The 8th Trondheim Conference on CO₂ Capture, Transport and Storage

An Open-Source Toolchain for Simulation and Optimization of Aquifer-Wide CO₂ Storage

Odd Andersen[a]*, Knut-Andreas Lie[a], Halvor Møll Nilsen[a]

[a]SINTEF ICT, Department of Applied Mathematics, P.O.Box 124 Blindern, N-0314 Oslo, Norway

Abstract

Planning and execution of large-scale, aquifer-wide CO₂ storage operations will require extensive use of computer modelling and simulations. The required computational tools will vary depending on the physical characteristics of the targeted aquifer, the stage of the project, and the questions asked, which may not always be anticipated in advance. In this paper, we argue that a one-size-fits-all simulation tool for the modelling CO₂ storage does not exist. Instead, we propose an integrated toolchain of computational methods that can be used in a flexible way to set up adaptive workflows. Although a complete toolchain will require computational methods at all levels of complexity, we further argue that lightweight methods play a particularly important role in addressing many of the relevant questions. We have implemented a number of such simplified methods in MRST-co2lab, a separate module to the open-source MATLAB Reservoir Simulation Toolbox (MRST). In particular, MRST-co2lab contains percolation-type methods that within seconds can identify structural traps and their catchment areas and compute spill paths and rough estimates of trapping capacity. The software also offers two-phase simulators based on vertical-equilibrium assumptions that can forecast structural, residual, and solubility trapping in a thousand-year perspective and are orders of magnitude faster than traditional 3D simulators. Herein, we apply these methods on realistic, large-scale datasets to demonstrate their capabilities and show how they can be used in combination to address optimal use of open aquifers for large-scale storage.

* Corresponding author. Tel.: +47-91785380;
E-mail address: odd.andersen@sintef.no

1. Introduction

If carbon capture and storage is to play a significant role in the mitigation of European greenhouse gas emissions, hundreds of megatonnes of CO_2 must be injected annually into geological formations for permanent storage. Operations at this scale represent a considerable scale-up from current practice and experience, and will require extensive mapping, analysis, planning, and monitoring of the selected storage sites to maintain sufficient confidence in their large-scale and long-term storage properties. The spatial and temporal scales involved are huge: tens of thousands of square kilometers and potentially thousands of years of migration for a typical large aquifer. Computer simulations will be indispensable in this process, from initial screening and ranking, through strategic injection planning, to day-to-day operation and subsequent long-term monitoring. However, each stage of analysis requires different computational methods and tools. Tools for rapid estimation of storage capacities and injection properties will play a key role in the initial exploration stage, whereas more advanced simulation tools will be needed to address actual utilization and realization of available storage potential. A large number of simulations are needed to explore the range of likely outcomes since data even in the best case will be limited and uncertain, and it is therefore necessary to minimize computational costs, particularly when forecasting long-term outcomes, with CO_2 migrating for thousands of years after operations have ceased. Computationally inexpensive model that can be gradually refined will also enable the use of mathematical optimization tools to guide injection planning and operations. During the operational phase, more detailed and computationally costly 3D models are necessary to study the local and short-term interplay among pressure buildup and multiphase, geomechanical, thermal, and geochemical effects, and can also be used to perform continuous integration of new data.

Potential storage sites will vary in operational constraints and in physical characteristics [1] such as seal quality, caprock shape and inclination, aquifer boundaries, rock properties, pressure regimes, thermal conditions, geochemistry, and impact of effects at the pore-scale like fluid relative permeabilities, capillary pressure, and dissolution into brine. Computer modelling and analysis should therefore be adapted on a case-by-case basis to adequately account for the relevant physical effects.

To address the considerations above, we have developed an integrated, open-source collection of software tools for investigating CO_2 storage at the basin-scale. These tools can be used in isolation but are developed to work together using common data structures, plotting and support routines to analyze large-scale aquifer systems in terms of storage capacities or to optimized utilization in terms of pressure buildup, leakage risk, and long-term migration and trapping. The open-source MATLAB Reservoir Simulation Toolbox [3] contains a separate module, MRST-co2lab [2], which emphasizes simplified models, for two reasons. First, whereas conventional 3D simulation is important to understand local development during the operational phase, such capabilities are already available in well-established simulators [4,5,6] and in other modules of MRST [27]. Secondly, computationally lightweight approaches have the ability to rapidly run a large number of simulations on large spatial and temporal domains, which not only enables more extensive exploration of uncertainties, but also makes tasks such as scenario specifications and continuous integration of new data amenable to nonlinear optimization algorithms [7]. An additional advantage is the higher degree of user interactivity compared with what is possible using full 3D models. Finally, we remark that all examples presented in the following are based on real aquifer models provided by the Norwegian Petroleum Directorate (NPD) [8] and the University of Texas at Austin [9].

2. Methods based on spill-point analysis of the aquifer caprock

The movement of CO_2 within a saline aquifer is driven by viscous, gravity and capillary forces. Viscous forces dominate flow close to the injection point, but diminish by distance and become negligible at some point compared to gravity and capillary effects if background flow is not present. After injection ceases, pressure buildup around the injection point will gradually dissipate, further reducing the role of pressure-driven CO_2 flow. When flow is primarily driven by gravity and capillary forces, simulations based on invasion-percolation theory can often provide a good description of CO_2 migration, as demonstrated for Sleipner [10].

Similar results can be obtained by assuming infinitesimal flow rate so that only gravity forces are taken into account. Because of the considerable density difference, the injected CO_2 will form a separate plume that starts to migrate upwards following the steepest ascent of the local caprock slope. When a local maximum is reached, CO_2

will start to accumulate and fill up the surrounding area. As CO_2 accumulates beneath the caprock in this *structural trap*, the local CO_2/water contact is pushed further down until the contact plane reaches a depth at which an alternative upward direction exists. CO_2 will then stop accumulating and any further inflow of CO_2 will exit the trap from the encountered *spill-point* and continue to migrate upwards along the steepest ascent until another local maximum is encountered, and so on. The expected migration from any given point in the aquifer can be predicted by analyzing caprock topography. This *spill-point analysis* provides the location, size, and shape of structural traps, spill-point(s) and spill paths in the upslope direction, and catchment areas (*spill regions*) associated with structural traps.

The modelled process has an analog in hydrology, where water catchment areas lead into lakes, which again spill out into rivers, leading to new lakes downstream, etc. Likewise, just as a detailed numerical simulation of fluid flow is not required to predict where rainfall eventually flows and accumulates, a spill-point analysis can give a good idea of where injected CO_2 will end up. The method also provides valuable information for assessment of storage capacity, as structural traps in the caprock represent the most easily exploitable trapping capacity in an open aquifer. On the other hand, spill-point analysis cannot forecast other trapping mechanisms (residual, dissolution), nor does it take into account non-geometric information and heterogeneous rock properties.

In MRST-co2lab, we have implemented two separate algorithms to run spill-point analysis on discrete, quadrangular 2D-meshes that either use cell centroids or cell vertices to representing the caprock surface [11]. Whereas the former is consistent with the way simulation grids are interpreted in a numerical simulation, the latter produces slightly more precise results. Each algorithm identifies all trap cells, spill regions and spill-point depths, as well as topological information such as connectivity between traps and the exact spill paths ("rivers") followed. Both algorithms are very fast, typically requiring only a few seconds for a grid with 100.000 cells. Once this information has been computed, the exact spill path and traps that would be reached from any hypothetical CO_2 injection point in the aquifer can be instantly computed and presented to the user in an interactive visualization tool. MRST also offers other lightweight tools for computing connected volumes, communication patterns, and timelines for fluid transport in heterogeneous 3D models (see [28]), but these are not discussed herein.

As an example, we have applied spill-point analysis on a simulation grid of the Statfjord formation, a large 150 by 300 km aquifer off the western coast of Norway at a depth of 1700-9000 m, identified by the NPD as a potential CO_2 storage site [8]. Using MRST-co2lab, we have constructed a simulation grid from the data provided by NPD as shown n the top plot of Figure 1. The location of the largest identified structural trap is displayed in dark brown, while the corresponding spill region that extends well beyond the trap itself is shown in light brown. The lower plot shows a complete system of structural traps and spill paths, superposed on a topographic map of the caprock. An

Fig. 1. Structural traps in the Statfjord formation. *Left:* Topographic map of caprock, with traps and spill paths. *Middle:* 3D plot with largest trap and associated spill region highlighted. *Right:* Traps coloured according to CO2 storage capacity (megatonnes).

intricate system of "rivers" and "lakes" can be observed. In some locations, injected CO_2 will migrate through a whole chain of structural traps before reaching the uppermost (eastern) boundary of the formation. The lower right plot reports estimates of the total trapping capacity each structural trap, obtained by multiplying the identified trap volumes with assumed porosity for the rock and density values of CO_2 that depend on local temperature and pressure conditions (assuming hydrostatic pressure and a constant temperature gradient). We note a large variation in trapping capacity, with three particularly large traps in the northern half. The largest has a capacity of 1.45 Gt, which is about the same as the two second-largest combined. Adding together all traps, the total storage capacity in structural traps for the aquifer is just short of 7 Gt. However, these figures are sensitive to inaccuracies in the caprock topography as well as our assumed values of rock porosity, local temperature, and pressure conditions. Altogether, the total computational time spent on the trap analysis was 4 seconds, less than the time it took to load and prepare the grid data from disk.

3. Methods based on a vertical-equilibrium assumption

As noted above, the use of spill-point analysis can rapidly provide rough capacity estimates and establish migration patterns that are useful for addressing several questions related to CO_2 storage. Nonetheless, to forecast the combined long-term effect of structural, residual, and solubility trapping, more comprehensive numerical simulations are required. State of the art conventional 3D simulators are highly sophisticated, but are not designed to handle grid models covering tens of thousands of square kilometres and simulations with timespans extending thousands of years. Moreover, under most relevant aquifer conditions, density and viscosity differences between CO_2 and the resident brine will quickly lead to phase segregation and fingering phenomena, in which a buoyant plume of CO_2 migrates as a thin wedge between the caprock and the brine zone below. Simulation grids with very high vertical resolution are therefore needed to capture the behaviour of the thin CO_2 layer, which increases computational costs and imposes severe time-step restrictions. Sufficient lateral resolution is also needed to model caprock undulations and their effect on gravity-driven flow. Computational times therefore quickly become prohibitive for addressing questions that require a large number of separate simulations.

In recent years, vertical-equilibrium (VE) models originating from the 1950's when computing resources were scarce have been reintroduced and adapted to the CO_2 storage problem to answer the associated computational challenges [12]. The key assumption for such models is that the fluid phases are in vertical hydrostatic equilibrium and fully segregated at all times. The injected CO_2 is assumed to form a separate plume above the brine phase, which has proved to be an excellent approximation for the aspect ratios and time scales generally considered. A number of studies, both on benchmark problems and real models, have shown that results from VE simulations compare well with full 3D ones [13, 14, 15, 16]. VE models not only reduce the dimensionality and the number of grid cells, but also contribute to reduce coupling and differences in time constants in the flow model. The lower plot in Figure 2 shows a 3D reservoir model grid of the Sleipner injection site whose general shape is close to that of a thin and almost flat sheet. The third dimension, with a vertical resolution of 34 grid cells, can only be discerned up close, and it is clear that the long-term migration primarily will take place in the lateral direction. A 2D grid representing the same domain with a much smaller number of cells, can be used for VE simulations that preserve the
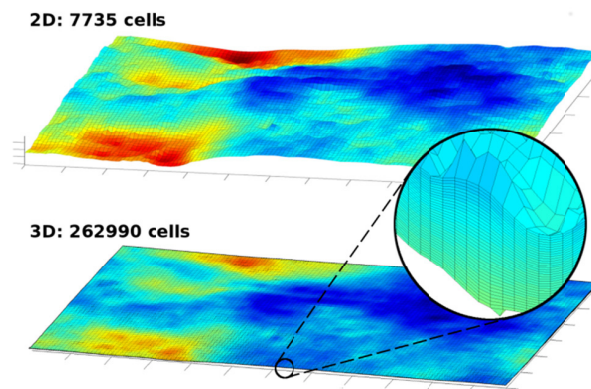

Fig. 2. Simulation grid model of the Sleipner injection site. Top: 2D model. Bottom: 3D model with correct aspect ratio.

fluid distribution profile, relative permeabilities, and rock heterogeneities from the 3D model in an integrated sense. Such VE models are particularly well suited to study large-scale, long-term migration scenarios, addressing questions related to capacity estimation, pressure build-up and the trapping state of CO_2 over time (inventories). The ability to rapidly simulate a large number of scenarios is very useful for assessing plausible outcomes in the face of scarce data, for interpretation/integration of new data in an evolving model, and for optimizing injection scenarios and operational parameters.

Another advantage of VE models is their flexibility in modelling physical effects. Although the basic formulation is simple, it can easily be extended to include a wide range of more advanced phenomena that affect two-phase flow. Recent literature has demonstrated the inclusion and impact of effects such as capillarity [17, 18], residual saturations and hysteresis [12, 19], dissolution and convective mixing [19, 20], subscale caprock topography [21, 22, 23], compressibility [24], brine leakage through caprock [12], geomechanics [25], and thermal effects [26].

In MRST-co2lab, we have implemented VE models that support most of the effects mentioned above, including capillarity, residual trapping, subscale caprock topography, dissolution, compressibility and heat transport, with geomechanical coupling currently under development. In addition, the software contains tools to create vertically integrated simulation grids from 3D stratigraphic models or depth and thickness maps [8], as well as fluid objects with density, viscosity, and enthalpy that depend on temperature and pressure. A finite-volume, fully-implicit numerical scheme is used to discretize the VE equations. The discretization is implemented using automatic differentiation [27], which provides the associated Jacobians of the system with no additional programming effort and hence enables rapid prototyping of new fluid models, as well as providing the necessary information for adjoint-based optimization, as exemplified in Section 4.To demonstrate the use of VE models with additional physical effects, we present two examples. Figure 3 shows the potential impact of CO_2 dissolution for a 1000 year migration scenario following the injection of CO_2 at three separate locations of the Bryne aquifer [8]. The upper left plot
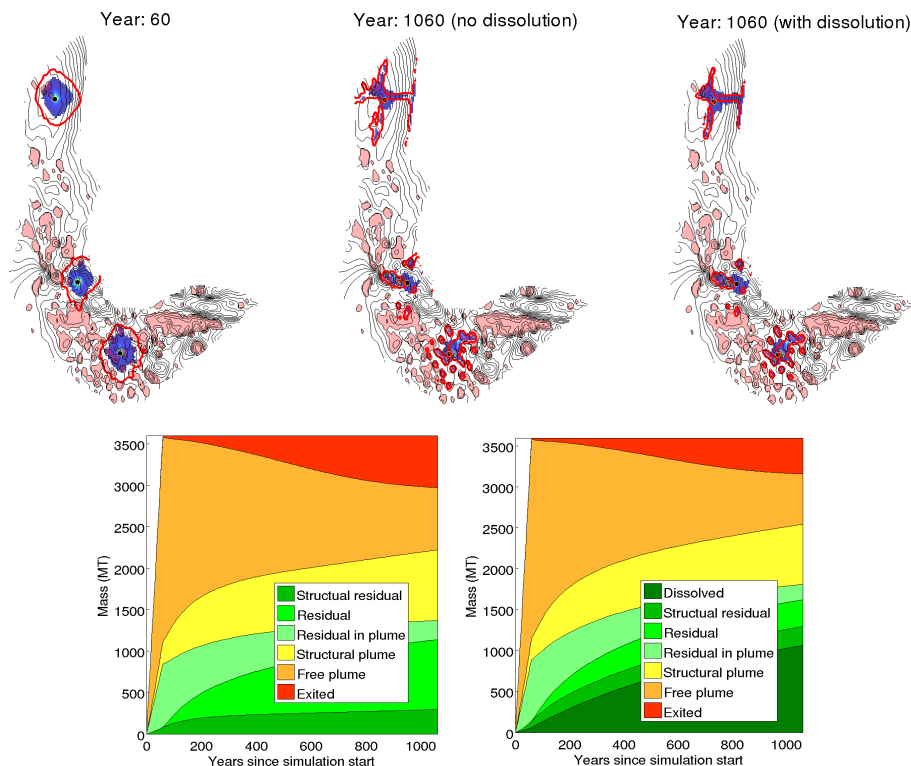

Fig. 3. Simulation of CO2 migration in the Bryne aquifer. Top row: Presence of CO_2 in aquifer just after injection end (left), after 1000 years, assuming no dissolution (middle), and after 1000 years, including dissolution (right). Red contour indicates edge of free-flowing CO_2 plume. Regions containing significant amounts of CO_2 (whether or not mobile) shown in blue. Bottom row: Trapping state of injected CO_2 as a function of time for the scenario without dissolution (left) and with dissolution (right).

shows a topographic map of the aquifer after 3.5 Gt has been injected over a 60-year period. Structural traps are indicated in pink, wells shown as black dots, the mobile CO_2 plume front traced in red, and regions with significant amounts of CO_2 (mobile or not) are coloured in blue. Whereas the two southern wells are positioned in regions with many large structural traps, the northernmost well is situated in a slope with few traps. The two following plots show the state of the aquifer after 1000 years of migration, simulated without and with inclusion of CO_2 dissolution. In both cases, most of the CO_2 injected in the two southern wells collects in nearby structural traps, with the remaining mobile plumes being smaller when dissolution is included. A larger impact can however be seen for the northernmost plume, which mostly does not collect in traps, but spreads out, moves upslope, and exits the simulated domain through the open eastern boundary.

When dissolution is included, the mobile CO_2 plume shrinks faster, more CO_2 is locally retained, and as a consequence, there is less migration out of the domain. The state of injected CO_2 at any point in time during migration is summarized in the two inventory plots in the second row of Figure 3. The coloured zones represent trapping states, with CO_2 exited across domain boundaries in red, the free and migrating plume shown in orange, and CO_2 immobilized by structural, residual, or solubility trapping shown in shades of green and yellow. We see on the rightmost plot how the impact of dissolution grows with time, having dissolved almost 30 percent of all injected CO_2 by the end of the simulation. Migration across boundaries is also significantly reduced compared to the case without dissolution – this is largely due to the impact on migration from the northernmost injection site.

In Figure 4, we show a very different example, where the basic VE model has been extended with energy conservation and conduction of heat. The scenario considered here is the intrusion of hot CO_2 of magmatic origin into a saline aquifer, assumed to have led to the creation of the present-day Bravo Dome natural CO_2 field in New Mexico [9]. In the figure, we show the end result of modelling 1000 years of continuous CO_2 intrusion from a point source close to the western boundary. For this scenario, the entering CO_2 has a temperature of 300 ºC, whereas ambient temperature is set to 20 ºC. Heat is transported with the CO_2 and diffused through the rock. Fluid flow limited to the aquifer itself and modelled using a VE formulation, whereas diffusion of heat is modelled on an extended grid that includes the over/underburden. The resulting discrete equations are solved as a fully coupled system. From the plots, we can see that whereas CO_2 spreads out widely in the aquifer, most of the introduced heat remains relatively close to the injection site. It should however be noted that this example is purely intended to demonstrate our modelling approach, and the choice of parameters should not be taken to accurately represent the historical event, which is still being studied.
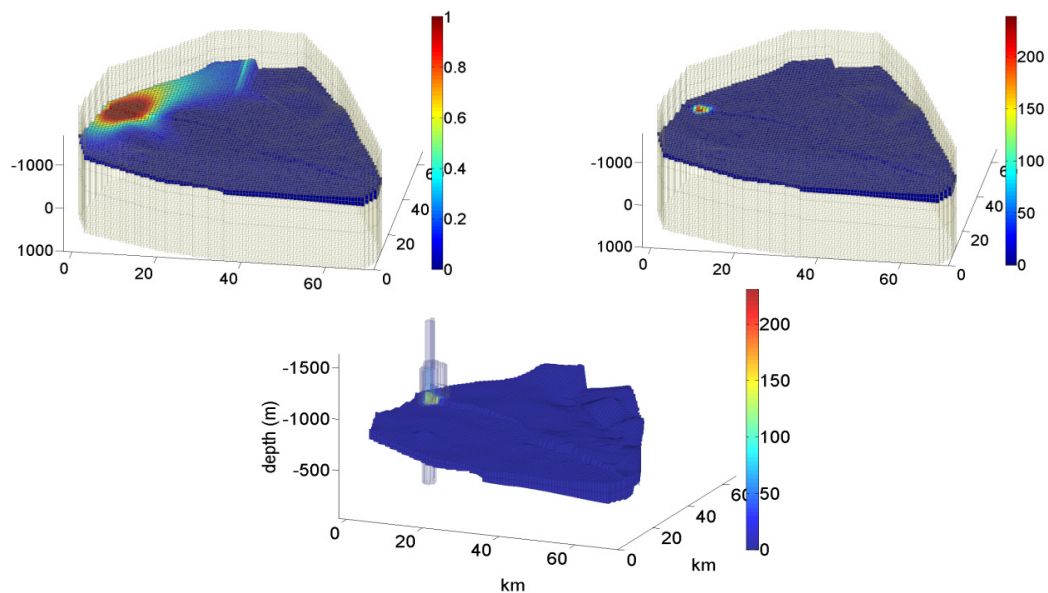

Fig. 4. Coupled thermal and two-phase flow simulation of hot CO_2 intrusion into the Bravo Dome field. *Upper left:* CO_2 saturation after 1000 years of injection. *Upper right:* Temperature increase (°K) in aquifer after 1000 years of injection. *Lower:* Heat transfer into overburden (°K).
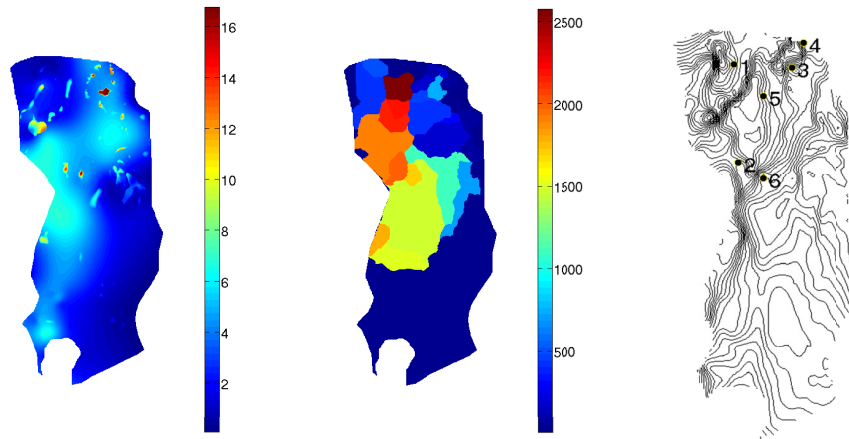
Fig. 5. Storage capacity of the Statfjord formation. *Left:* Map of combined total storage capacity from residual, structural, and solubility trapping mechanisms [megatonnes/m^2]. *Middle:* Map of structural capacity reachable by gravity-driven migration from any given point [megatonnes]. *Right:* Injection locations chosen to maximise amount of structural trapping reached.

4. Outline of an integrated toolchain

By "integrated toolchain", we here refer to the idea that individual modelling methods, tools, data-objects and other MRST functionality can be combined in a flexible way to investigate larger questions related to CO_2 storage. The details of the resulting workflow will necessarily depend on the questions asked, the underlying assumptions made, and the particularities of any specific site. We here exemplify the idea though an approach that integrates the use of EOS-based fluid properties, spill-point analysis, VE simulations, and nonlinear optimization to investigate storage capacity and optimal utilization of the Statfjord aquifer in a large-scale, multi-site injection scenario.

The left plot of Figure 5 displays the local, combined trapping capacity of the Statfjord aquifer, taking structural, residual and dissolution into account, using the methodology of [29,30] and considering the impact of local reservoir conditions on the density of injected CO_2. Adding up the numbers, a total of 95 Gt of CO_2 could be retained in the aquifer by the mechanism of structural (6.95 Gt), residual (69.6 Gt), and dissolution (18.3 Gt) trapping. However, these values are not realistically achievable as they assume 100% sweep efficiency. Structural trapping is the only mechanism that is independent of time and sweep, and can as such be considered the most easily exploitable component of the total capacity. Even so, not all traps can be reached since there will be constraints on the number of injection sites for any real scenario.

One strategy for placing wells could be to maximize utilization of structural traps. The middle plot of Figure 5 displays the maximum mass that can accumulate in structural traps as a result of gravity-driven migration from any specific injection point in the aquifer. Appling the "greedy" algorithm described in [11] to select optimal placement of six wells causes all wells to be placed in the northern half of the aquifer (see Figure 5), where structural traps are larger and more abundant than in the south. Since the algorithm does not take into account other trapping mechanisms, the southern half of the aquifer ends up underutilized, and the method should primarily be used for guidance. Nevertheless, for the purpose of the rest of this section, we will use this well configuration as a starting point to determine injection rates that will optimize use of both structural *and* residual trapping. For any choice of rates, VE simulations will provide a detailed inventory of the state of injected CO_2, as seen in Figure 3. We can thus define an *objective function* that takes a choice of well rates as input and computes a single value representing the "desirability" of the resulting outcome. As our implementation of the VE equations is based on automatic differentiation [27], the Jacobian of the system equations is always available. We can therefore use a continuous, adjoint-based, nonlinear optimization algorithm already available in MRST to determine well rates that represent a local maximum of this function. To this end, VE simulations are essential since any general nonlinear optimization procedure will usually require many evaluations of the objective function, which again necessitates a complete simulation of the migration scenario

We assume that the Statfjord aquifer has open boundaries with constant pressure and aim to maximize the total amount of CO2 injected over 50 years, while minimizing the amount of CO2 that leaves the domain over the next 2900 years. Our objective function thus equals the amount of injected CO2, minus the amount of CO2 that eventually exits the domain multiplied by a penalization factor of ten.

As a starting point for the nonlinear optimization algorithm, we choose injection rates for each well that correspond to the amount of structural capacity reachable from that well (see above). These rates are indicated as blue bars in the upper-right plot of Figure 6, while red bars show the new rates obtained by the optimization procedure. These rates are sometimes quite different from the initial suggestion. In particular, the injection rate of Well 1 has been adjusted drastically downwards. The reason why can be inferred by examining the left plot in Figure 6. During injection, the flow is mainly driven by pressure, and not gravity as assumed by the spill-point analysis. Rather than directly migrating upslope, the CO_2 from Well 1 spreads out into an oblong shape, whose front already touches the northern boundary at the end of the injection period. It is clear that any higher injection rate would lead to immediate migration across the boundaries. The difference between initial and optimal injection rates for the other wells should be understood as a consequence of the effects of residual saturation and pressure-driven flow, which are not captured by the spill-point analysis. The CO_2 inventory from the simulation with optimized rates is presented in the lower right plot of Figure 6. We see that a total of 2.9 Gt is injected, and only a tiny fraction of this amount ends up leaving the domain.

We emphasize that our objective function was chosen subject to the assumption of an open aquifer. If we instead had considered the aquifer to be closed, a more important objective might be to prevent excessive pressure buildup. We could then have specified an objective function that penalizes large pressures, or pressures above some given threshold. Such an objective function is easy to define since pressure is explicitly solved for in the simulation. Moreover, if we had introduced production wells to limit pressure buildup, their production rates could easily be included as additional unknowns in the optimization problem. Linear constraints on the input variables can also be specified so that, for instance, the amount of water produced should balance the amount of CO_2 injected. Finally, we remark that the optimization algorithm used can be easily extended to include time-dependent well rates or other effects such as dissolution. This, however, comes at a higher computational cost.
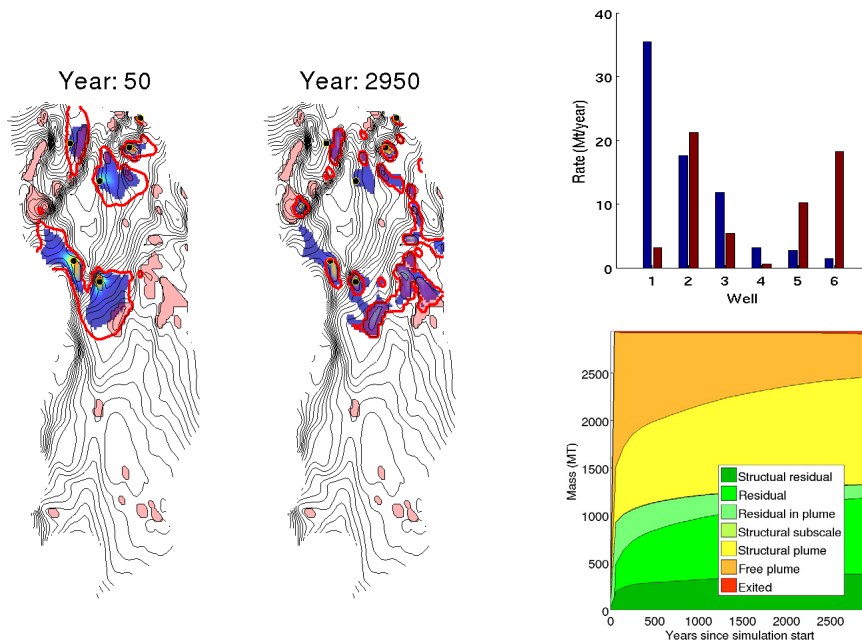

Fig.6. Optimization of injection rates for a 6-well storage scenario in the Statfjord Formation. Left: Presence of CO_2 in aquifer after end of injection, and after end of simulated migration period. Red contour indicates edge of free-flowing CO_2 plume. Regions containing significant amounts of CO_2 (whether or not mobile) shown in blue. Upper right: Initial (blue) and optimized (red) injection rates. Bottom right: Trapping state of injected CO_2 as a function of time.

5. Conclusion

Modelling and understanding CO_2 storage is a highly complex, nonlinear, multiscale, multiphase problem and any computational forecast will necessarily rely on a large number of assumptions, given the limited amount of input data that realistically can be obtained for a given site. In this paper, we suggest that the problem is best approached using a number of methods with different strengths, to be applied independently or combined as components in an integrated workflow consisting of tools that adapt to the specific scenario and questions asked. Figure 7 shows one example of such a workflow. We further emphasize the importance of simplified methods with low computational cost, discuss two such methods, namely spill-point analysis and VE simulation, and demonstrated by example how these can act as components in a more comprehensive analysis. However, we do not intend to suggest that they form a complete toolchain by themselves, nor that other simplified methods are not important in the context of CO_2 storage. A well-equipped toolchain would also include sophisticated 3D modelling tools, as well as a large range of other methods, e.g., statistical tools for assessing parameter uncertainty and model sensitivity, single-phase solvers to assess pressure build-up, flow diagnostic tools that identify volumetric connections and timelines for multiphase displacements, and specialized tools for history-matching and integration of new data. While not a part of MRST-co2lab, several of these tools are available in other modules of MRST.
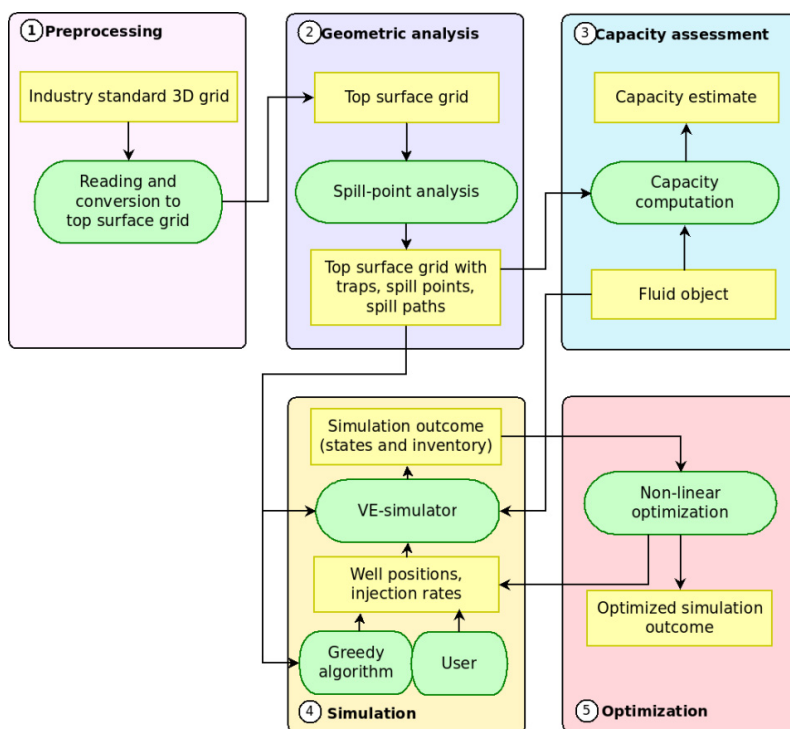
Acknowledgements

Fig.7. Flow chart for the type of workflow discussed herein divided into stages of analysis, starting with the preprocessing of 3D aquifer models from industry-standard input and ending with the proposal of optimal injection points and rates. Yellow boxes are data objects (specified input or computed output), while green ovals represent data-processing stages (software and user).

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