivation is somewhat simpler when deriving the practical method, but we believe that our derivation gives a better description of the combined approximations of the VE assumptions and the numerical implementations in a realistic setting.

Appendix B: the black-oil equations

The predominant way of simulating multiphase flow in petroleum reservoirs is through the so-called ‘black-oil model’ in which various chemical species are lumped together to form two components at surface conditions, a denser ‘oil’ component and a lighter ‘gas’ component. At reservoir conditions, these two components can be partially or completely dissolved in each other depending on pressure and temperature, forming two hydrocarbon phases, a liquid oleic phase, and/or a gaseous phase, that may coexist with an aqueous phase.

By convention, the black-oil equations are formulated as conservation of the gas, oil, and water component at standard surface conditions combined with a simple PVT model that uses pressure-dependent functions to related fluid volumes at surface and reservoir conditions. To state the equations, we define the inverse formation-volume factors $b_\ell = V_\ell^s/V_\ell$, where V_ℓ^s and V_ℓ denote the volumes occupied by a bulk of component ℓ at surface and reservoir conditions, respectively. The solubility of gas in oil is usually modeled through the pressure-dependent solution gas-oil ratio, $r_{so} = V_g^s/V_o^s$ defined as the volume of gas, measured at standard conditions, that at reservoir

conditions is dissolved in a unit of stock-tank oil. The black-oil framework also opens for oil vaporized in gas, and the presence of the hydrocarbon components in the aqueous phase and water in the gaseous and oleic phases, but these possibilities are not needed for our purpose herein. With this, we can now write the system of continuity equations for our three-component, three-phase system as:

$$\begin{aligned} \partial_t(\phi b_o s_o) + \nabla \cdot (b_o \vec{v}_o) - b_o q_o &= q_o, \\ \partial_t(\phi b_w s_w) + \nabla \cdot (b_w \vec{v}_w) - b_w q_w &= q_w, \\ \partial_t[\phi(b_g s_g + b_{or_{so}} s_o)] + \nabla \cdot (b_g \vec{v}_g + b_{or_{so}} \vec{v}_o) \\ &\quad - (b_g q_g + b_{or_{so}} q_o) = q_g. \end{aligned}$$

In addition, we need various closure relationships, which particularly includes relations that express the capillary pressures as functions of phase saturations

$$p_o - p_w = P_{cow}(s_w, s_o), \quad p_g - p_o = P_{cgo}(s_o, s_g).$$

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