

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

CCUS Innovation 2.0

Key Knowledge Deliverable 3.2

Key Knowledge Deliverable Cover Sheet

This Key Knowledge Deliverable (KKD) has been produced by Imperial College London as part of the DESNZ CCUS Innovation 2.0 programme. The document is reflective of the status of the project at the time of writing. The material presented could have been subject to change as the project matured. These documents should not be considered a full representation of the final project.

Description of the project: In StrataTrapper we translate cutting edge research carried out at Imperial College London and the University of Cambridge on the geological fluid dynamics and trapping of CO₂ into innovative characterisation and modelling software tools that will be used by industry to reduce risks and costs of CO₂ storage projects. The tools will be commercialised through incorporation into the CO₂ reservoir simulation platform OpenGoSim, in addition to being made open-source. We will work with industry partners bp, Storegga, and Drax power to demonstrate the applicability of these tools to the Endurance field in the Southern North Sea and the East Mey Site in the Central and Northern North Sea. The result of the work will be the commercialisation of the StrataTrapper reservoir simulation tools for the rapid screening, risking, project design, and management of CO₂ storage.

This report describes Key knowledge Deliverable 3.2, analysing the impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites. Note that the models are not designed to forecast how CO₂ storage will take place at these sites, but rather to demonstrate the features of dynamic plume migration captured in using the StrataTrapper modelling approaches.

The following is the full list of KKD's to be published under StrataTrapper:

KKD1.1 Open-source research codes for the characterisation of multiphase flow heterogeneity and conversion to flow functions for reservoir simulation

KKD1.2 A report detailing the workflows for reservoir characterisation, and model creation and use

KKD2.1 Open-source research codes for the rapid estimate of the impacts of heterogeneity on lateral plume migration, residual and dissolution trapping

KKD2.2 A report detailing the use and limitations of reduced physics models for various applications, including screening and probabilistic analysis

KKD3.1 Publicly available models of the Endurance and East Mey sites

KKD3.2 A report analysing the impacts of multiphase flow heterogeneity on CO₂ migration and trapping in the case study sites

KKD4.1 StrataTrapper user interface in Stratus

KKD4.2 Accelerated OGS simulator

KKD4.3 StrataTrapper Workshop to CCS project developers

KKD5.1 Annual reports

KKD5.2 Project final report



© Crown copyright 2026

This publication is licensed under the terms of the Open Government Licence v3.0 except where otherwise stated. To view this licence, visit nationalarchives.gov.uk/doc/open-government-licence/version/3 or write to the Information Policy Team, The National Archives, Kew, London TW9 4DU, or email: psi@nationalarchives.gsi.gov.uk.

Where we have identified any third-party copyright information you will need to obtain permission from the copyright holders concerned.

Any enquiries regarding this publication should be sent to us at: nzip@energysecurity.gov.uk

Contents

Numerical reservoir simulation of case study sites	5
Summary	5
Prerequisites	6
Endurance site	7
Capillary heterogeneity upscaling results	10
Dynamic simulation results	10
Risk-related measurements: boundary CO2 saturation	12
Proxy modelling	14
East Mey site	16
Factorial experiment design	18
Capillary heterogeneity upscaling results	18
Dynamic simulation results	19
Derived statistics	20
References	23
Simplified physics modelling of case study sites	24
Description of Mathematical Model	24
Applications	25
East Mey	25
Sleipner	27
Injection Rate Sensitivity	29
Topographic Sensitivity	30

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

Numerical reservoir simulation of case study sites

Maksim Elizarev, Ann Muggeridge, and Samuel Krevor, Imperial College London

Uncertainty-driven numerical case studies were conducted on Endurance and East Mey site models using the StrataTrapper Upscaling Toolkit.

Summary

1. We used the StrataTrapper upscaling approach to study the impact within a framework of a factorial experiment. Within the framework, we arranged a polynomial proxy modelling workflow to analyse correlations and patterns associated with parameters of small-scale capillary heterogeneity.
2. For the Endurance model, flow patterns of StrataTrapper upscaling preserved the effects of small-scale capillary heterogeneity. It predicts slower vertical migrations, faster lateral migration, and greater sweep efficiency.
3. StrataTrapper upscaling yields different simulation results for the wide range of relevant inputs, particularly injection rate, capillary pressure curve shape, and layered heterogeneity strength.
4. For the given injection model and the chosen spilling risk metric, StrataTrapper upscaling predicts the same level of risk as the conventional upscaling method at well injection rates of ~100 Mt/year/well slower.
5. For the East Mey model, we observed derived statistics over the conducted factorial experiment. We observed similar changes in behaviour as for the Endurance model: decrease in vertical migration in favour of the lateral, increased sweep efficiency and trapping.

StrataTrapper Upscaling Toolkit web page:

imperialcollegelondon.github.io/StrataTrapper

Changelog of the StrataTrapper Upscaling Toolkit on GitHub:

github.com/ImperialCollegeLondon/StrataTrapper/blob/main/CHANGELOG.md

“StrataTrapper-models” data repository web page:

imperialcollegelondon.github.io/StrataTrapper-models

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

More results of case studies are available at:

Elizarev, Maksim and Wenck, Nele and Krevor, Samuel and Muggeridge, Ann,
Upscaling Algorithm to Preserve Effects of Small-Scale Capillary Heterogeneity: Field-Scale Studies on CO₂ Storage Sites (December 23, 2024).
Proceedings of the 17th Greenhouse Gas Control Technologies Conference (GHGT-17)
20-24 October 2024,
Available at SSRN: <https://ssrn.com/abstract=5068897>
or <http://dx.doi.org/10.2139/ssrn.5068897>

Prerequisites

More detailed specifications of the Endurance and the East Mey models can be found in (Wenck et al., 2025; Elizarev et al., 2024; Elizarev, 2024). In the described experiments, we simulated heterogeneities by generating spatially correlated porosities and absolute permeabilities. Correlations are simulated by ellipsoidal averaging with semi-axes $c_{[x,y,z]}$.

The impacts of multiphase flow heterogeneity on CO2 migration and trapping at case study sites

Table 1: Nomenclature (primarily in chronological order)

Entry	Definition	Physical dimensions
M	Unit mass	M
L	Unit length	L
T	1. Unit time (in the right-most column of this table) 2. Total simulated time interval	T
P_c	Capillary pressure	$ML^{-1}T^{-2}$
$S_{[w,g]}$	Saturation of water or gas/CO2	1
ϕ	Porosity	1
$K, K_{[x,y,z]}$	Absolute permeability tensor and its diagonal components	L^2
$J_{\min (\text{ref})}$	Leverett J-function minimum (reference value)	MT^{-2}
$S_{w,\text{irr}}$	Irreducible water saturation	1
λ	Pore distribution parameter	1
$c_{[x,y,z]}$	Geological correlation length along x, y, or z	L
Q_{inj}	Well mass injection rate	MT^{-1}
$N_{[x,y,z]}$	Number of fine layers in coarse cell along each direction	1
K_{ijk}, ϕ_{ijk}	Isotropic permeability and porosity of fine cell (i, j, k)	$L^2, 1$
$S_g^{[\text{bound}, \text{top}, \text{side}]}$	Boundary gas saturation (total, top-boundary, and side-boundary)	1
S_g^{cell}	Gas saturation in a cell	1
$A_{[\text{bound}, \text{top}, \text{side}]}^{\text{cell}}$	Surface area of a cell included in a model's boundary (total, top-boundary, and side-boundary)	L^2
p	Parameters in factorial experiment	Arbitrary
y	Nonlinear measurement for p	Arbitrary
f	Estimator for y	Same as estimated y
$\alpha, \beta_i, \gamma_{ij}, \delta_{ijk}$	Parameters of polynomial proxy model for $y(p)$	Depends on y and p
t	Time in dynamic simulations	T
$S_{g,[\text{base}, \text{upsc}]}^*$	Gas saturation in models upscaled conventionally / with StrataTrapper	1

Endurance site

Figure 1 describes the relations between inputs and outputs in the designed experiment. We generated a fine-scale model for every tested combination of variable inputs specified in Table 2. Porosity and permeability fields were generated geostatistically using distributions from

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

Wenck et al. (2025). Each fine-scale model was upscaled in a ‘conventional’ way and via the StrataTrapper approach. Then, each coarse model was put into dynamic simulation. We took the “four-wells” setup from (Elizarev, 2024) and simulated 25 years of injection and 25 more years. To simulate open boundary conditions, we created a numerical aquifer by amplifying pore volumes of the side-boundary cells in the model.

Dynamic simulation results were summarised quantitatively by computing the dynamics of total gas saturation in areas close to the model’s boundaries. We derived secondary measurements using these quantities: disagreement of upscaling algorithms and maximum side-boundary saturation for a given upscaling algorithm and injection rate. Finally, we trained polynomial proxy models on the entire ensemble of simulations to predict the derived quantities for parameters within the simulated range.

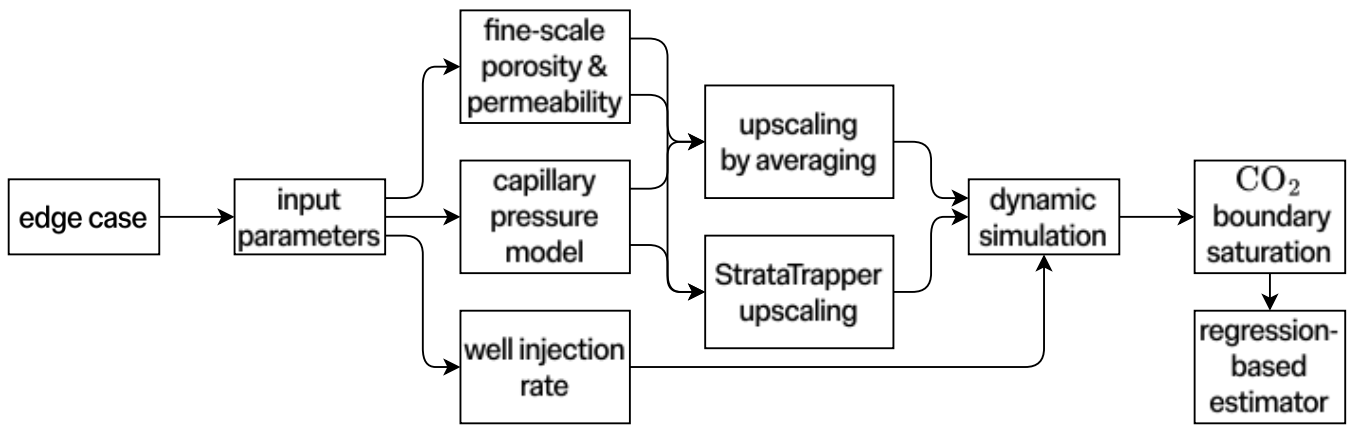


Figure 1. Diagram of the factorial numerical experiment conducted for the Endurance site model.

Table 2. Variable parameters of the Endurance model in the factorial experiment with their respective ranges (edge cases) and base values. Base values originate from previous characterisation studies (Wenck et al., 2025). The base injection rate is an arbitrary point inside the corresponding range.

Parameter	Base value	Range	Units
c_z	4	[2, 8]	m
c_y	760	[80, 1000]	m
c_x/c_y	$\frac{1000}{760}$	[1, 2]	1
$\frac{J_{\min}}{J_{\min, \text{ref}}}$	0.032/0.032	[0.01, 1.2]	1
$1/\lambda$	1/1.75	[0.3, 1]	1
Q_{inj}	250	[3, 1000]	$\frac{\text{kt CO}_2}{\text{year}}$

The impacts of multiphase flow heterogeneity on CO2 migration and trapping at case study sites

We refer to the conducted experiment as factorial since we simulated all possible combinations of variable factors' minima and maxima. The base value was an additional directly simulated point. Figure 2 visualises the tested combinations in a way that captures the shape of the covered area in the parameter space.

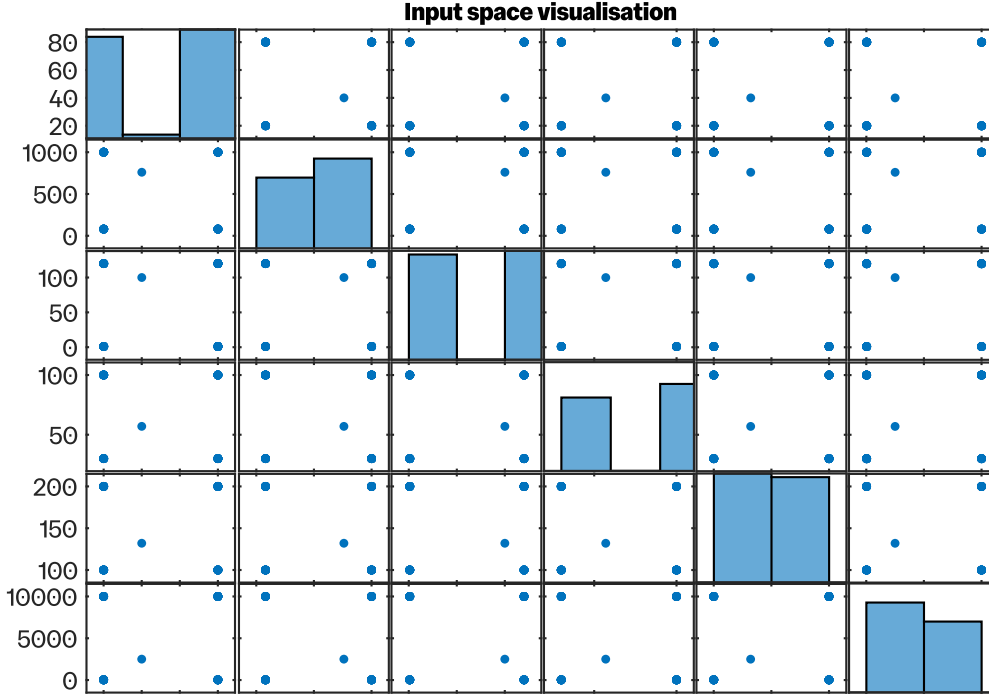


Figure 2. Visualisation of multi-dimensional input points for the factorial experiment. All parameter pairs are scatter-plotted.

The following equation (and its equivalents for K_x and K_y) was used for absolute permeability upscaling in the ‘conventional’ homogeneous approach (“upscaling by averaging”) compared to the StrataTrapper approach.

$$K_z = \frac{N_z}{N_x N_y} \left[\sum_k \left[\sum_{ij} K_{ijk} \right]^{-1} \right]^{-1}$$

The following equation was used for porosity upscaling in both tested approaches.

$$\varphi = \frac{1}{N_x N_y N_z} \sum_{ijk} \varphi_{ijk}$$

The Leverett J-function approach to capillary pressure modelling was the source of capillary heterogeneity for both upscaling approaches. The equation below was used for fine-scale capillary pressure computation and homogeneously upscaled dynamic models. For simplicity of the equation, the term $J_{\min}$ is a multiple of dimensionless value, surface tension and contact angle

$$P_c(S_w, \varphi, \mathbf{K}) = J_{\min} \left(\frac{S_w - S_{w,irr}}{1 - S_{w,irr}} \right)^{-\frac{1}{\lambda}} \sqrt{\frac{\varphi}{(K_x + K_y) \cdot 0.5}}$$

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

Capillary heterogeneity upscaling results

Parallel coordinate plots in Figure 3 show the upscaling results of the StrataTrapper toolkit v0.10.0. Statistically significant decrease in entry capillary pressure and reduced vertical gas permeabilities from Wenck et al. (2025) were reproduced.

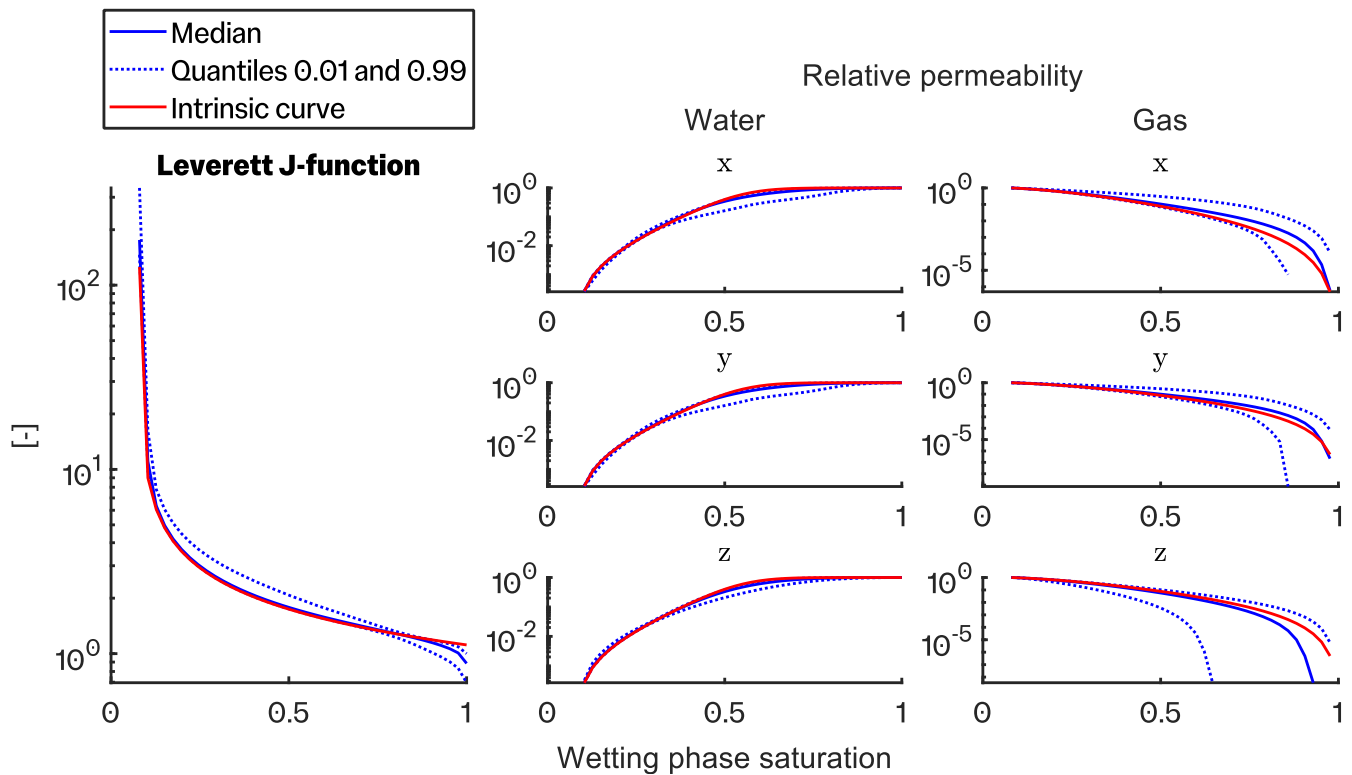


Figure 3. StrataTrapper upscaling summary given the base values from Table 2. “Intrinsic curves” are the original fine-scale viscous-limit inputs used in the standard upscaled models that do not incorporate capillary heterogeneity effects.

All the following figures of an individual Endurance simulation correspond to the base values from Table 2.

Dynamic simulation results

Figure 4 and Figure 5 show CO₂ saturation predicted by the ‘conventional’ and the StrataTrapper upscaling, respectively.

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

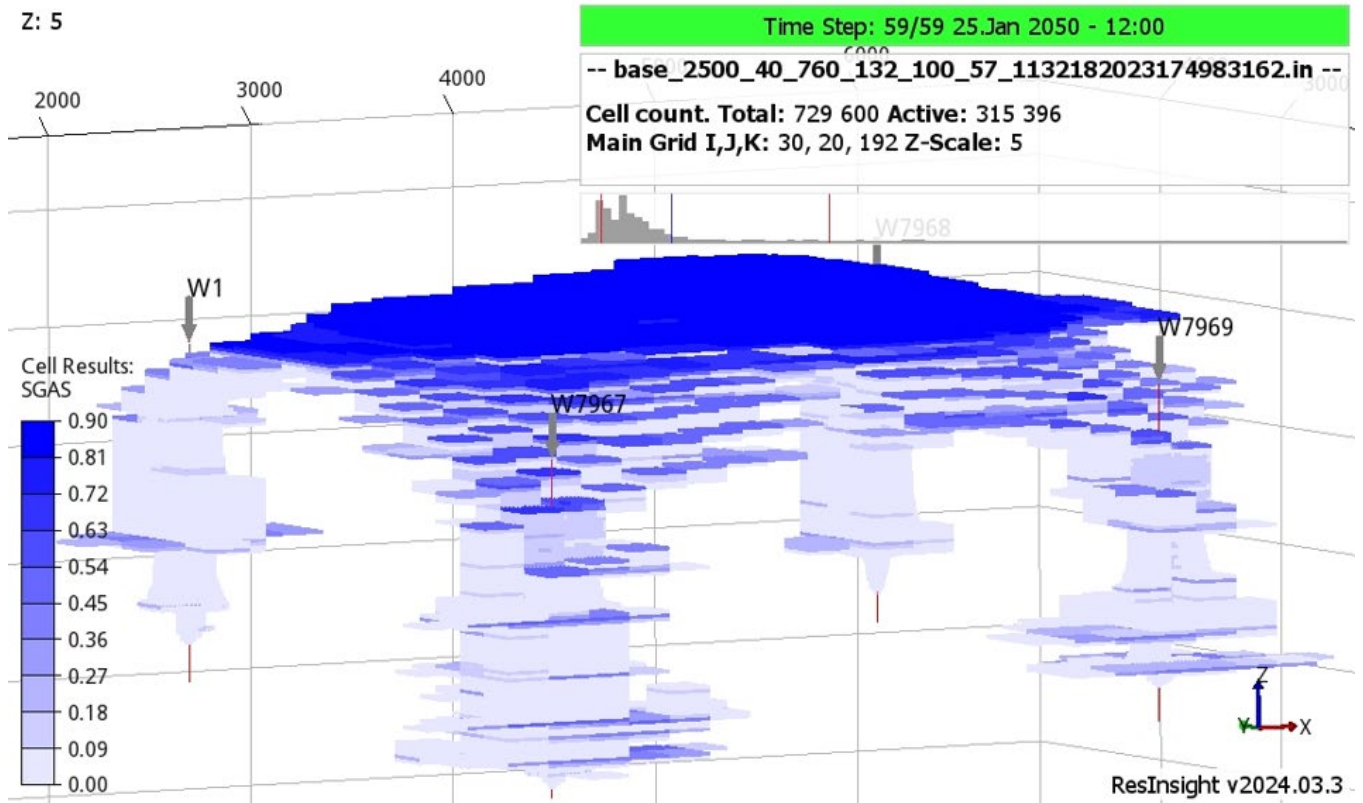


Figure 4. End of coarse-scale dynamic simulation without capillary heterogeneity upscaling: resulting CO₂ saturation given the base values from Table 2.

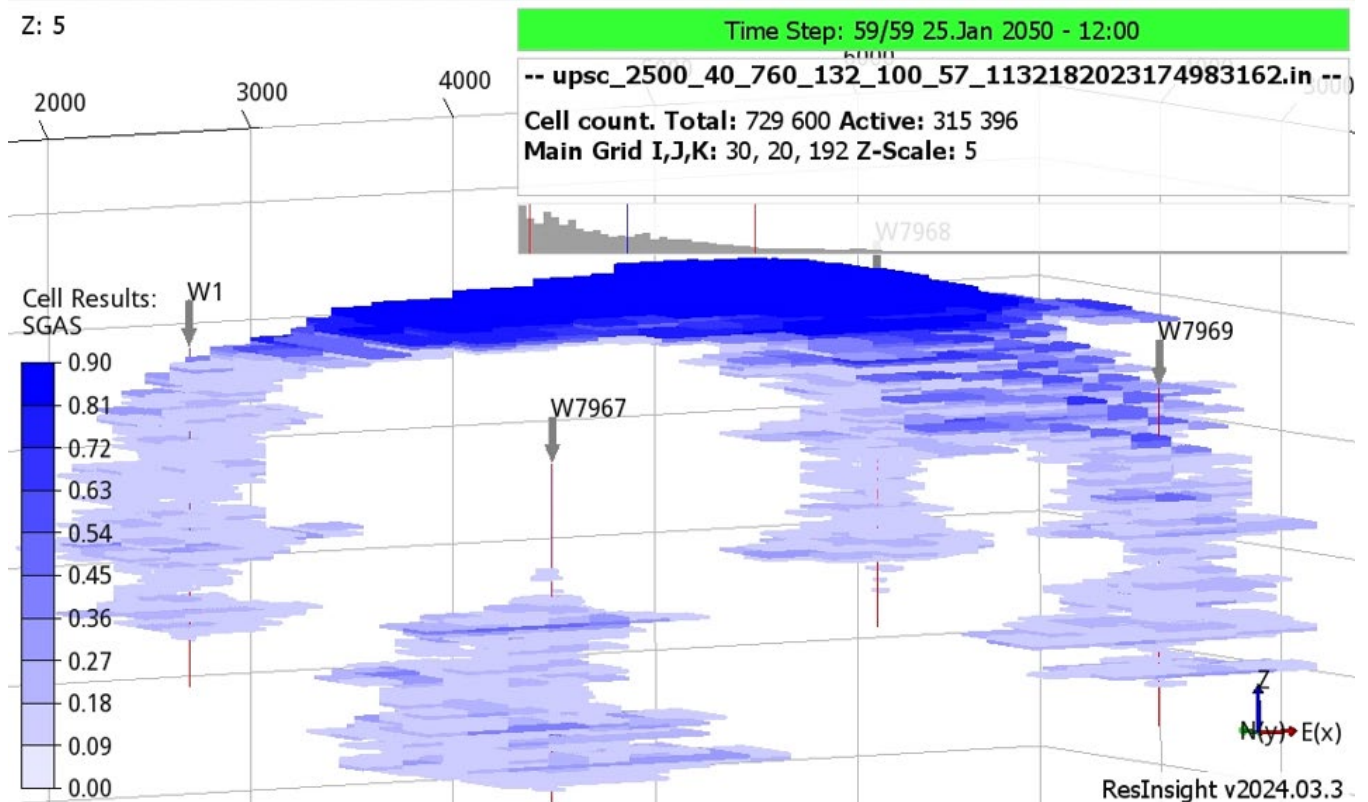


Figure 5. End of coarse-scale dynamic simulation with the StrataTrapper upscaling: resulting CO₂ saturation given the base values from Table 2.

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

With the StrataTrapper upscaling approach, the dynamic simulation predicts greater sweep efficiency around the wellbores and reduced vertical migration compared to the ‘conventional’ upscaling. Figure 6 visualises areas of increased and decreased saturation by colour.

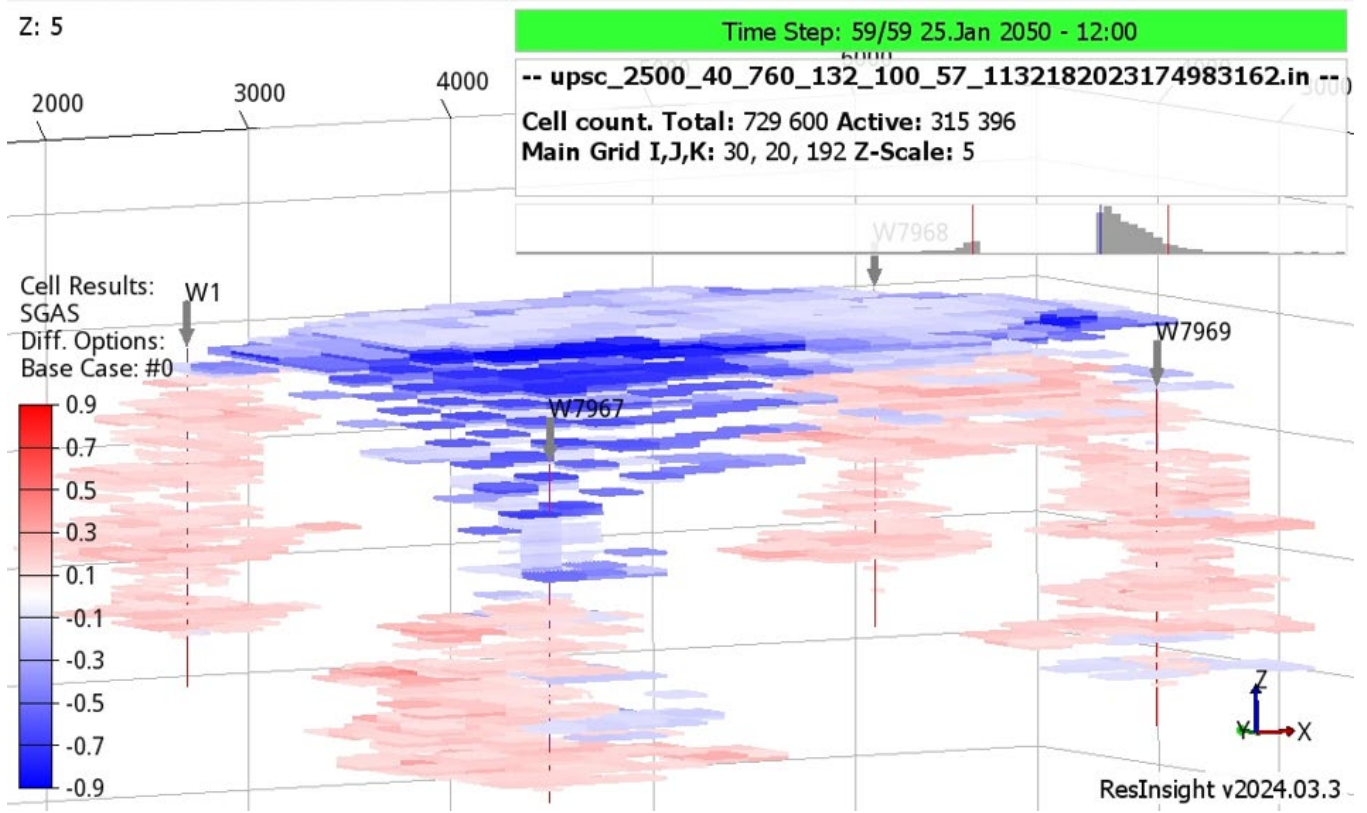


Figure 6. Visualised difference in CO₂ saturation between the two in Figure 5 and Figure 4.

Risk-related measurements: boundary CO₂ saturation

Following the equation below, we computed boundary gas saturations for each reported timestep of every dynamic simulation.

$$S_g^{\text{boundary}} = \frac{\sum_{\text{cell} \in \text{boundary}} S_g^{\text{cell}} \cdot A_{\text{boundary}}^{\text{cell}}}{\sum_{\text{cell} \in \text{boundary}} A_{\text{boundary}}^{\text{cell}}}$$

The boundary regions we considered were:

1. top: cells contacting the dome and their upper surface areas
2. side: cells contacting the numerical aquifer and the areas of their corresponding surfaces.
3. bound: a union of top and side, entire boundary region

Figure 8 summarises differences from Figure 6 in terms of change in top and side CO₂ saturations.

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

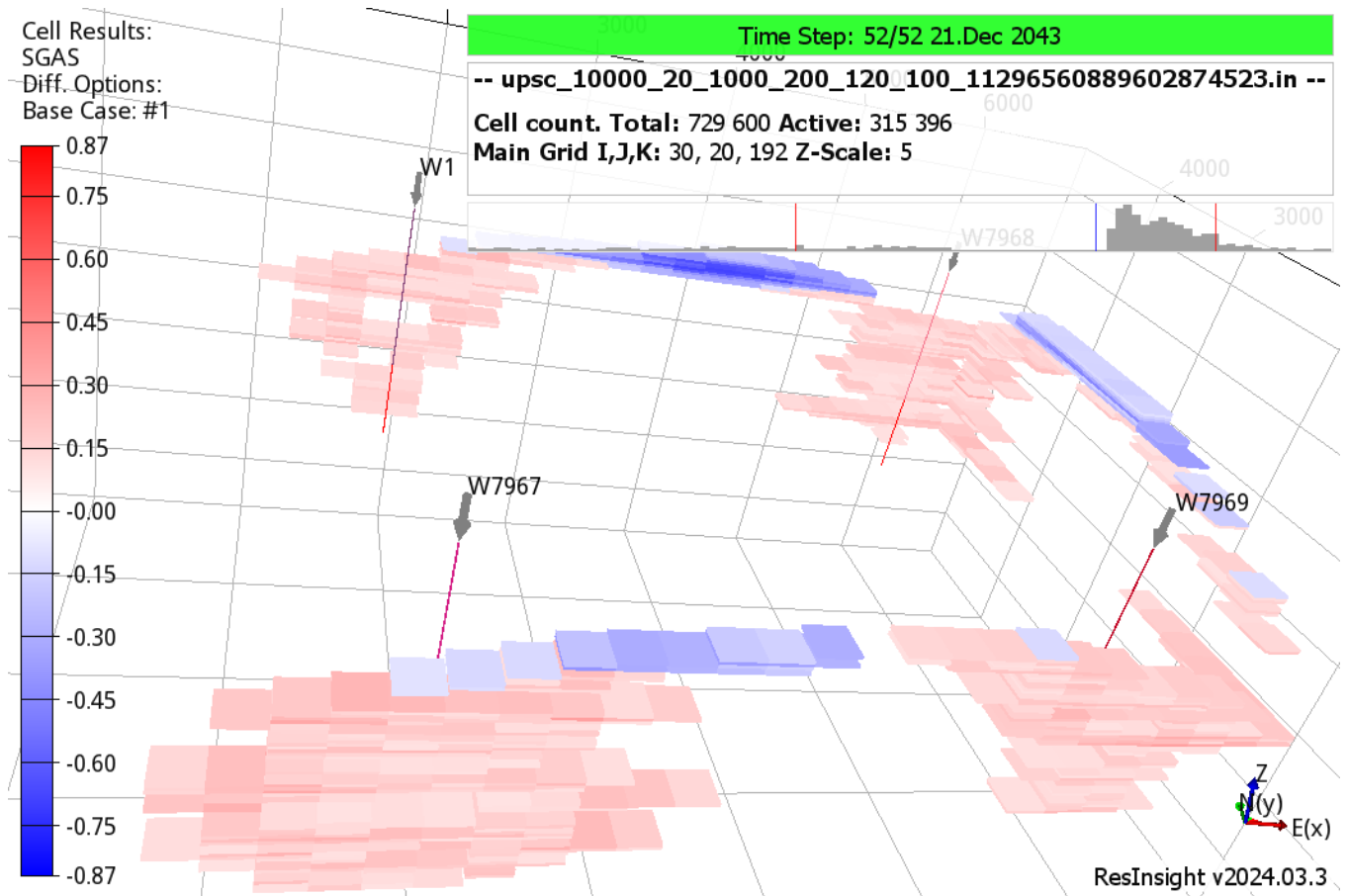


Figure 7. Example: visualised final difference in side-boundary CO₂ saturation for one of the edge cases of the factorial experiment.

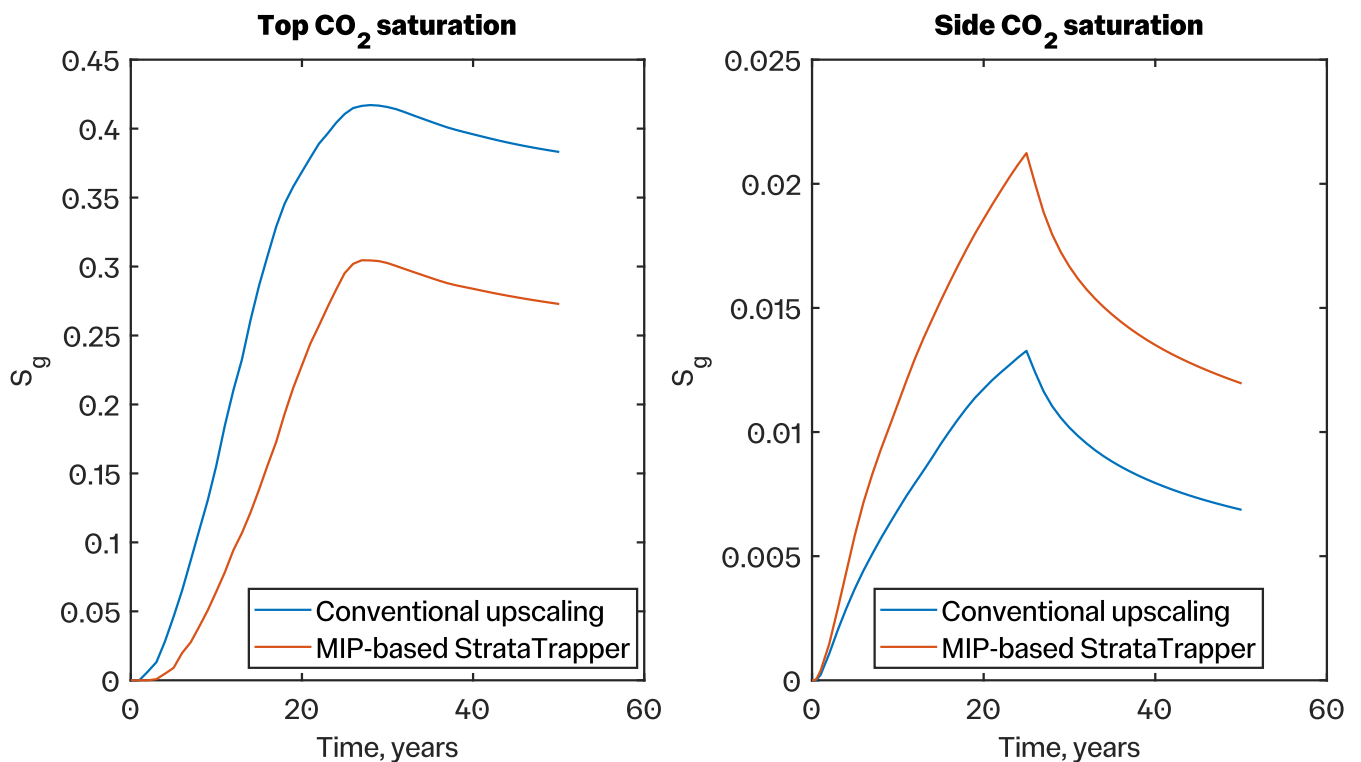


Figure 8. Comparison of boundary CO₂ saturation for the base values from Table 2. “Conventional upscaling” refers to homogeneous upscaling that does not incorporate capillary heterogeneity effects.

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

Proxy modelling

If $p = [p_1 \dots, p_6]$ — variable parameters of factorial experiment, and $y(p)$ — corresponding measurement, then the polynomial proxy model $f(p)$ for $y(p)$ had the following form.

$$y(p) \approx f(p) = \alpha + \sum_i \left[\beta_i p_i + \sum_{j < i} \left[\gamma_{ij} p_i p_j + \sum_{k < j} \delta_{ijk} p_i p_j p_k \right] \right]$$

Parameters of proxy models were evaluated via linear regression.

We derived and analysed two quantities:

1. Disagreement of upscaling algorithms $f_{\text{diff}}(p) \approx y_{\text{diff}}(p)$

$$y_{\text{diff}}(p) = \frac{1}{T} \int_0^T |S_{\text{g,upsc}}^{\text{bound}}(t; p) - S_{\text{g,base}}^{\text{bound}}(t; p)| dt$$

2. Maximum side-boundary gas saturation $f_{\text{side}}(p) \approx y_{\text{side}}(p)$

$$y_{\text{side}}(p) = \max_t S_{\text{g}}^{\text{side}}(t; p) \rightarrow f_{\text{side}}(p)$$

Sensitivity analysis of capillary heterogeneity upscaling

Using $f_{\text{diff}}(p)$ proxy model, we conducted sensitivity analysis of simulated CO₂ migration to the model's boundary (Figure 9).

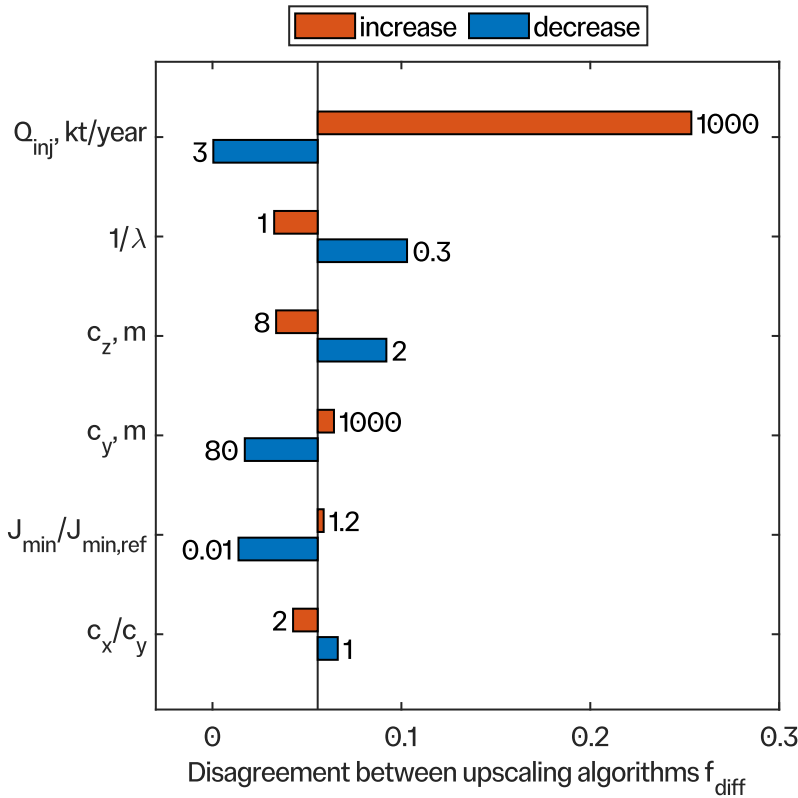


Figure 9. Sensitivity analysis of the difference in boundary CO₂ saturation predicted with different upscaling algorithms. Estimates are made by the trained polynomial proxy model. The vertical baseline corresponds to the base values from Table 2. In each row, only the respective parameter is changed to one of the edge cases.

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

Within the tested range of parameters, the most significant variations in predicted CO₂ migration were caused by changes in well injection rate, shape of capillary pressure curve, and vertical correlation length. Notably, the increase in f_{diff} correlated with the decrease in c_z , which represents layered heterogeneity.

Impact of capillary heterogeneity on spilling risks assessment

Figure 10 shows maximum side boundary saturations predicted by the two upscaling methods we compared. It also shows differences between directly simulated saturations and those predicted by proxy models.

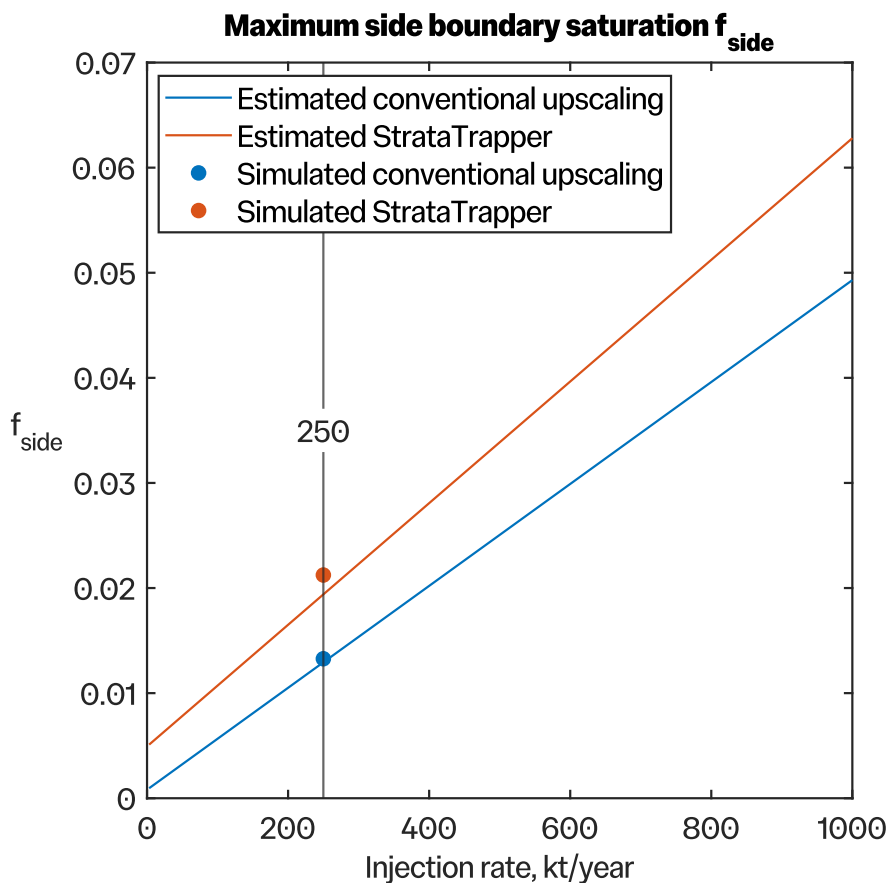


Figure 10. Proxy-modelling of the maximum side-boundary CO₂ saturation for the base values from Table 2 (with variable well injection rate) based on two upscaling approaches. Lines represent proxy modelling, while dots represent coarse-scale simulations.

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

East Mey site

We took the well placement “1” from Elizarev (2024) and simulated 34 years of injection and 44 years afterwards. Four injection wells in Figure 11 were split into two injection scenarios: wells G1–G2 only and all wells G1–G4. To simulate open boundary conditions, the model included a numerical aquifer. The given East Mey site model had frequently alternating layers of shale rock simulated as virtually impermeable.

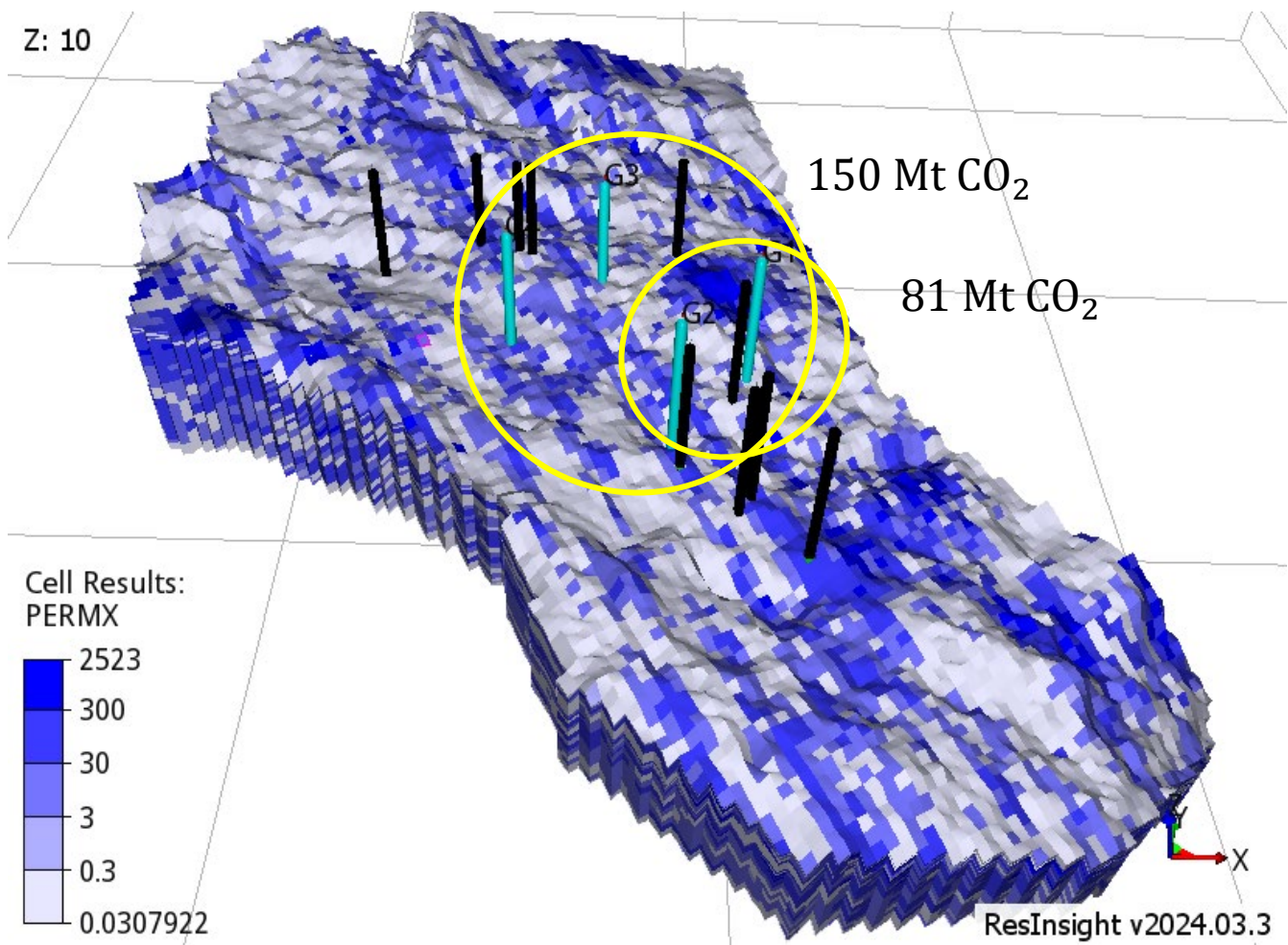


Figure 11. Visualisation of lateral absolute permeability in the given East Mey model. Gas injection wells are coloured cyan. A subset of legacy wells around gas injection wells is coloured black. Two injection scenarios are represented by two encircled sets of gas injectors, each with its respective total injected mass.

Using the given coarse East Mey site model, we investigated the re-upscaling approach to modelling with the StrataTrapper toolkit. We assumed porosity and logarithm of permeability were distributed normally at the fine scale, and corresponding coarse values in the model were produced by volume-weighted averaging. Accordingly, to scale a coarse cell down to the original fine-scale resolution, we implemented the following procedure for porosity and the lateral permeability logarithm:

1. Sample sub-scale values from a normal distribution with the mean equal to the given coarse value and the standard deviation of the empirical coarse-scale distribution (see Figure 12).

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

2. Apply spatial correlation lengths (c_x, c_y, c_z) that do not exceed the respective cell dimensions.
3. Re-normalize spatially correlated realisations to match the mean and the standard deviation from step 1.

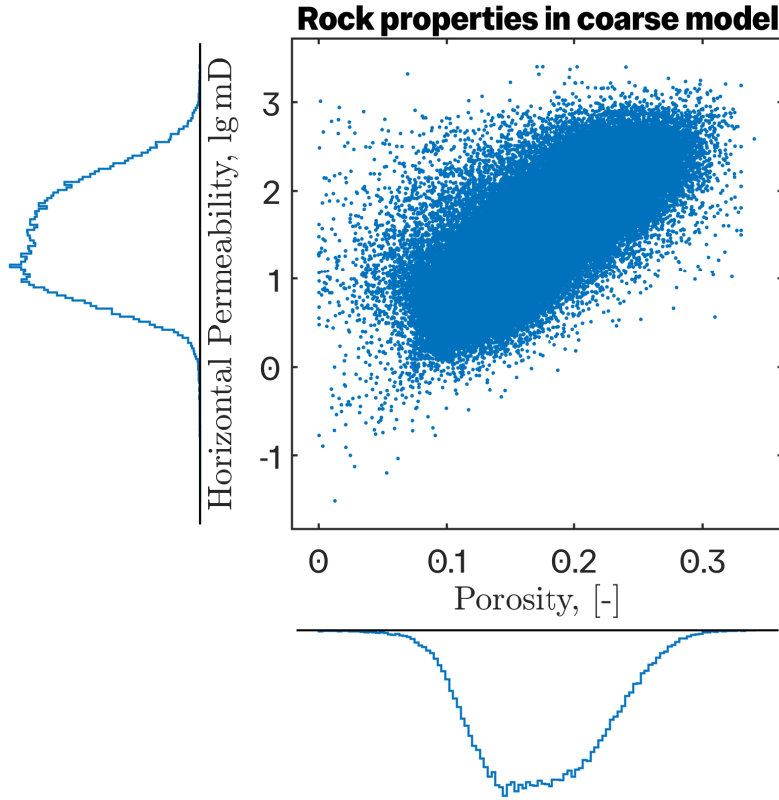


Figure 12. Distribution of porosity and lateral absolute permeability in the given East Mey model.

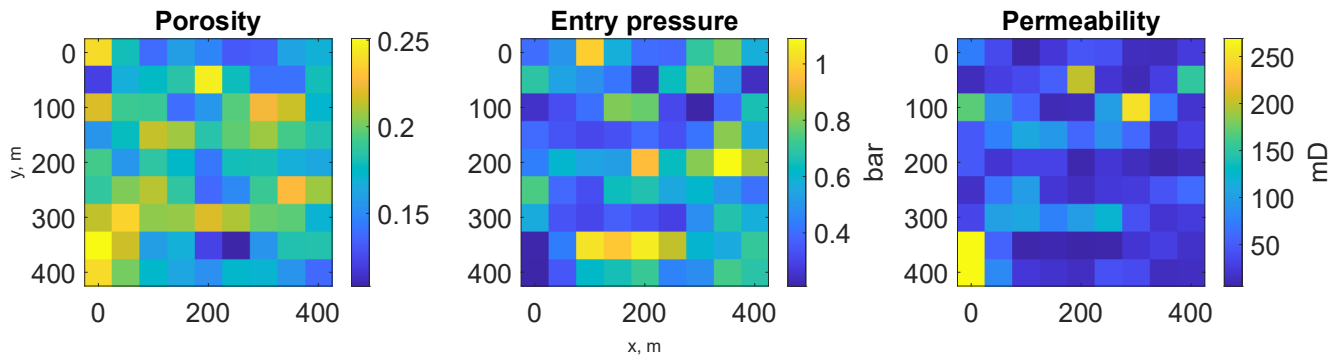


Figure 13. Example of a downscaled coarse block of the East Mey model with $c_x > c_y$. Figures represent a horizontal cross-section at the middle of a coarse cell.

Regarding absolute permeability, the coarse model was laterally isotropic with vertical anisotropy equal to 0.5. We generated lateral permeabilities following the procedure above for consistent fine-scale reconstruction and then applied vertical anisotropy of 0.5 to obtain fine-scale vertical permeabilities.

The given model did not include capillary pressure. We adopted the equation used for the Endurance model for the factorial experiment with East Mey.

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

Factorial experiment design

Using the sensitivity analysis results shown in Figure 9, we excluded lateral anisotropy from the parameter space of the East Mey factorial experiment. Also, we analysed two injection scenarios independently.

Table 3. Variable parameters of the East Mey factorial experiment (both scenarios) with their respective ranges (edge cases) and an arbitrarily selected internal point.

Parameter	Internal point	Range	Unit
c_z	4	[1, 22]	m
$c_x = c_y$	60	[60, 400]	m
$\frac{J_{\min}}{J_{\min, \text{ref}}}$	1	[0.01, 1.2]	1
$1/\lambda$	1	[0.5, 1]	1

Then, we followed the workflow from Figure 1 to produce and simulate the ensemble of re-upscaled dynamic models. Those simulations were compared to simulations with originally provided rock properties and zero capillary pressure to investigate the impact of re-introduction of small-scale heterogeneities. Finally, we analysed the derived statistics for the re-upscaled ensemble.

Capillary heterogeneity upscaling results

Parallel coordinate plots in Figure 14 show the upscaling results of the StrataTrapper toolkit v0.10.0. In this case, we observed a significant decrease in gas permeability for small gas saturations down to the introduction of non-zero effective critical gas saturations. Across the ensemble, we observed a decrease in entry capillary pressure, a common effect of macroscopic invasion percolation.

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

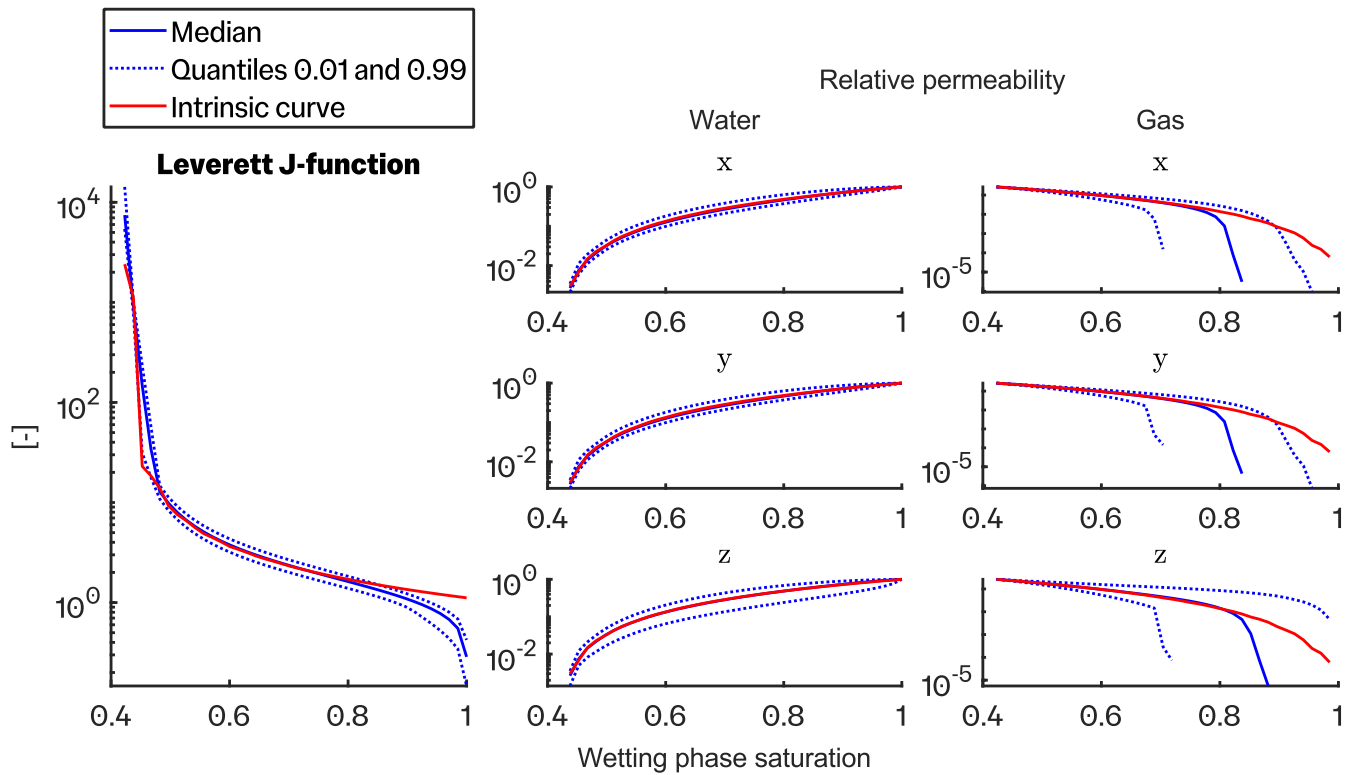


Figure 14. StrataTrapper upscaling summary given the internal point from Table 3. “Intrinsic curves” are the original inputs used in the standard upscaled models that do not incorporate capillary heterogeneity effects.

Dynamic simulation results

As shown in Figure 15, introduction of capillary pressure within re-upscaling with the StrataTrapper toolkit impacted East Mey simulations in the same way observed during experiments with the Endurance model: reduced vertical migration in favour of lateral, increased sweep efficiency and trapping.

The impacts of multiphase flow heterogeneity on CO2 migration and trapping at case study sites

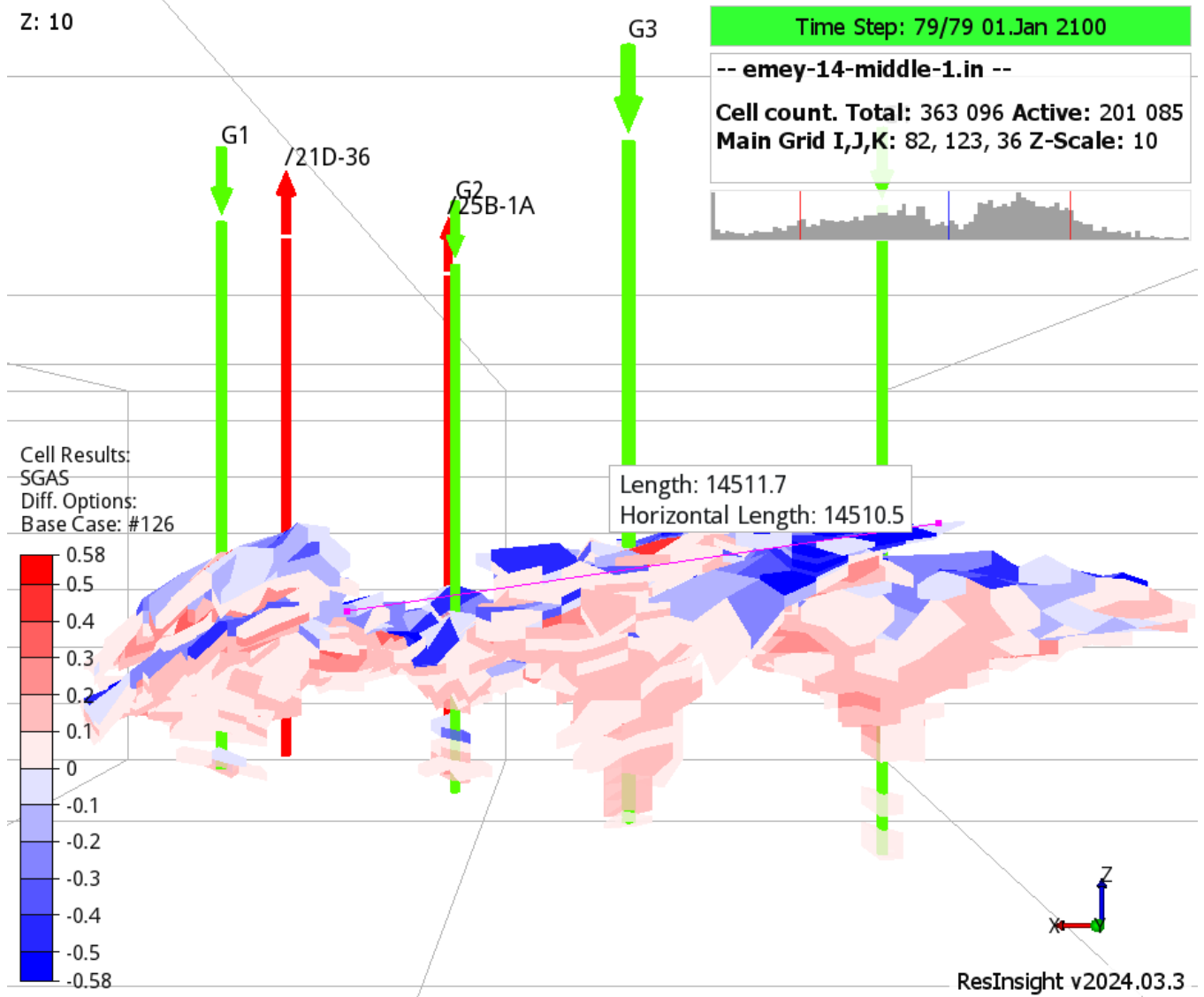


Figure 15. East Mey: visualised difference in final gas saturation, scenario with 150 Mt CO2 injected. The internal point from Table 3 (re-upscaled model) is compared to the original coarse model.

Derived statistics

Figure 16 shows the impact of uncertainty in small-scale capillary heterogeneity on uncertainty in simulated gas saturation: the standard deviation of gas saturation across the ensemble can reach magnitudes close to the maximum gas saturation in the model. Figure 17 shows local uncertainty in gas saturation around one of the wells close to the injection wells.

The impacts of multiphase flow heterogeneity on CO2 migration and trapping at case study sites

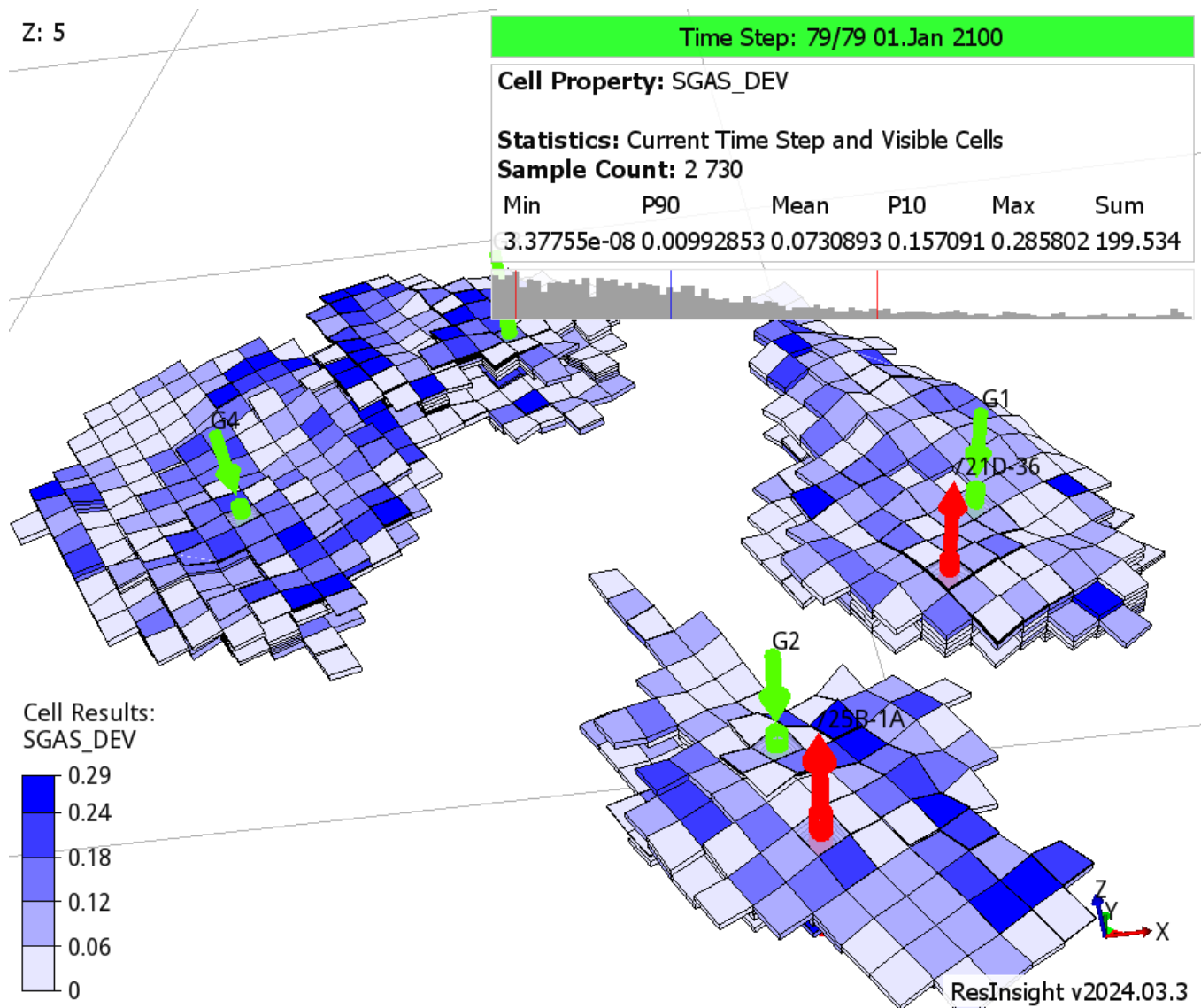


Figure 16. East Mey: derived statistics over the ensemble computed for the 150 Mt scenario. The visualised is the standard deviation in the final CO2 saturation.

The impacts of multiphase flow heterogeneity on CO2 migration and trapping at case study sites

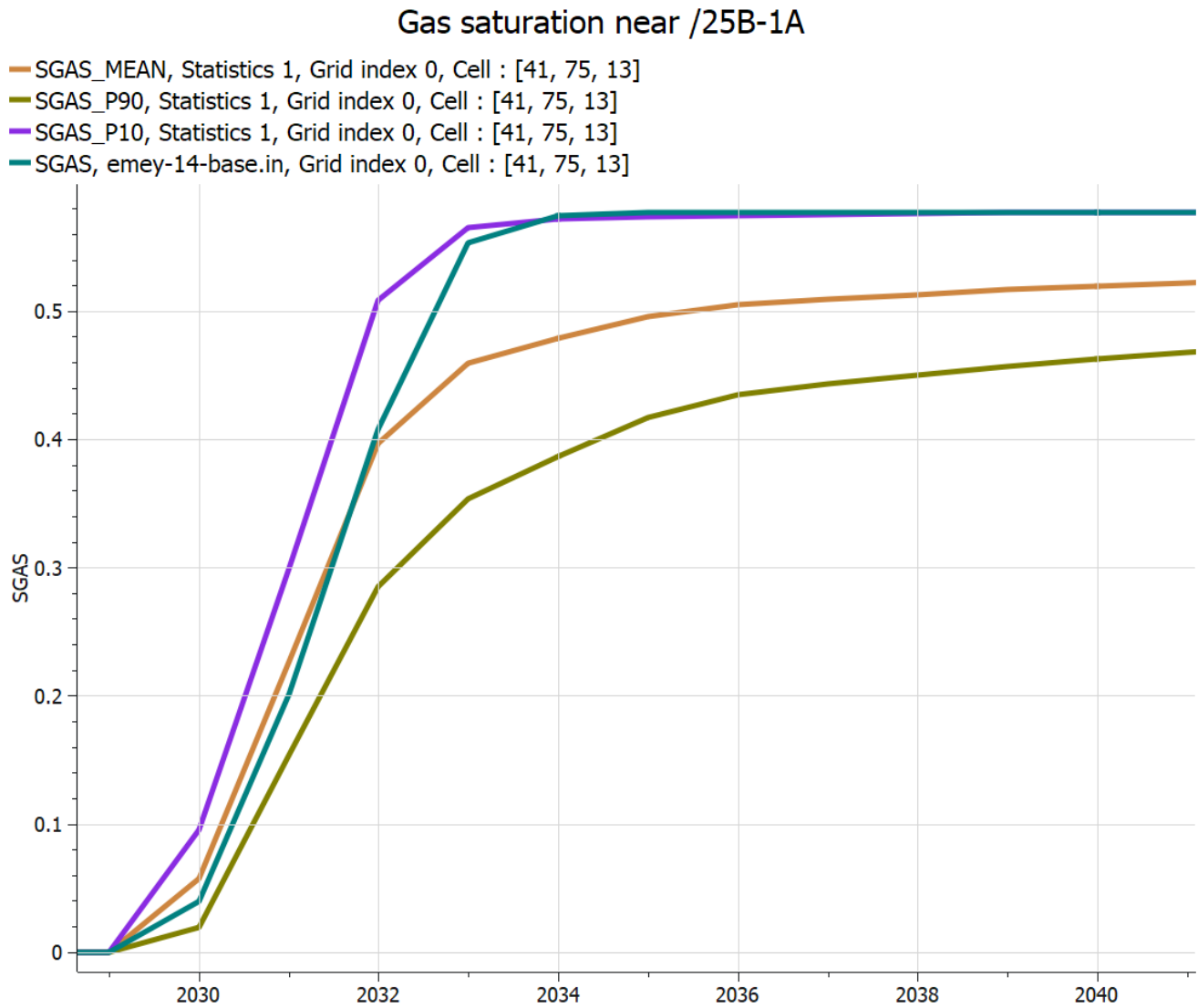


Figure 17. East Mey: derived statistics over the ensemble computed for the 150 Mt scenario. The visualised is CO2 saturation at the top active coarse cell at the lateral location of legacy well /25B-1A: original coarse model, ensemble mean, ensemble's P10 and P90.

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

References

Elizarev, M. (2024) *ImperialCollegeLondon/StrataTrapper-models: Models upscaled with StrataTrapper*. 2024. github.com. <https://github.com/ImperialCollegeLondon/StrataTrapper-models> [Accessed: 20 January 2025].

Elizarev, M., Wenck, N., Krevor, S. & Muggeridge, A. (2024) Upscaling Algorithm to Preserve Effects of Small-Scale Capillary Heterogeneity: Field-Scale Studies on CO₂ Storage Sites. *SSRN Electronic Journal*. doi:10.2139/SSRN.5068897.

Wenck, N., Muggeridge, A., Jackson, S., An, S. & Krevor, S. (2025) The Impact of capillary heterogeneity on CO₂ plume migration at the Endurance CO₂ storage Site in the UK. *Geoenergy*. doi:10.1144/GEOENERGY2024-029.

Simplified physics modelling of case study sites

CO2GraVISim (CO2 Gravity-dominated Vertically Integrated Simulator), a reduced-physics model for geological carbon storage developed as part of the StrataTrapper project, has been used to investigate CO2 injection for both East Mey and Sleipner. For East Mey we get good agreement with simulations performed with a traditional reservoir simulator. For Sleipner we investigate the sensitivity of the CO2 plume to injection strategy and uncertainty in caprock topography.

Description of Mathematical Model

The reduced-physics model developed as part of WP2 of the StrataTrapper project describes the field-scale behaviour of CO2 injected into a subsurface, fluid-saturated reservoir. The model relies on two widely applicable assumptions about the flow of the CO2:

1. The flow of the CO2 is predominantly horizontal,
 2. The time for the CO2 to migrate to the caprock of the storage interval is short compared to the total migration time.
- Under these assumptions, we can picture the flow as shown in Figure 1.

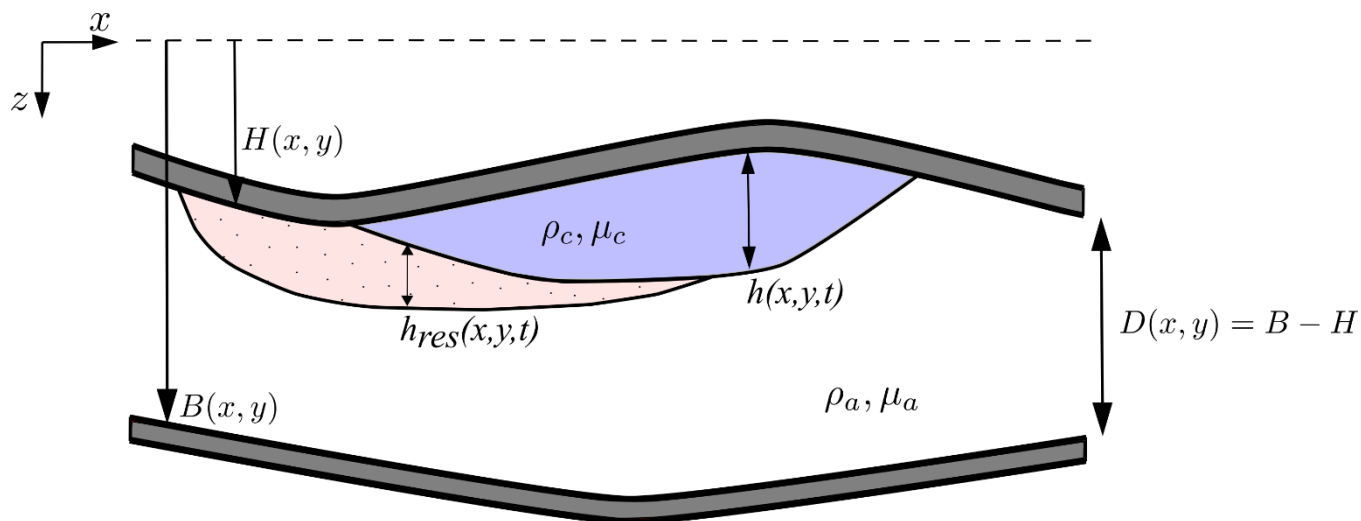


Figure 1: Schematic of the reservoir and flow setup used in the mathematical model. The reservoir is divided into regions of mobile CO2 (purple), residually trapped CO2 (spotted, light red), and pure ambient fluid (the remainder of the reservoir).

This splits the reservoir into three distinct flow regions:

- Mobile region ($H \leq z \leq H + h$), consisting of mobile free-phase CO2 and immobilised, irreducible ambient water,
- Trapping region ($H + h \leq z \leq H + h + h_{res}$), consisting of residually trapped free-phase CO2 and mobile ambient water,

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

- Ambient region ($H + h + h_{res} \leq z \leq B$), consisting purely of mobile ambient water.

Under these assumptions, the vertical variation of pore pressure in the reservoir is predominantly due to gravity (i.e. hydrostatic) and we can vertically integrate the governing equations across the flow regions described above. This vertical integration encodes the vertical structure of the reservoir while producing a simpler set of governing equations for this model that now only involve derivatives in terms of x and y , and no longer in z . This order reduction means that this model can be solved numerically much more quickly than those used by traditional Full Physics simulators, while still retaining the key physical mechanisms governing the behaviour of the CO₂, e.g. the heterogeneity of reservoir properties such as topography, porosity, and permeability.

For more details, see *StrataTrapper: WP2 D2.1 - Reduced Physics Models of Fluid Flow and Trapping*.

The software implementing this reduced physics model, called CO₂GraVISim (**CO₂ Gravity-controlled Vertically Integrated Simulator**), is publicly available on GitHub at <https://github.com/ajobutler/CO2GraVISim>. It consists of

- Fortran files comprising the main solver,
- Python scripts to preview reservoir structure, post-process the results from individual and ensemble runs, and to generate simple reservoir geometries,
- Batch scripts to facilitate performing ensembles of runs in a parallelised fashion.
- Further details can be found in the documentation provided in the GitHub repository.

Applications

East Mey

Using the East Mey reservoir model developed as part of WP3 and the StratusAPI developed as part of WP4, it is straightforward to run a CO₂GraVISim simulation of the flow of CO₂ from the 4 injector wells in the East Mey model. The East Mey geomodel has a high degree of heterogeneity in terms of permeability and porosity, as well as a large number of inactive cells. Despite this, the CO₂GraVISim simulation runs without issue, with a mass-balance error of less than 0.09% by the end of the simulation period. This simulation, covering a total simulation period of 90 years, took 56 seconds to run in Unconfined mode on a standard laptop¹.

¹ 10th Generation Intel® Core™ i7-10510U Processor, 12GB RAM, purchased in 2020.

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

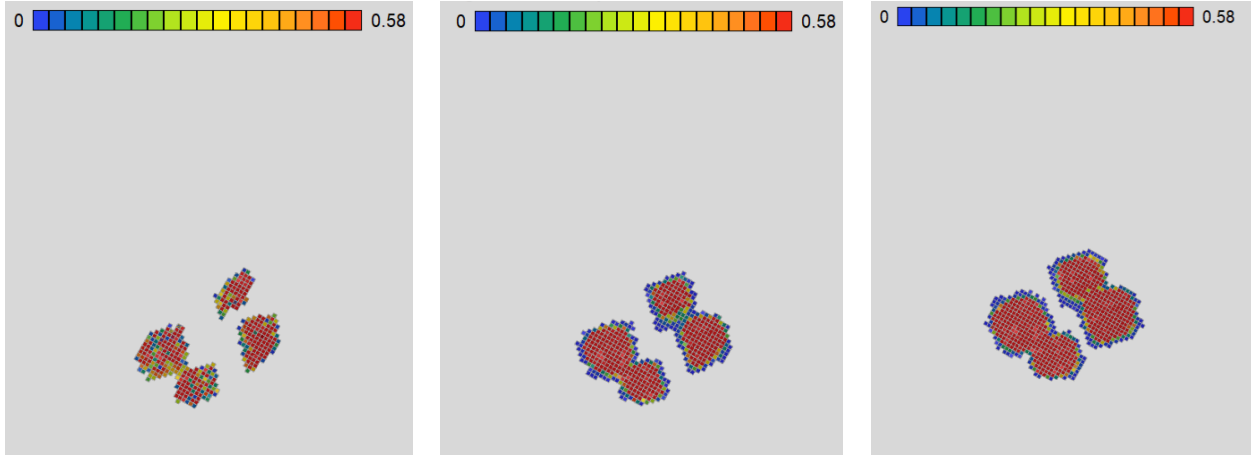


Figure 2: The final saturation distributions from a simulation for the heterogeneous East Mey model using Cirrus (right) and CO₂GraVISim (centre), and a homogeneous version of East Mey using CO₂GraVISim (right).

Figure 2 shows a comparison between the saturation distribution profiles at the end of the simulation from both CO₂GraVISim and Cirrus (formerly PFLOTRAN-OGS), showing a very good agreement in terms of plume shape and saturation distribution despite the simplifying assumptions made in the model. For comparison, an equivalent simulation has been run using CO₂GraVISim for a homogeneous variant of the East Mey geomodel, with porosity and permeability set to their mean values from the heterogeneous version. We see in Figure 2 that this results in faster migration away from the injection wells, with broader, and correspondingly thinner, CO₂ plumes.

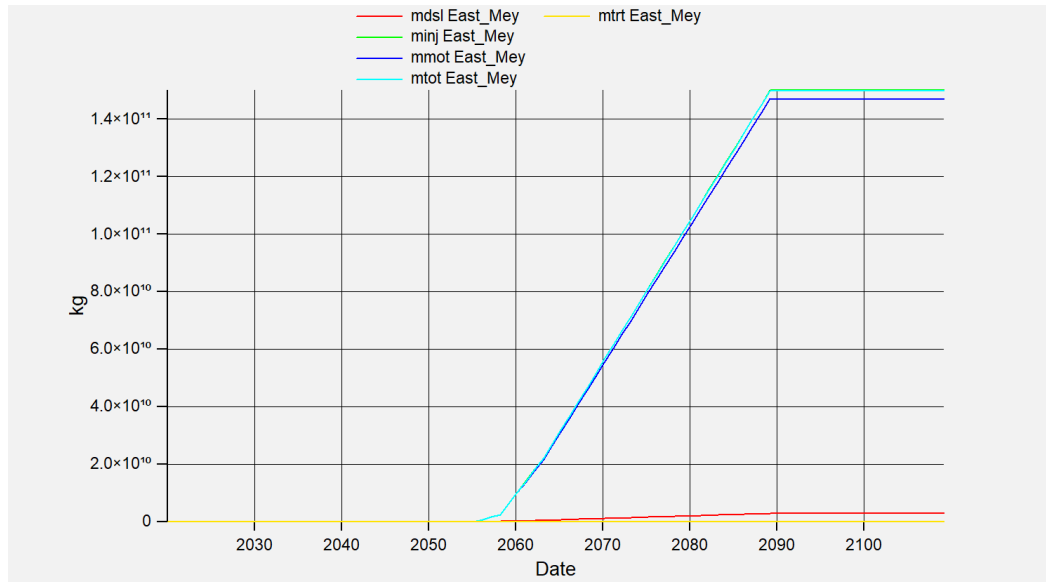


Figure 3: A plot over time of the various masses in the CO₂GraVISim simulation for East Mey. See main text for details.

Figure 3 shows a time-series plot of the various masses accounted for in the simulation. These are the total mass of CO₂ injected (minj, green); total mass in the simulation (mtot, light blue); the total mobile mass (mmot, dark blue), the total residually trapped mass (mtrt, yellow), and the total dissolved mass (mdsl, red).

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

The results in Figure 3 are shown with a nominal start date of 1st Jan 2020, and include an initial period without any injection that corresponds to a period of Production Well activity in the Cirrus simulation. By the end of the simulation, we see that the total mass in the simulation matches the total mass injected, as expected, and that the majority of the CO₂ is still mobile, with only $\approx 2\%$ of the CO₂ dissolved in the ambient brine by this stage. These simulations were performed without the effects of residual trapping.

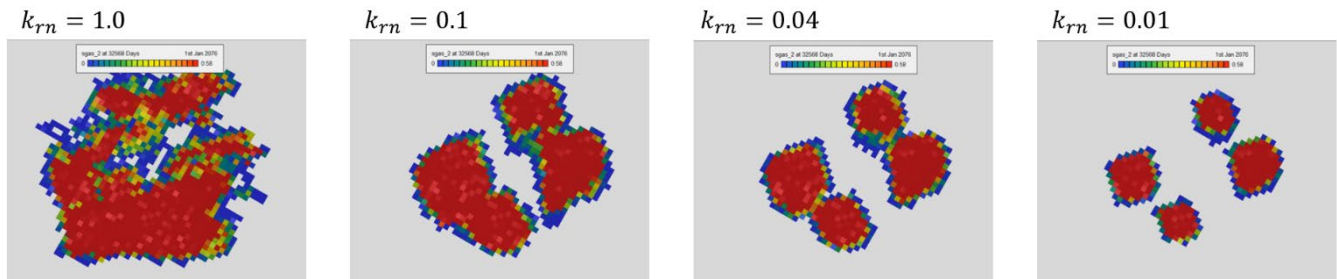


Figure 4: A comparison of the final plume profile as the non-wetting relative permeability k_{rn} is varied.

The CO₂GraVISim results shown in Figures 2 and 3 were calculated using a relative permeability coefficient of k_{rn} for the CO₂ (the non-wetting phase) of $k_{rn} = 0.04$. Figure 4 shows the final saturation distributions for a range of different k_{rn} values and highlights the importance that this effect can have on the simulation results. Despite the full saturation curves used in Full Physics simulations being boiled down to a single value for the mobile region here, we are still able to get strong agreement between the two simulation methods.

Sleipner

We have also considered the effect of topographic heterogeneity, using the Sleipner project as a test case. For this we have used a modified version of the Sleipner 2019 Benchmark Model, publicly available on the CO₂DataShare website: <https://co2datashare.org/dataset/sleipner-2019-benchmark-model>.

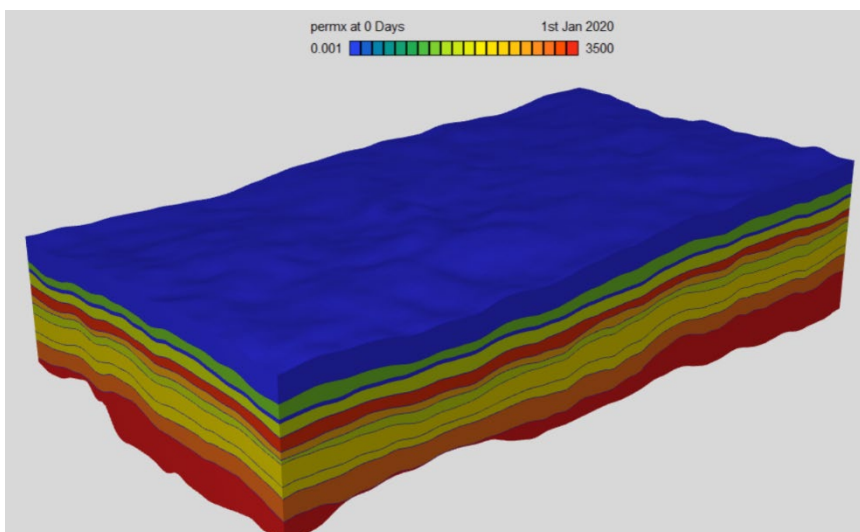


Figure 5: The permeability structure of the Sleipner geomodel. The storage interval considered here, Layer 1, is shown in red at the bottom of the geomodel.

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

This geomodel consists of 9 high-permeability layers, separated by low-permeability interfaces. Here we have chosen to use the deepest high-permeability section of the model, Layer 1, assuming an impermeable interface with the layer above (i.e. with no leakage to shallower depths). This subsection of the geomodel corresponds to a storage interval with $64 \times 118 \times 58$ grid points in x , y , and z ; horizontal grid spacings $dx = dy = 50m$; a permeability of $3483.09mD$; and a porosity of 0.36. The mean vertical extent of this storage interval is $85m$.

The base case of our simulations consists of a constant injection rate of 0.2 Mt/yr for 3 years followed by a post-injection period continuing to a total simulation period of 270 years. This simulation takes about 90 seconds on the standard laptop. The simulations discussed in this section were run in Unconfined mode, where the effect of the injection of the CO₂ is assumed to have a negligible effect on the ambient water and so the dynamic pressure is assumed to be $P_a = 0$, resulting in a simpler form for the governing equations.

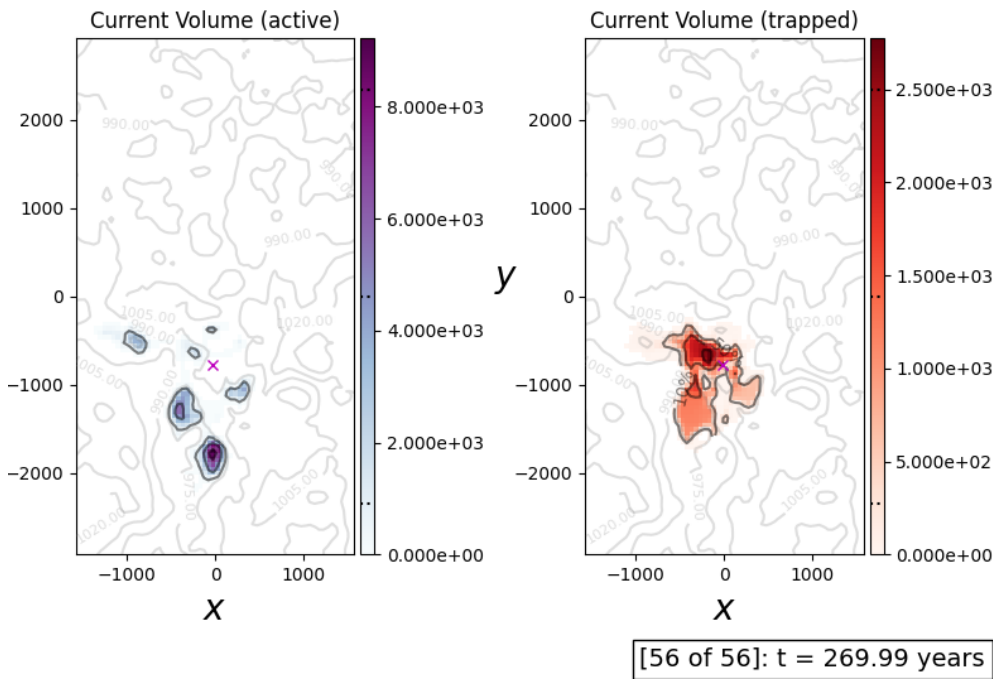


Figure 6: The free-phase CO₂ volume distribution at the end of the simulation – mobile phase (left, purple) and residually trapped (right, orange). Volumes here are measured in m^3 and distances in m .

Figure 6 shows the final volume distributions at the end of the simulation for both the mobile and residually trapped CO₂. We find that at the end of the simulation, 3% of the total volume is trapped via dissolution, 36% is residually trapped, and 61% remains in the mobile phase and is stratigraphically trapped.

Since this simulation is quick to run, we can perform a large of runs with variations of the input parameters or geomodel data in order to study the ensemble behaviour. We have used this to investigate the sensitivity of the CO₂ plume to variations in the injection rate and variations in caprock topography.

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

Injection Rate Sensitivity

To study the sensitivity of the CO₂ plume to how it is injected, we consider 30 variants of the base case discussed above: we inject the same total mass of 0.6 Mt at the same location, varying the injection rate from 0.02 Mt/yr ($0.1 \times$ the base case value) to 2 Mt/yr ($10 \times$ the base case value), adjusting the injection period appropriately.

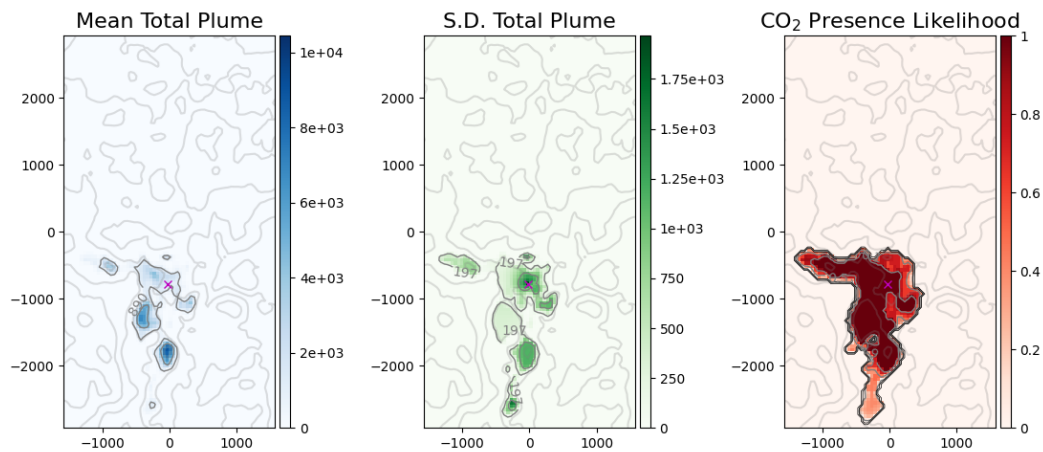


Figure 7: The ensemble plume behaviour for varying injection rate with fixed total volume. The first and second panels show the mean and standard deviation, respectively, of the volume of free-phase CO₂ (i.e. mobile and trapped) at each location measured in m^3 . The third panel shows for each location the proportion of runs that had CO₂ there at any point in the simulation.

Figure 7 shows the mean and standard deviation of this ensemble of simulation results, as well as the proportion of runs that had CO₂ at each location at any point in the simulation. Values close to 1 or 0 are thus where the runs agree on the presence or absence of CO₂, while intermediate values are where the results are more variable. For an uncontrolled, random parameter such as topographic variation discussed below, this can be interpreted as a likelihood map of encountering CO₂ at each location.

We can thus see that for this injection location the choice of injection rate can have a significant effect on the ultimate behaviour of the CO₂ plume. Some runs were able to migrate close to the southern boundary of the simulation domain, which may be of significant regulatory concern when considering the licenced region in which the CO₂ must remain. For this ensemble of injection scenarios, it was the simulations with a weaker injection rate (over a longer injection period) that were able to migrate farther south; those with a stronger injection rate remained closer to the injection location and had a higher overall sweep efficiency.

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

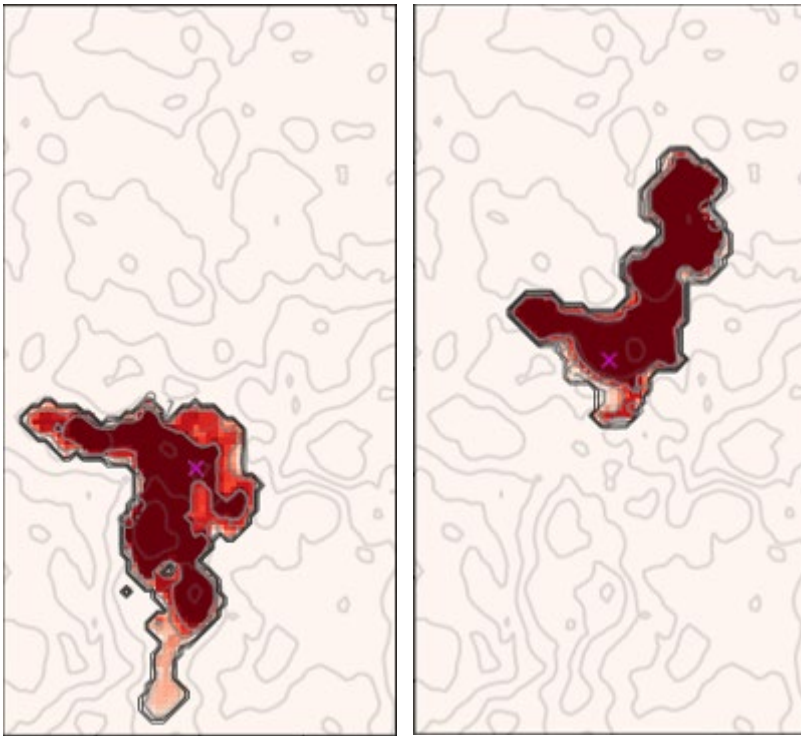


Figure 8: A comparison of the likelihood maps for the same injection-variation ensemble runs carried out at two neighbouring injection locations

Figure 8 shows a comparison between the likelihood maps for the ensemble run discussed above and shown in figure 7, and the same set of injection scenarios simulated at a neighbouring injection location. The two injection locations have grid indices (31,43) and (31,60), and so are only 850 m apart. However, due to the caprock topography they have significantly different drainage basins, and the second injection location has a much lower variability in CO₂ distribution – a much smaller proportion of the CO₂ footprint has intermediate likelihood values (lighter red colours), suggesting a more secure storage location.

Topographic Sensitivity

As well as variables that can be controlled by site operators, such as injection rates, we can also look at the sensitivity of the CO₂ plume to variables that cannot be controlled, such as uncertainty in caprock topography.

Dr. Sophie Tobin, a Postdoc at the University of Cambridge, has developed a process to quickly generate variants for given topography. Here we use 50 variants that are normally distributed around the base topography, with mean variation amplitude of 1 m and a correlation length of 300 m. We then use the injection scenario from the base case (0.2 Mt/yr for 3 years) and simulate the CO₂ behaviour for each variant.

Each simulation again took $\approx 90s$ to run the standard laptop. In series this would take $\approx 1hr\ 15mins$, but run in 4 parallel batches we are able to reduce this to 18 mins, $\frac{1}{4}$ of the series time.

The impacts of multiphase flow heterogeneity on CO₂ migration and trapping at case study sites

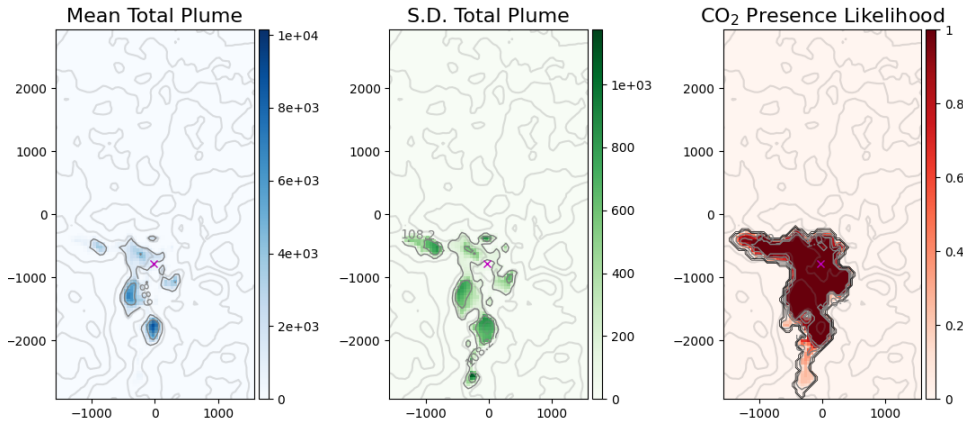


Figure 9: The ensemble plume behaviour for varying caprock topography. The first and second panels show the mean and standard deviation, respectively, of the volume of free-phase CO₂ (i.e. mobile and trapped) at each location measured in m^3 . The third panel shows for each location the proportion of runs that had CO₂ there at any point in the simulation.

Figure 9 shows the ensemble results for injection at (31,43), the injection location considered in the base case. Again, we see a significant degree of variability in the CO₂ footprint across this ensemble of runs, in this case resulting from comparatively small variations in topography (1m compared to a range of ≈ 80 m of depth values for the base caprock topography) that lie within the uncertainty of seismic measurements. These results, together with the injection variation results above, suggest that there is a key topographic low point in the base-case caprock topography preventing migration of the plume to the southern extent of the domain, but that it can be overcome by relatively small changes in injection rate or topography.

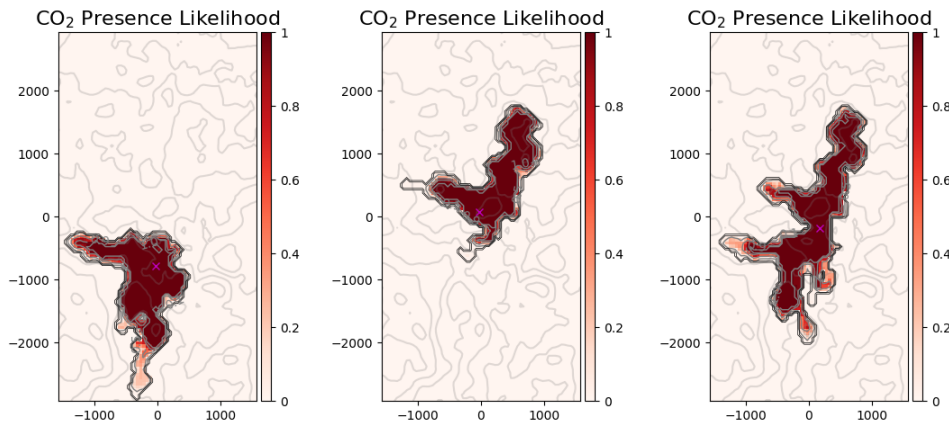


Figure 10: The likelihood maps for the topographic variation simulations at three different injection location.

Figure 10 shows a comparison of the likelihood maps for the same ensemble study of topographic variation – using the same topography variants in each case – at three different injection locations: the two locations considered in figure 8, and a third at (35,55) that lies in between. We again see similar results for the second injection location when compared to the injection variation study. The third injection location lies on a watershed dividing the drainage basins of the first and second injection locations.

If you need a version of this document in a more accessible format, please email alt.formats@energysecurity.gov.uk. Please tell us what format you need. It will help us if you say what assistive technology you use.