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SPE11: Convergence Study and Extension to Realistic Physics

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Abstract

The SPE11 comparative solution project presents a benchmark for geological carbon storage in an aquifer, as the development of sufficiently accurate CO₂ sequestration models is critical for predicting the distribution of CO₂ during and after injection. In this paper we present a convergence analysis of the SPE11 benchmark simulation using the Delft Advanced Research Terra Simulator (open-DARTS). Open-DARTS, an open-source simulation framework designed for forward and inverse modeling, as well as uncertainty quantification, employs a unified thermal-compositional formulation and operator-based linearization. In our convergence analysis the SPE11b (2D - reservoir conditions) starts to converge at a grid resolution of 1340 × 240, after which added resolution provides diminishing returns. In addition the three-dimensional SPE11c benchmark is simulated with 8M grid blocks. However, 2D results from SPE11b suggest that a greater resolution is required for a truly converged solution. Furthermore, we extend the SPE11b benchmark to include H₂S as a trace impurity in the injection stream.

Introduction

During geological carbon sequestration (GCS), CO₂ is captured from industrial point sources, transported and injected into geological formations. To ensure permanent storage, these geological storage complexes must comprise a combination of permeable reservoirs and impermeable sealing units. Therefore, saline aquifers and depleted oil and gas reservoirs are considered suitable for GCS. Deep saline aquifers have the advantage of offering the largest proven volumes for CO₂ storage, whereas depleted hydrocarbon reservoirs demonstrate a proven ability to store buoyant fluids, are well-characterized, and have existing infrastructure in place (Ringrose, 2020).

Once injected, CO₂ is trapped through a combination of various trapping mechanisms, including structural, residual and solubility trapping. In the shorter time scale, structural and residual trapping mechanisms are expected to dominate, while dissolution trapping occurs over longer time scales (Metz et al., 2005). During structural trapping, the injected CO₂ accumulates under a capillary barrier or impermeable sealing layer. Residual trapping occurs when the CO₂ plume migrates due to buoyancy. In this process, CO₂ at the tail of the plume is immobilized at the pore scale during CO₂ drainage when the wetting phase is imbibed back into the pore space (Krevor et al., 2015). At this point, the CO₂ exists as a series of disconnected

ganglia separated by water. During solubility trapping, CO₂ dissolves into the aquifer water. This molecular diffusion process occurs slowly and is enhanced by the convective mixing of the brine and CO₂ (Neufeld et al., 2010). Convective mixing starts at the interface between CO₂ and water. As CO₂ dissolves into the brine, density-driven flow is induced which in turn increases the dissolution rate. To accurately model this process, high-fidelity models are run for large time spans, as the onset of convective mixing can occur over tens to thousands of years (Pruess and Nordbotten, 2011; Riaz et al., 2006; Pau et al., 2010). CO₂ dissolution is one of the primary mechanisms with which CO₂ will be permanently and safely stored in the subsurface in the long term.

Previous intercomparisons by Pruess et al. (2004) have shown a good agreement between solutions obtained with different numerical simulators. The authors attribute discrepancies to differences in the descriptions of fluid properties. However, convective dissolution always introduces a significant challenge to the modeling of long-term CO₂ sequestration at the reservoir scale. Elenius et al. (2015) present for the first time a numerically converged solution for a large-scale plume migration problem encompassing a wide range of dominant physical phenomena, including enhanced CO₂ dissolution. The first benchmark study fully linking experiments and simulations of enhanced dissolution processed was proposed by Nordbotten et al. (2022). A representative heterogeneous geometry based on typical North Sea reservoirs was constructed in a meter-scale rig, filled with unconsolidated sands of different types. The forecasts reported by different numerical simulation groups were analyzed in the presence of physical ground truth, provided by a series of repeated experiments on the experimental rig (Flemisch et al., 2024). Several advanced methodologies including data assimilation based on tracer test results (Tian et al., 2024) and the use of Multi-Point Flux Approximation (Wapperom et al., 2024) were reported as the result of this benchmark study.

The SPE11 comparative solution project (CSP) borrows its geometry from the FluidFlower experiment and offers a baseline for simulation of CO₂ storage in aquifers (Nordbotten et al., 2024). The reservoir is a heterogeneous reservoir storage complex resembling those found on the Norwegian continental shelf. Three versions of the benchmark are presented in the CSP. The first, 11a is a 2D lab-scale geometry at surface conditions. The second, 11b, is geometrically identical to 11a but at reservoir scale and conditions. The third and last, 11c, is a 3D extruded version of 11b that includes an anticline. The aim of the CSP is to provide a reference case for the development of numerical simulation of GCS by comparative study. The SPE11 CSP explicitly specifies all reservoir and fluid properties in Nordbotten et al. (2024). In this study, the convergence analysis of the SPE11 benchmark simulation utilizing the Delft Advanced Research Terra Simulator (DARTS) is presented. Furthermore, the original physics of the benchmark is extended to include impurities in the CO₂ injection stream. This follows the experience with the largest and longest running CO₂ storage projects where trace amounts of other gasses, such as H₂S and CH₄, are injected. In the case of the Sleipner field, CO₂ is injected with a 0.5 — 2% fraction of methane (Eiken et al., 2011) and hydrogen sulfide is injected with CO₂ in the case of the Weyburn project (Whittaker et al., 2004).

Planning CO₂ storage projects requires developing an understanding of the storage conditions, and fluid flow behavior. To this extent, reservoir simulation is used to predict the migration of CO₂ pressure and storage capacity of the reservoir. Accurate modeling of CO₂ sequestration necessitates the inclusion of complex physical processes, including gravity, capillarity, diffusion, mechanical dispersion, and multiphase flow. To accurately capture the effect of dissolution trapping, it is necessary to solve the highly nonlinear, coupled system of equations, accounting for all these effects, with sufficient resolution and over extended timescale. This study utilizes open-DARTS, an open-source simulation framework designed for forward and inverse modeling, as well as uncertainty quantification (Voskov et al., 2024). Open-DARTS employs a unified thermal-compositional formulation and operator-based linearization (Voskov, 2017). This approach allows users to easily adjust the terms of the PDEs and model various complex physical phenomena. Additionally, open-DARTS leverages GPU parallelization, enabling simulations to run close to an order of magnitude faster compared to CPU implementation (Khait and Voskov, 2021).

In this study, we begin with a brief description of governing equations, thermodynamic properties, reservoir description and boundary conditions for SPE11 benchmark. Next, we present a convergence study for SPE11b reservoir, followed by a comparison of the converged solution with the results of the high-resolution SPE11c simulation. Subsequently, we present the results of the more realistic version of the SPE11b model, which includes typical impurities in the CO₂ stream. Finally, we conclude this study with lessons learned and suggestions for future work.

The SPE11 - Comparative Solution Project

What follows is an abbreviated description of the SPE11 comparative solution project. For a complete description of the CSP please refer to the official technical description by [Nordbotten et al. \(2024\)](#). As CO₂ is frequently injected at lower temperatures than the reservoir a thermo-compositional formulation is used. In DARTS the advective-diffusive multiphase multicomponent formulation is used ([Lyu and Voskov, 2023](#)). The mass conservation equation for component c is written as,

$$\frac{\partial}{\partial t} \left(\phi \sum_{j=1}^{np} \rho_j S_j x_{cj} \right) + \nabla \cdot \left(\sum_{j=1}^{np} x_{cj} \rho_j \mathbf{u}_j + \mathbf{J}_{cj} \right) = 0, \quad c = 1, \dots, n_c \quad (1)$$

where ϕ is porosity, S_j is phase saturation, ρ_j is molar phase density and x_{cj} is molar fraction of component c in phase j . Additionally, the thermal equation for multiphase flow accounts accounts for advective and conductive heat flow and contains contributions from both fluid and rock,

$$\frac{\partial}{\partial t} \left(\phi \sum_{j=1}^{np} \rho_j S_j U_j + (1 - \phi) U_r \right) + \nabla \cdot \left(\sum_{j=1}^{np} h_j \rho_j \mathbf{u}_j + \kappa \nabla T \right) = 0, \quad (2)$$

where U_j is specific internal energy of phase j , U_r is rock specific internal energy and κ is effective heat conductivity. The phase velocity $\mathbf{u}_j$ follows Darcy's law for multiphase flow,

$$\mathbf{u}_j = -\mathbf{K} \frac{k_{rj}}{\mu_j} (\nabla p_j - \rho_j g \nabla z), \quad (3)$$

where $\mathbf{K}$ is the permeability tensor, k_{rj} is relative phase permeability, μ_j is phase viscosity, p_j is phase pressure, g is gravitational acceleration, and z is depth. The diffusive flux $\mathbf{J}_{cj}$ of component c in phase j is described by Fick's law as

$$\mathbf{J}_{cj} = -(\phi S_j D_{cj} + E |\mathbf{u}_j|) \nabla (\rho_j x_{cj}), \quad (4)$$

where D_{cj} is diffusion coefficient of component c in phase j , E is dispersivity coefficient, equal for all components in all phases. This formulation accounts for the dispersion term, scaled by the scalar dispersivity coefficient and the magnitude of Darcy's velocity. The velocity vector is reconstructed at cell centers using a least-squares solution of fluxes across all cell's interfaces, then averaged between neighboring cells and explicitly incorporated into the numerical approximation of the dispersion term. This system of equations is closed by capillary, thermal and thermodynamic equilibrium assumptions.

Thermodynamics and physical properties

A negative flash procedure with successive substitution is employed for resolving thermodynamic equilibrium calculations ([Michelsen, 1982](#); [Whitson and Michelsen, 1989](#)). The fugacities of the vapor phase are evaluated using a cubic equation of state ([Peng and Robinson, 1976](#)) and the fugacities of the water phase are calculated using an activity model based on Henry's constants ([Ziabakhsh-Ganji and Kooi, 2012](#)). Using this hybrid-model approach, the implementation of a separate model for the aqueous phase

maintains the simplicity of solving phase equilibrium problems with cubic equations of state while obtaining an accurate thermodynamic description of the aqueous phase (Wapperom et al., 2025).

The property correlations for SPE11 and open-DARTS are presented in Tab. 1. The properties of pure phases of the SPE11 CSP are defined in accordance with the NIST database (Lemmon et al., 2023). Wapperom et al. (2024) compared the results of our modelling approach with those of NIST and found good agreement. Fig. 1 presents the results of DARTS, verified against various data sets available in the literature. The considered properties are highly dependent on pressure and temperature, with the exception of the dissolved H₂O in the CO₂-rich phase at field conditions. At elevated pressures, changes in pressure exert minimal influence on solubility when the CO₂ is in a dense phase. Conversely, at low pressures, CO₂ in a vaporous state results in a greater concentration of H₂O within the CO₂ phase. As pressure decreases, the transition from the vapor phase to the dense phase gives rise to a pronounced decline in solubility.

Table 1—Fluid properties of 11b and 11c

Properties	SPE11	open-DARTS
CO ₂ density, kg/m ³	Lemmon et al. (2023)	Peng and Robinson (1976)
H ₂ O density, kg/m ³	Garcia (2001)	
CO ₂ viscosity, cP	Lemmon et al. (2023)	Fenghour et al. (1998)
H ₂ O viscosity, cP	Lemmon et al. (2023)	Islam and Carlson (2012)
CO ₂ enthalpy, kJkmol ^{−1}	Lemmon et al. (2023)	Peng and Robinson (1976)
H ₂ O enthalpy, kJkmol ^{−1}	Lemmon et al. (2023)	Ziabakhsh-Ganji and Kooi (2012)
Mutual solubilities	Spycher et al. (2003)	Wapperom et al. (2025)
Gas diffusion coefficient, m ² /s	2×10^{-8}	
Water diffusion coefficient, m ² /s	1×10^{-9}	

Table 2—Porous media properties

Properties	Values
Dispersivity, E	10
Immobile gas saturation, $s_{n,imm}$	0.1
Max capillary pressure, $p_{cap, max}$, Pa	3×10^7
Shape exponent capillary pressure, c_2	1.5
Rock specific heat capacity, C_s , kJkg ^{−1} K ^{−1}	8.5×10^{-1}
Rock density, ρ_s , kgm ^{−3}	2500
Shape exponents relative permeability, $c_{a,1}$	1.5
Normalized saturations, $s_{j,n}$	$\max \frac{s_j - s_{j,imm}}{1 - s_{j,imm}}$
Relative permeability, k_{rj}	$(s_{j,n})^{c_{a,1}}$
Entry pressure, p_{entry} , bar	$\sqrt{\phi/k_x} 6.12 \times 10^{-3} Nm^{-1}$

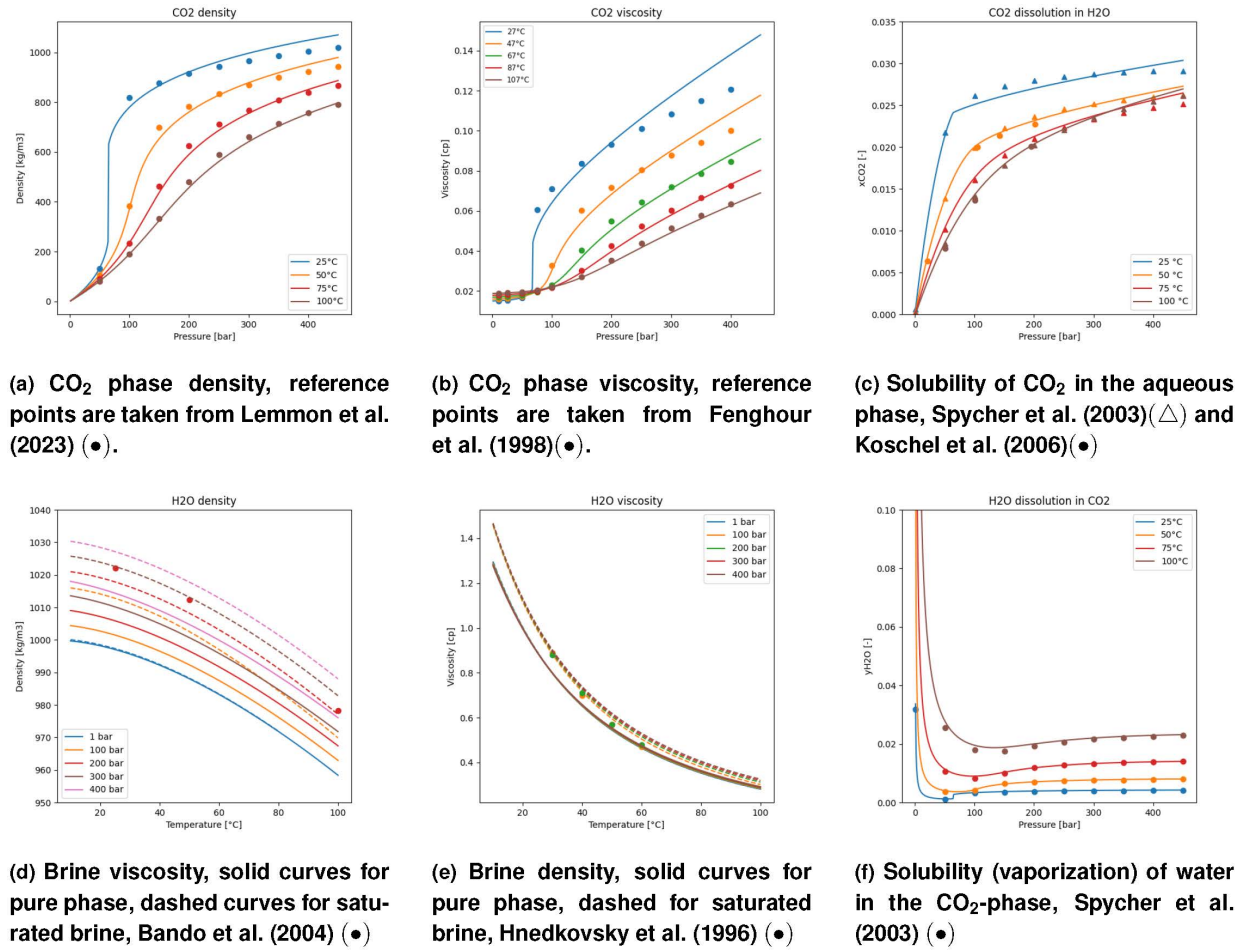


Figure 1—Fluid properties computed in this work.

In addition, the capillary pressure p_c , defining pressure drop between wetting and non-wetting phases, is governed by the following relationship

$$p_c(s_w) = p_{c, \max} \cdot \operatorname{erf} \left(\left(p_{\text{entry}}(s_{w,n})^{-1/c_2} / p_{c, \max} \right) (\sqrt{\pi} / 2) \right), \quad (5)$$

where $p_{c, \max}$ is maximum capillary pressure, p_{entry} is entry pressure, c_2 is empirical parameter. The exact values of these properties are provided in Tab. 2.

Reservoir

Seven different facies are defined in both the 11b and 11c reservoir models. Facies 1 represents the storage complex and serves as a capillary barrier to migrating CO₂. Facies 2 through 5 consist of permeable reservoir sands, while Facies 6 corresponds to fault infill. Finally, Facies 7 forms an impermeable barrier. The facies distribution is shown in Fig. 2 for 11b model. The 11c model is an extruded version of the 11b model and, in addition, it includes anticline. Note that in SPE11, the reservoir geometry defines the z-axis at the base of the reservoir. Facies properties are identical for both models and are listed in Tab. 3. The vertical permeability of each of the facies is one-tenth of its horizontal permeability. Model geometries of the three SPE11 variants are hosted on the GitHub repository: <https://github.com/Simulation-Benchmarks/11thSPE-CSP>. Reservoir geometries are provided in the GMSH geometry format and available in the SPE11 repository. In our model, the geometry of the FluidFlower model is converted to the reservoir scale following the SPE11's description. For all simulations, a structured mesh is constructed and populated according to the facies descriptions.

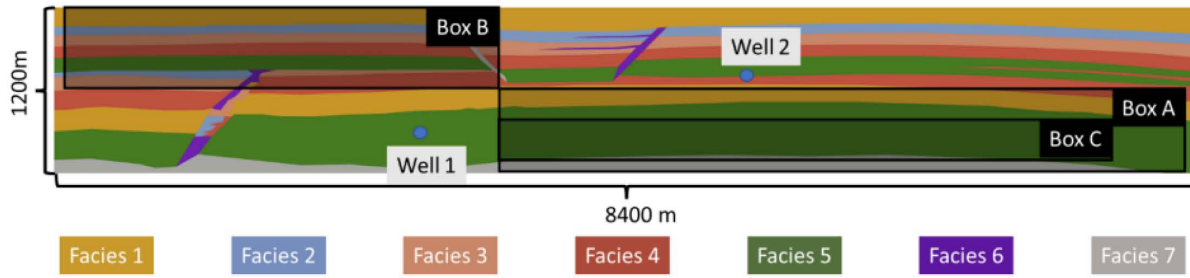


Figure 2—11b reservoir with corresponding reporting boxes and well locations. Image from Nordbotten et al. (2024).

Table 3—Facies properties of 11b and c.

Facies no.	Permeability k , mD	Porosity ϕ	$S_{w,imm}$	κ , $\text{W m}^{-1} \text{ K}^{-1}$
1	0.101	0.10	0.32	1.90
2	101	0.20	0.14	1.25
3	202	0.20	0.12	1.25
4	507	0.20	0.12	1.25
5	1013	0.20	0.12	0.92
6	2027	0.25	0.12	0.26
7	0	0	0.10	2.00

Initial/boundary conditions

In the SPE11b and 11c models, temperatures at the top and bottom boundaries are fixed, all boundaries are impermeable and the boundary volumes are increased to $5 \times 10^4 \Delta z$. No CO_2 is present in the system prior to injection. A geothermal gradient of $25^\circ \text{C km}^{-1}$ is applied along with a temperature of 70°C maintained at the bottom boundary. The initial reservoir pressure is hydrostatic and defined as,

$$p_{w, initial} = 3 \times 10^{-7} \text{ Pa} - g \int_{300 \text{ m}}^z \rho_w(p, T) dz, \quad (6)$$

where ρ_w is water phase density. The model undergoes an equilibration step lasting 1000 yr prior to injection, with $t = 0 \text{ yr}$ defined as the start of injection. Both the 11b and 11c models include two injection wells. In model 11b, well 1 is located at (2700, 300), and well 2 at (5100, 1100). For model 11c, well 1 is horizontal, it perforates reservoir between points (2700, 1000, 300) and (2700, 4000, 300). Well 2 perforates reservoir between points (5100, 1000, 700) and (5100, 4000, 700). In both models injection starts in well 1 at $t = 0 \text{ yr}$ and continues until $t = 50 \text{ yr}$. Well 2 starts injection at $t = 25 \text{ yr}$, lasting until $t = 50 \text{ yr}$. In the post-injection period, the simulation continues until $t = 1000 \text{ yr}$. In both wells, CO_2 is injected at 10°C . In 11b the injection rate is equal to 3024 kg d^{-1} and in 11c 50 kg s^{-1} .

Solution strategy

A finite-volume discretization is employed, using the backward-Euler scheme in time and two-point flux approximation with upstream weighting in space. Operator-based linearization (OBL) is used to manage the computational cost of property evaluation and Jacobian assembly. In OBL, the governing equations are represented through state-dependent and spatial operators. State-dependent operators aggregate variables that depend on the physical state into a single term, i.e. operator. The state-operators are resolved on a uniform mesh introduced in the physical space. While the operators undergo exact evaluation at the nodes of this mesh, multilinear interpolation ensures a continuous representation of the operators between the nodes. The mesh resolution provides a key control over the nonlinearity of the problem, simulation performance,

and robustness of the simulation (Khait and Voskov, 2017). Therefore, to accurately capture multiphase flow in the presence of capillarity and buoyancy a resolution of 100 points is used for pressure and 1000 points for composition space (Lyu et al., 2021).

Results

Time series and spatial data are used for the SPE11 CSP. The spatial maps are shown in their native resolution and are not projected to the SPE11 reporting grid. Time series values include: pressure at two observation points (S1) and (S2), convective mixing M in box C and mass of CO_2 . The mass of CO_2 contained in boxes A and B as well as in the seals is reported. The location of the boxes with respect to the injection wells is visualized in Fig. 2. Convective mixing is quantified by the following integral

$$M = \int \nabla \left| \frac{x_{\text{CO}_2}^w}{x_{\text{CO}_2, \text{max}}^w} \right| dV, \quad (7)$$

where $x_{\text{CO}_2}^w$ is the mass fraction of CO_2 in water and $x_{\text{CO}_2, \text{max}}^w$ the solubility limit of CO_2 in water.

SPE11b

This study compares the simulation results of the SPE11b model obtained with various grid resolutions on a structured grid. The exact grid specifications are reported in Tab. 4. The models with 50 and 100 thousand grid blocks are considered low-resolution, whereas the models with 300 and 600 thousand grid blocks are high-resolution models. The spatial solutions are shown in Figs. 3 and 4. Injection starts in well 1. Initially, the lower temperature of the injected CO_2 causes it to sink downward due to its higher density compared to the surrounding reservoir water. However, as the CO_2 equilibrates with the reservoir temperature, it migrates upwards due to buoyancy. From there, the majority of CO_2 migrates along the bottom of the overlying capillary barrier, while a portion migrates via the adjacent fault to the upper sand units.

Table 4—Grid specifications

No. grid blocks	$n_x \times n_z$	$dx \times dz$	Runtime (GPU)
52, 500	525×100	$16m \times 12m$	1h
100, 800	840×120	$10m \times 10m$	2h
321, 600	1340×240	$6.27m \times 5m$	7h
604, 800	1680×360	$5.0m \times 3.3m$	11h

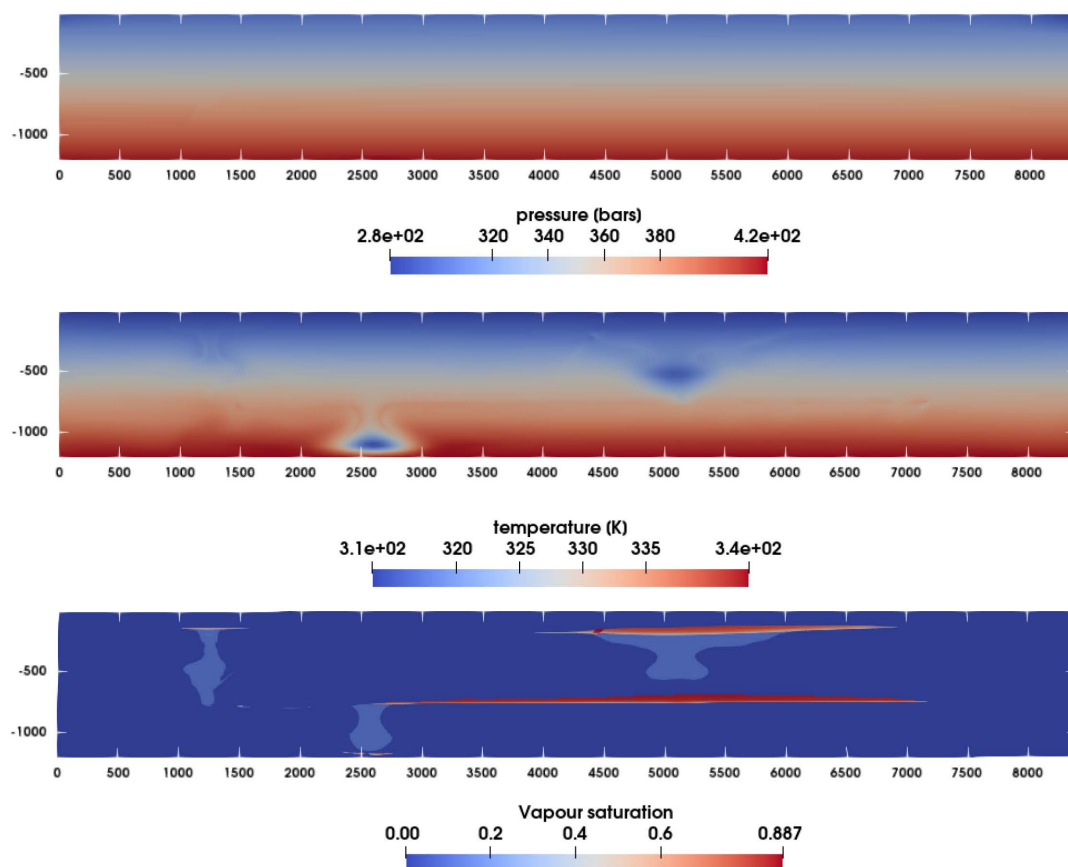


Figure 3—Pressure, temperature and gas saturation at year 300; the model has a resolution of 600K grid blocks.

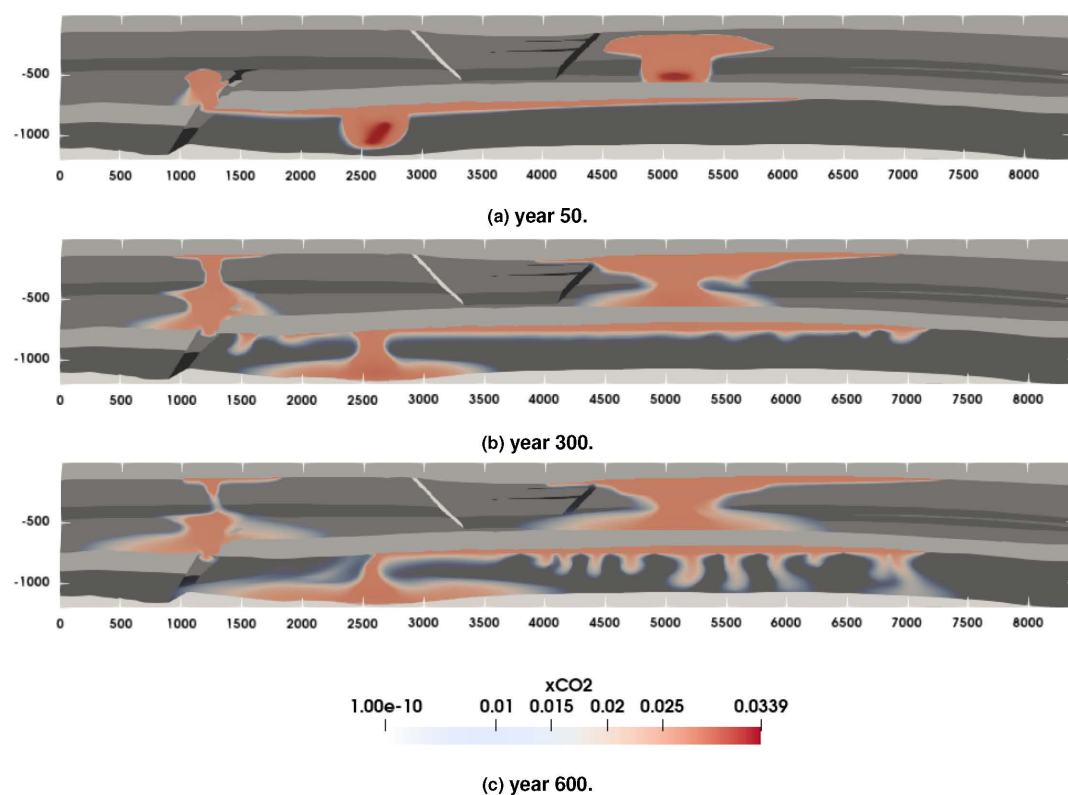


Figure 4—CO₂ fraction in liquid phase; the model has a resolution of 600K grid blocks.

As the CO₂ plume migrates upwards to box B, residual trapping takes place. In box A, two principal processes are observed: first, the CO₂ diffuses into the capillary barrier; second, the CO₂ starts to dissolve into the reservoir water. This dissolution alters the water's density, making it heavier, inducing instabilities, and leading to the formation of dissolution fingers—narrow, finger-like patterns of CO₂-saturated water. These fingers enhance the dissolution process by increasing the surface area for interaction between CO₂ and water, thereby accelerating mixing and promoting the permanent storage of CO₂.

Several observations can be derived from Fig. 5. Convective mixing increases as CO₂ dissolves into the aquifer water. The onset of dissolution can be identified as an inflection point in the curve for convective mixing and occurs in year 300. By year 600, the amount of convective mixing decreases as the more of the water column is in contact with CO₂ and density contrasts decrease. Post-injection CO₂ begins to diffuse into the sealing unit at an increasing rate.

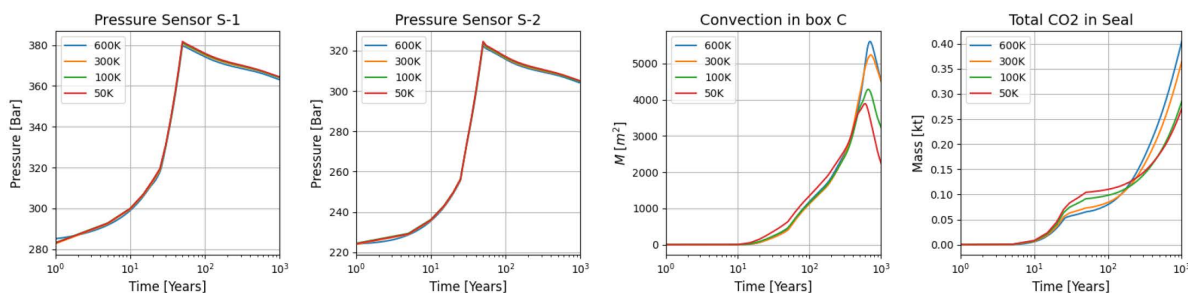


Figure 5—SPE11b time series data.

In box A, Fig. 6, minor differences are observed in the amounts of dissolved and mobile CO₂ across varying resolutions. Around year 300, the amount of mobile CO₂ begins decreasing, coinciding with the onset of enhanced dissolution and an increased dissolution rate. Nevertheless, the higher-resolution models exhibit a lower quantity of immobilized CO₂ compared to the lower-resolution models. Furthermore, the final amount of CO₂ accumulating in the seal increases with finer resolution.

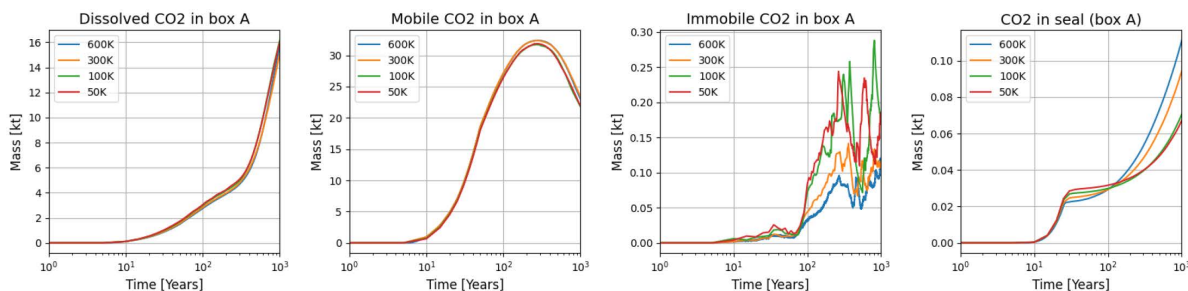


Figure 6—SPE11b, box A - bottom left (3300, 0), top right (8300, 600).

CO₂ enters the box B at approximately year 20. In box B, Fig. 7, the amount of mobile CO₂ consistently increases with finer resolutions, whereas it remains virtually unchanged for the 300 and 600 thousand grid block models. Similarly, the higher-resolution models also exhibit greater amounts of CO₂ in seal B and higher levels of dissolved CO₂, indicating a strong resolution-dependent trend across all models. No density-driven fingering is observed in box B, and greater amounts of CO₂ are immobilized compared to box A. Therefore, residual trapping is identified as the dominant trapping mechanism in box B, while solubility trapping dominates in box A.

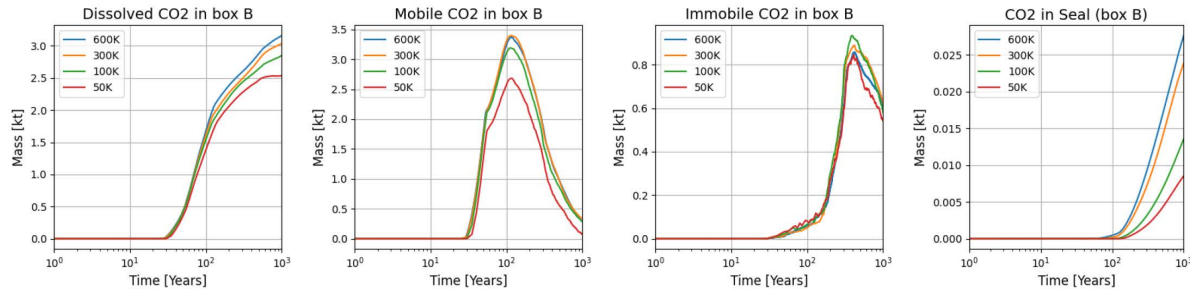


Figure 7—SPE11b, box B - bottom left (100, 600), top right (3300, 1200).

SPE11c

In addition, the full SPE11c model is run using the GPU version of DARTS. The model consists of $n_x = 840$, $n_y = 250$, $n_z = 120$ blocks per dimension, corresponding to 8,041,864 active reservoir blocks. The 3D representation with two profiles across the model at $x = 2700$ and $x = 6000$ are shown in Fig. 8, depicting the fraction of CO₂ in liquid phase at 600 years of simulation. The results at three different time steps for cross-sections along the model at $y = 2600$ are presented in Fig. 9.

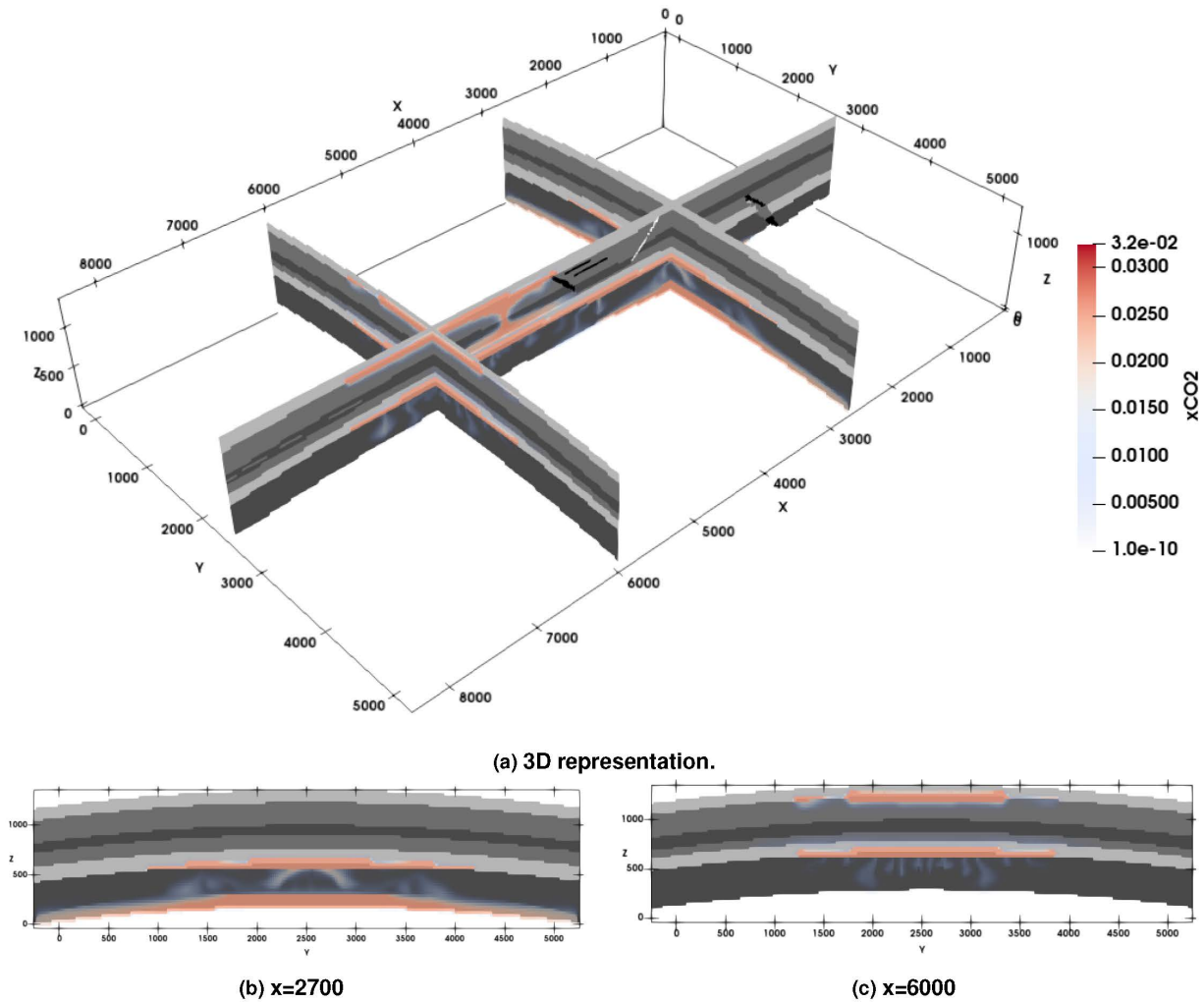


Figure 8—8M grid block model at year 600 with two cross-section across the model.

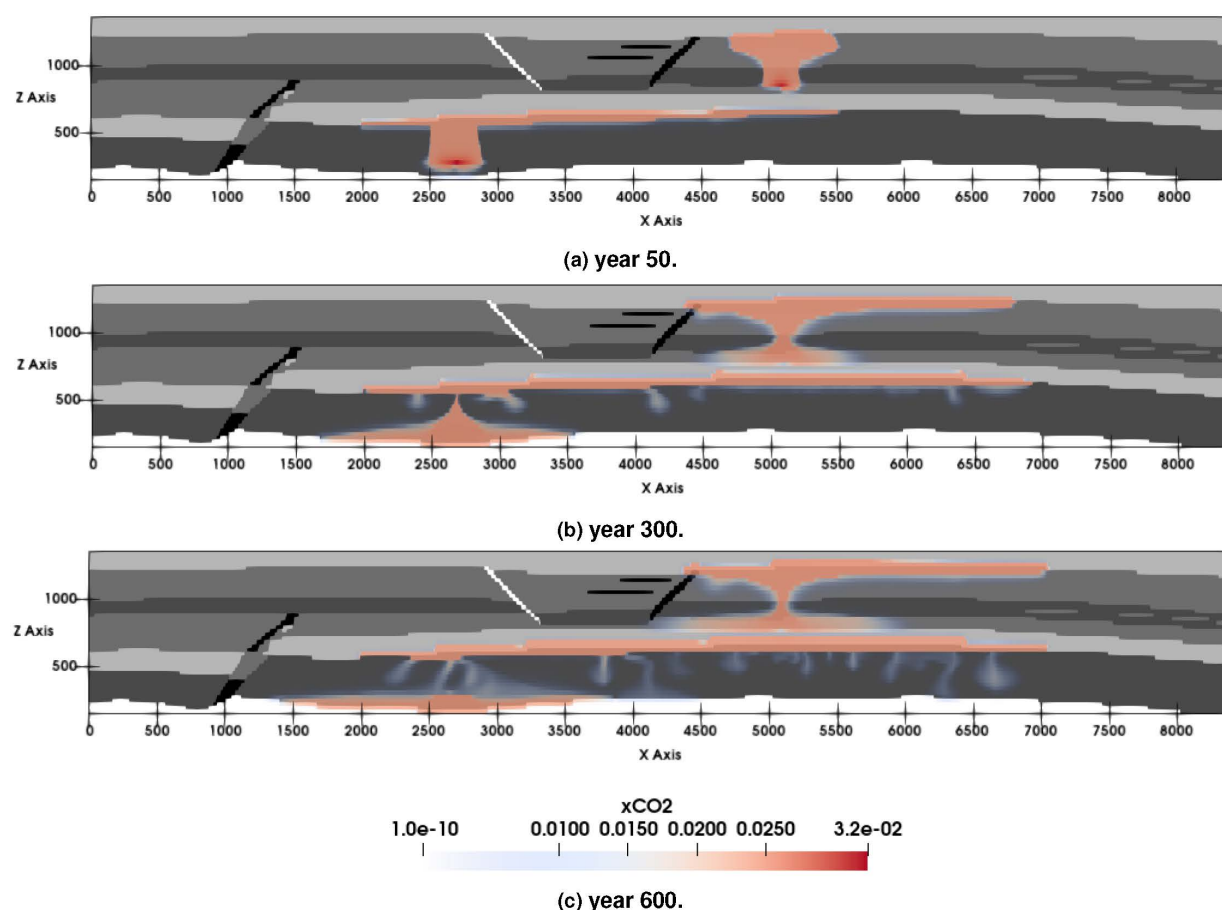


Figure 9—CO₂ fraction in liquid phase - of the SPE11c model at y = 2600.

Several differences can be derived from the comparison of Fig. 4 and Fig. 9. First, the results indicate that CO₂ does not spill through the left-most fault, which is attributed to the dipping of the reservoir. Moreover, it is quite obvious that the current resolution of the SPE11c model is insufficient to accurately capture the dynamics of enhanced dissolution, as the simulation does not resolve the characteristic length of fingers and their general dynamics.

SPE11b with impurities

In this section, we study the effect of impurities included in the injection stream of the SPE11b benchmark. There is relatively little experimental data available of H₂S-CO₂ systems at reservoir conditions. However, the experimental data show that the solubility of CO₂ decreases in the presence of H₂S (Savary et al., 2012). Field observations, experiments (Bachu and Bennion, 2009) and numerical simulations (Zhang et al., 2011) show that the leading edge of the gas plume contains higher concentrations of CO₂. This chromatographic partitioning can be explained by the higher solubility of H₂S in water and different characteristics close to the leading shock of displacement (F.M.Jr.Orr, 2007). This indicates that the inclusion of H₂S in the injection stream may reduce the storage capacity of the reservoir. Furthermore, Zaidin et al. (2024) investigate the effect of H₂S on CO₂ storage in saline aquifers. In their study they measure the solubility of H₂S-CO₂ mixtures and model the effect on CO₂ storage at the reservoir scale. Their findings indicate that H₂S has a negligible effect on CO₂ as in their model the amount of dissolved CO₂ decreases only slightly.

In this simulation, 5 mol% H₂S is co-injected with CO₂. The injection schedules per well are identical to the SPE11b benchmark but the total injection rate is reduced to 2800kgd⁻¹. In Fig. 10, the molar fraction of each component in the aqueous phase is shown at year 600. Evidently, the solution to the flow problem is

similar to that of the original SPE11b benchmark. However, the characteristic wavelength of the dissolution fingers is smaller in size.

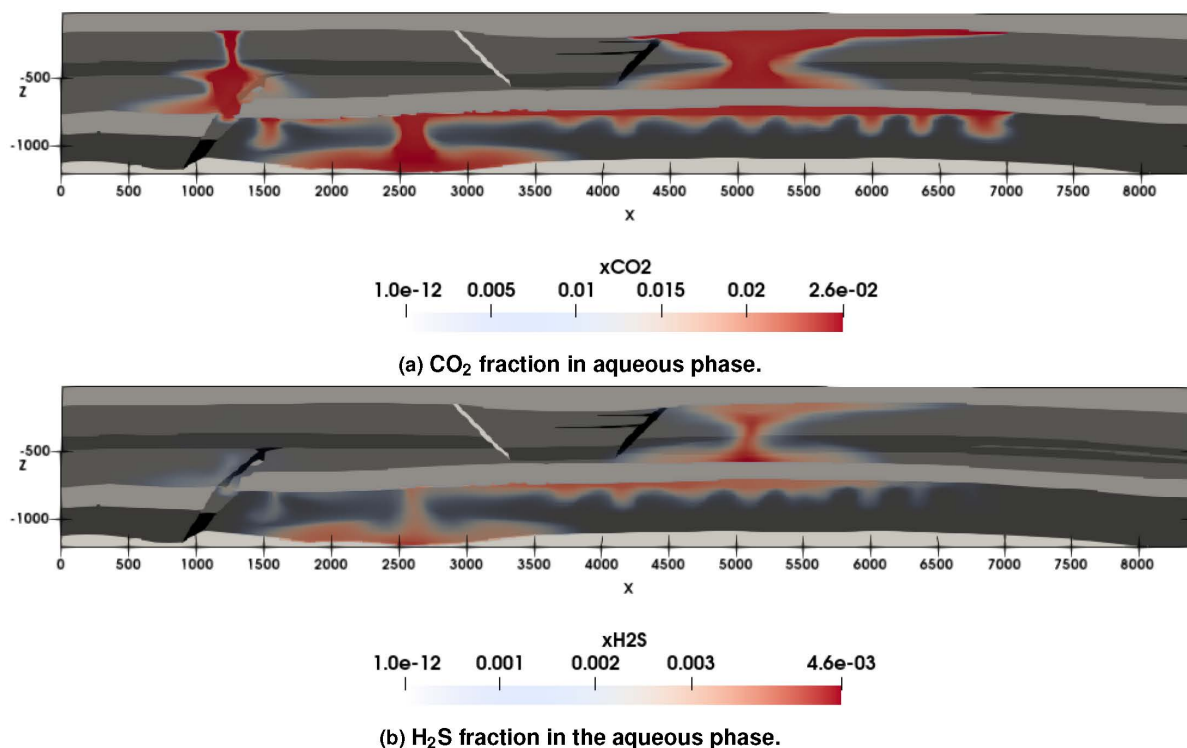


Figure 10—Simulation results of SPE11b with CO₂- H₂S coinjection in year 600.

Conclusion and recommendations

The solubility of CO₂ in aquifer water, the buoyancy of gaseous CO₂, diffusion and capillary forces are critical factors for accurate simulation of Geological Carbon Storage (GCS). In this study, the SPE11b and SPE11c benchmark models are simulated using the open-DARTS framework. In both models, CO₂ is effectively trapped under the capillary barriers, migrates across different units and dissolves into the aquifer brine. For the 11b model, a structured mesh is employed at various resolutions ranging from roughly 50K to 600K gridlocks. The results indicate that the solution for the SPE11b benchmark starts to converge at a vertical resolution of 1340 and horizontal resolution of 240 blocks per dimension, resulting in a 300K grid, with regards to dissolved mobile and immobile CO₂. However, the amount of CO₂ in the sealing units is found to be highly resolution-dependent, which we attribute to the use of a structured grid. Previous studies by [Wapperom et al. \(2024\)](#) clearly demonstrate that a similar reservoir structure is susceptible to grid-orientation effects.

The SPE11c benchmark model which is an extruded version of the SPE11b, is simulated with a grid resolution of about 8M active gridlocks. Comparison with the 2D simulation results of SPE11b reveals that this resolution is insufficient to produce an accurate solution. Generally, the SPE11 benchmark requires high-resolution and high-performance computing resources to obtain a converged solution due to a combination of many complex physical mechanisms.

One of the limitations of the SPE11 benchmark is the representation of the injection stream as pure CO₂. In real-life industrial applications, the stream of injected gas is expected to be a combination of CO₂ and various impurities depending on the source of CO₂. For this reason, the proposed benchmark is extended to include impurities in the injection stream and tested on the SPE11b structural model keeping most of the other parameters the same. In our simulation, H₂S was co-injected with CO₂ in the injection stream.

The results demonstrate chromatographic partitioning of the injected components which can be used for monitoring of CO₂ plume dynamics.

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