StrataTrapper

Final Project Report

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Contents

Executive Summary

In StrataTrapper we translate cutting edge research 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. Through the project, the tools are commercialised through incorporation into the CO2 reservoir simulation platform OpenGoSim, in addition to being made open-source. We 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 has been the commercialisation of the StrataTrapper reservoir simulation tools for the rapid screening, risking, project design, and management of CO2 storage.

Reservoir simulations of injected CO2 plumes are central to the successful engineering and management of CO2 storage. Plume migration rates and direction determine the storage efficiency and significance of potential leakage pathways. The extent of residual and dissolution trapping are quantified through simulation based history matching. Increasing simulation accuracy can de-risk and lower costs throughout the lifetime of a storage project including appraisal, project design, implementation, and abandonment.

Past work at Imperial College London and University of Cambridge has identified that major inaccuracies in current modelling approaches are due to previously ignored impacts of small scale (cm-m) heterogeneities in multiphase flow properties. Plume migration rates, and the extent of residual and dissolution trapping in a field can all be enhanced by over 200% by these flow heterogeneities. The research has demonstrated the importance of these processes. In this project we have taken advantage of the opportunity to commercialise the research into simulation tools for site screening, appraisal, and forecast modelling of use by practitioners.

The structure of StrataTrapper is designed to realise the commercial potential of the research advances in flow physics. Consortium partners BP, Storegga, and Drax are project developers of CCUS clusters in the UK, and provide invaluable guidance on the demands placed on the commercial use of these tools. OpenGoSim provides the commercial platform necessary for these and other industrial organisations to make use of these research advances. The open publication of the research basis and engagement with additional practitioners has facilitated broader uptake.

Project Outline, aims and objectives

Work Package 1 – Core-to-field reservoir simulation

Aims

To develop the core-to-field numerical upscaling techniques of Jackson & Krevor (2018) from 2D to 3D models, apply them to case studies in WP3, and provide codes for generating flow functions from field data to WP4 for commercial incorporation into OpenGoSim.

Objectives

(O1.1) Define the StrataTrapper approach to reservoir characterisation (O1.2) Define the StrataTrapper approach to reservoir simulation.

Deliverables

(D1.1) Open-source research codes for the characterisation of multiphase flow heterogeneity and conversion to flow functions for reservoir simulation (D1.2) A report detailing the workflows for reservoir characterisation, and model creation and use.

Work Package 2 – Reduced physics models of fluid flow and trapping

Aims

In WP2 the models previously developed at ICL and Univ. Cambridge will be extended to incorporate spatially variable reservoir architecture. We will develop automated upscaling functions for application to case studies in WP3 and incorporation into the OpenGoSim simulator in WP4. In addition, a standard methodology for characterising uncertainty will be developed and directed towards probabilistic forecasts of the plume spread.

Objectives

(O2.1) Create open-source codes of reduced physics models of CO2 storage (O2.2) Develop workflows for applying these codes for screening and probabilistic analysis of injection.

Deliverables

(D2.1) Open-source research codes for the rapid estimate of the impacts of heterogeneity on lateral plume migration, residual and dissolution trapping (D2.2) A report detailing the use and limitations of reduced physics models for various applications, including screening and probabilistic analysis.

Work Package 3 – Case Studies: The Endurance Field and the East Mey Storage Site

Aims

In WP3 we will classify heterogeneity types within the Endurance and East Mey Storage sites, supplementing existing data with analysis of core material in WP1. We will construct models of the sites using the StrataTrapper workflow and demonstrate the impacts of heterogeneities on flow and trapping, with implications for site development, management, and closure. We will evaluate primary and further stage development plans of the sites with injection rates ranging from 0.3 – 8 Mt yr-1 by 2030.

Objectives

(O3.1) StrataTrapper analysis of the Endurance Field (O3.2) StrataTrapper analysis of the East Mey Site (O3.3) Analysis of latter stage field development scenarios.

Deliverables

(D3.1) Publicly available models of the Endurance and East Mey sites (D3.2) A report analysing the impacts of multiphase flow heterogeneity on CO2 migration and trapping in the case study sites.

Work Package 4 – Commercialising the StrataTrapper Numerical Toolset

Aims

We will commercialise the StrataTrapper toolset by incorporation into the software platform OpenGoSim. There are two groups of activities that will take place in parallel. One group translates techniques and research codes from WP1 and 2 into the OpenGoSim simulator, PFLOTRAN-OGS. The second develops GPU support for the simulator, dramatically enhancing the computational performance so that high spatial resolution simulations of heterogeneity can be performed. We will hold a workshop with storage project developers in the final year to further encourage uptake.

Objectives

(O4.1) Develop the StrataTrapper Pseudo and reduced physics packages for OpenGoSim (O4.2) Develop GPU solver capability for OpenGoSim.

Deliverables

(D4.1) StrataTrapper User Interface implemented for OpenGoSim (D4.3) High-performance version of PFLOTRAN-OGS supporting the StrataTrapper extensions (D4.4) StrataTrapper Workshop for CCS Project Developers.

Work Package 5 – Management

Aims

The Principal Investigator (PI), Sam Krevor, is responsible for the project performance. The PI will be advised by the General Assembly (GA) which will comprise one member of each partner. A Work Plan will be agreed by the GA. A regular teleconference will take place to track progress, monthly for the first 6 months, and quarterly thereafter. The PI and the GA will be responsible for monitoring progress including maintaining a RAG dashboard of project risks. The GA will formally approve milestones and deliverables and will be the decision-making body for changes to the scope.

Objectives

(O5.1) Create a project management infrastructure to efficiently deliver the project (O5.2) Successfully carry out the project management plan and provide timely delivery of the project outcomes.

Deliverables

(D5.1) Project reports to BEIS (D5.2) Project final report.

Roles and contributions of each project partner

Imperial College London – Project lead; Lead and sole contributor to WP1; co-lead for WP3, and lead for WP5

University of Cambridge – Lead and sole contributor to WP2; co-lead for WP3, and contributor to WP5

OpenGoSim – Lead and sole contributor to WP4; co-lead for WP3, and contributor to WP5

bp – Guidance and feedback on the activities in WP1, WP2, and WP3

Storegga – Guidance and feedback on the activities in WP1, WP2, and WP3; Data for WP3

Drax – Guidance and feedback on the activities in WP1, WP2, and WP3

Description of activities and work packages, milestones, and final results

Work Package 1: Numerical Upscaling Toolkit and Reservoir Simulation

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

Open-source research codes for characterising multiphase flow heterogeneity and conversion to flow functions for reservoir simulation.

A research software toolkit, written in MATLAB, was created to facilitate the conversion of information about the properties of a reservoir to be used in the StrataTrapper modelling approach. The purpose of the software is to accurately incorporate information about the reservoir's heterogeneity, particularly the capillary pressure heterogeneity, into an upscaled model used for reservoir simulation. The algorithm's input is spatial statistical information about reservoir properties, including means, variances, and correlation lengths of flow properties. The output is a 3D reservoir model with upscaled flow properties, including relative permeability and capillary pressure, that may be used for dynamic reservoir simulation.

The upscaling approach closely follows the approach presented in Jackson & Krevor (2020) but includes a few key developments: The upscaling has been extended from 2D to 3D models; the calculation of upscaled relative permeability is now performed within the code and without calls to reservoir simulation software, significantly improving the computational performance.

The software toolkit is publicly available via the GitHub repository: https://github.com/ImperialCollegeLondon/StrataTrapper.

The `` `main` `` branch of this repository is a release branch. We recommend using and referring to the latest state of this branch. The repository has a `` `README` `` file that describes the purpose and contents of the repository, as well as our guidelines for users and potential contributors.

The StrataTrapper GitHub project has the web page: https://imperialcollegelondon.github.io/StrataTrapper/

This development was built on top of the work of Jackson and Krevor (2020) and the doctoral thesis of Wenck (2023). The more efficient analytical approach was derived and implemented within the project to evaluate upscaled relative permeabilities without any calls to external reservoir simulations. Those works in turn are developments of the upscaling approaches presented in Wolff et al., (2013) and Yang et al., (2013).

Key References

The upscaling approach implemented in this toolkit is described in detail in:

Samuel J. Jackson, Samuel Krevor
Small-Scale Capillary Heterogeneity Linked to Rapid Plume Migration During CO2 Storage
Geophysical Research Letters | 2020
https://doi.org/10.1029/2020GL088616

Nele Mareike Wenck
The Impact of Capillary Heterogeneity on Subsurface Carbon Dioxide Storage
PhD Thesis, Imperial College London, Department of Earth Science and Engineering | 2023

Those works developed this toolkit, building on the upscaling approaches presented in:

Wolff, M., Flemisch, B., & Helmig, R. (2013). An adaptive multiscale approach for modeling two-phase flow in porous media including capillary pressure. Water Resources Research, 49(12), 8139-8159.

Yang, Z., Tian, L., Niemi, A., & Fagerlund, F. (2013). Upscaling of the constitutive relationships for CO2 migration in multimodal heterogeneous formations. International Journal of Greenhouse Gas Control, 19, 743-755.

Initial release

StrataTrapper v0.1.0
https://github.com/ImperialCollegeLondon/StrataTrapper/tree/v0.1.0

StrataTrapper v0.1.0 Technical Reference
https://github.com/ImperialCollegeLondon/StrataTrapper/blob/v0.1.0/Reference/user-manual.pdf

Later releases

Since the initial release v0.1.0, the toolkit and its development infrastructure have been improving continuously.

Changelog of the StrataTrapper Upscaling Toolkit on GitHub:
github.com/ImperialCollegeLondon/StrataTrapper/blob/main/CHANGELOG.md

Implementation/infrastructure improvements

1. Reduced code duplication.

2. Cleaner toolkit interface and data structures.
3. Implemented routines of continuous integration (CI): automated checks of new code (static analysis, tests) and documentation (spell checks, hyperlink checks), automated releases, automated website deployment, etc.
4. Substantially reduced memory use. It also improves computation speeds and allows for the calculation of larger models.
5. Improved single-thread performance.
6. Support for parallel computing. Since v0.2.0, each coarse cell can be processed in parallel using MATLAB's Parallel Computing Toolbox. Such computations are effectively independent, so parallelisation results in speedups approximately proportional to the number of parallel computing units (threads or processes).
7. Reduced numerical errors of permeability upscaling by choice of units (solved for millidarcies instead of metres squared).
8. Introduced compatibility of the toolkit's data structures with MATLAB Reservoir Simulation Toolbox (MRST): grid structures, unit conversion multipliers, etc.

New capabilities

1. Support for anisotropic permeability at fine scale.
2. Support for the additional hydrostatic pressure term at the percolation step.
3. Progress visualisation via waitbar with computation time estimates.
4. Provided out-of-the-box statistical plot to visualise fine-scale and upscaled flow functions.
5. Export of upscaled models to the PFLOTRAN-OGS input deck format.
6. Partial processing of a model. Might be used for performance tests or separate processing of regions with different fine-scale flow functions.
7. Performance logging
8. Miscellaneous: utility functions to analyse and debug complex MATLAB scripts (were used to prepare release v0.2.0)

Examples

The code in Figure 1 is similar to the code from the demo script.

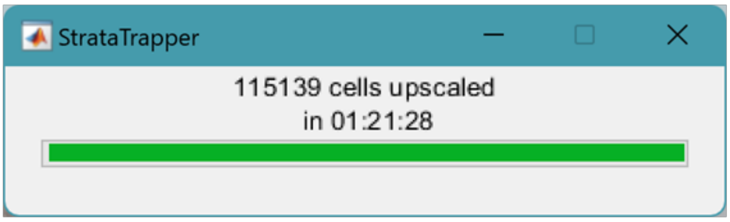
https://github.com/ImperialCollegeLondon/StrataTrapper/blob/main/demo.m

It shows the top-level abstractions of the toolkit and how to use them.

```
params = Params(krw,krg,cap_pressure,rho_gas,rho_water);

options = Options();
options.hydrostatic_correction = false;

strata_trapped = strata_trapper(grid, sub_rock, params, ...
    mask=mask, ...
    options=Options(), ...
    enable_waitbar = true,...
    parfor_arg = 36 );
```



115139 cells upscaled
in 01:21:28

```
plot_result(strata_trapped);
```

Figure 1. The main top-level functions and data structures of the StrataTrapper toolkit. Some of the latest features are highlighted in bright orange. An example of a live progress bar at the end of a computation is also provided.

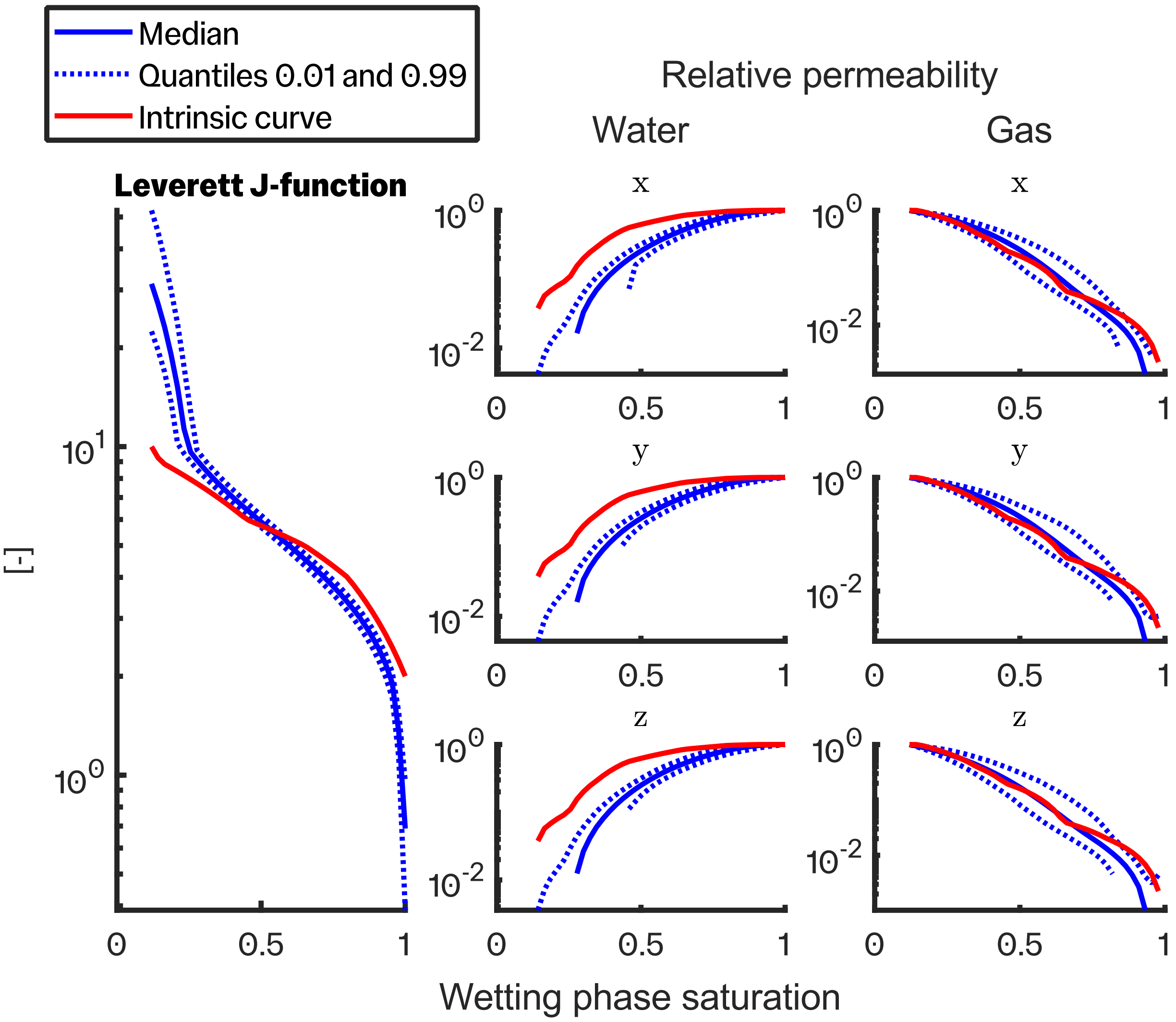


Figure 2. An example of the summary plot produced by the “plot_result” function. “Intrinsic curves” are the original fine-scale viscous-limit inputs used in the standard upscaled models that do not incorporate capillary heterogeneity effects.

Performance

Since v0.10.0, the StrataTrapper toolkit logs performance. It records the processing times of each coarse cell along with the parameters of the entire computation. The following equation is an experimentally derived hardware-specific constant that can be used to predict computation times on a given hardware for large $N_{\mathrm{sub,n}}$.

$$\langle P_{\mathrm{single}} \rangle \approx \frac{(2N_{\mathrm{sat}} + 1)}{T_{\mathrm{run}}} \sum_{n=1}^{N_{\mathrm{coarse}}} N_{\mathrm{sub,n}}^{k\approx 1}$$

$$P_{\mathrm{total}} = \langle P_{\mathrm{single}} \rangle \cdot N_{\mathrm{parallel}}$$

- N_{sat} — number of water saturation points
- N_{coarse} — number of coarse cells in the run
- $N_{\mathrm{sub,n}}$ — number of sub-cells in a coarse cell n

- T_{run} — upscaling run time
- $N_{parallel}$ — number of parallel units

Table 1 summarises changes in performance, accompanied by more detailed statistics in Figure 3.

Table 1. Performance comparison of StrataTrapper v0.1.0 and v0.10.0

Version	N_{coarse}	N_{sub}	N_{sat}	$N_{parallel}$	T_{run}	P_{single}	P_{total}
v0.1.0	2100	8	42	n/a	53 sec	27 kHz	n/a
v0.10.0	115139	248	40	36	44 min	40 kHz	881 kHz

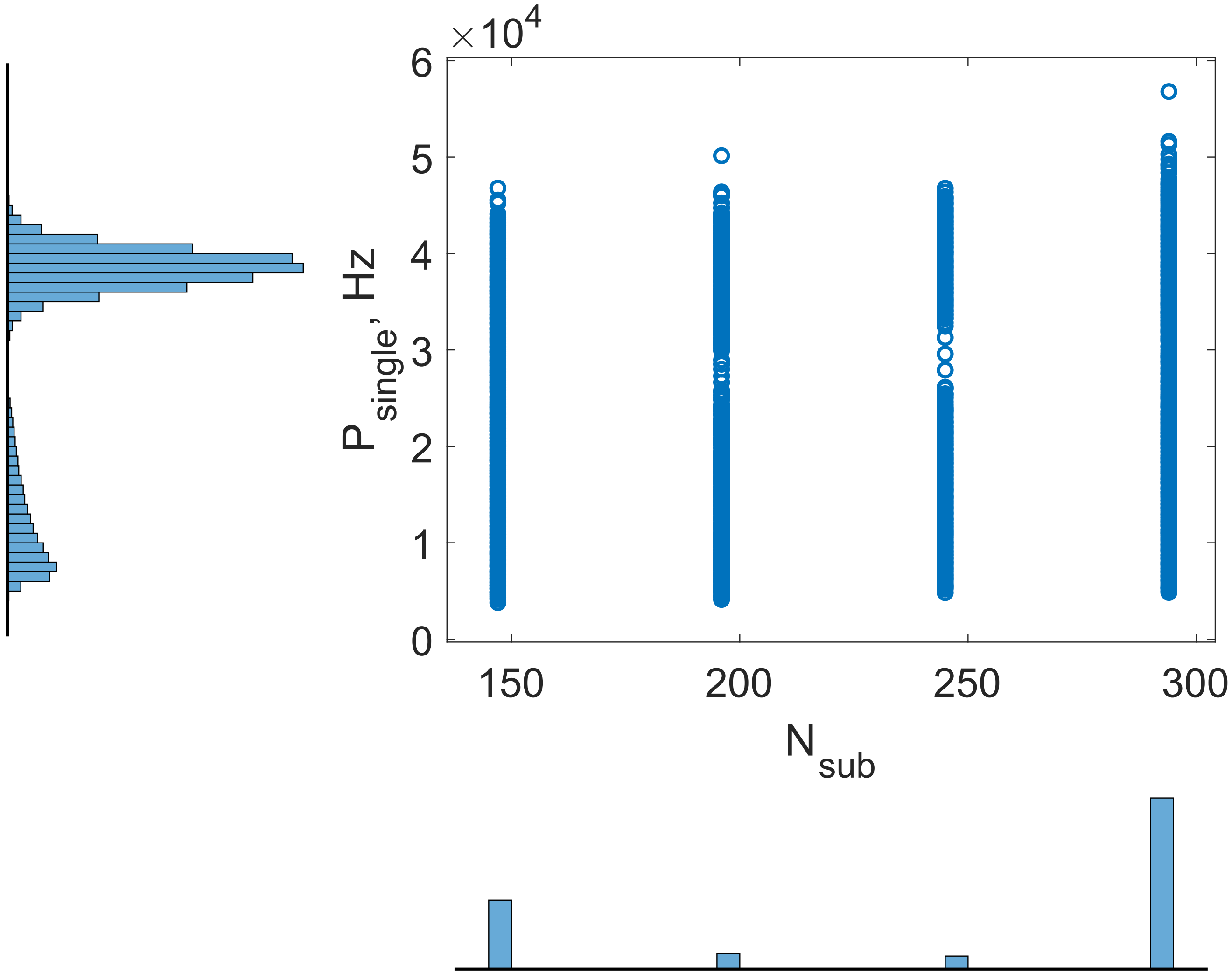


Figure 3. Detailed performance statistics in Table 1 for v0.10.0. Each dataset entry corresponds to an individual coarse cell. The second distribution mode with lower performance is likely associated with using “efficiency cores” controlled by the operating system.

References

[1] N. Wenck, A. Muggeridge, S. Jackson, S. An, and S. Krevor, ‘The Impact of capillary heterogeneity on CO2 plume migration at the Endurance CO2 storage Site in the UK’, *Geoenergy*, Feb. 2025, doi: 10.1144/GEOENERGY2024-029.

[2] M. Elizarev, N. Wenck, S. Krevor, and A. Muggeridge, ‘Upscaling Algorithm to Preserve Effects of Small-Scale Capillary Heterogeneity: Field-Scale Studies on CO2 Storage Sites’, *SSRN Electronic Journal*, Dec. 2024, doi: 10.2139/SSRN.5068897.

Work Package 2: Reduced Physics Modelling

University of Cambridge: Adam Butler and Jerome Neufeld

*CO2GraVISim (****CO2 Gra****vity-dominated* ***V****ertically* ***I****ntegrated* ***Sim****ulator) is a reduced-physics model for geological carbon storage, developed as part of the StrataTrapper project. By vertically integrating the governing Darcy Flow equations, the resulting system can be solved numerically much more quickly than traditional simulation approaches while retaining the key physical mechanisms that control the behaviour of the CO2, allowing us to consider a much wider range of potential storage scenarios and reservoir properties.*

Model Description

The mathematical model implemented here, developed as part of WP2 of the StrataTrapper project, describes the field-scale behaviour of supercritical CO2 injected into a sub-surface, fluid-saturated reservoir. The model relies on two key assumptions about the behaviour of the CO2:

9. The flow of the CO2 is predominantly horizontal (i.e. the characteristic vertical:horizontal aspect ratio for the flow is small),
10. The time taken for the CO2 to reach the caprock is short compared to the total migration time.
11. With these assumptions, we can picture the flow within the reservoir as shown in Figure 4.

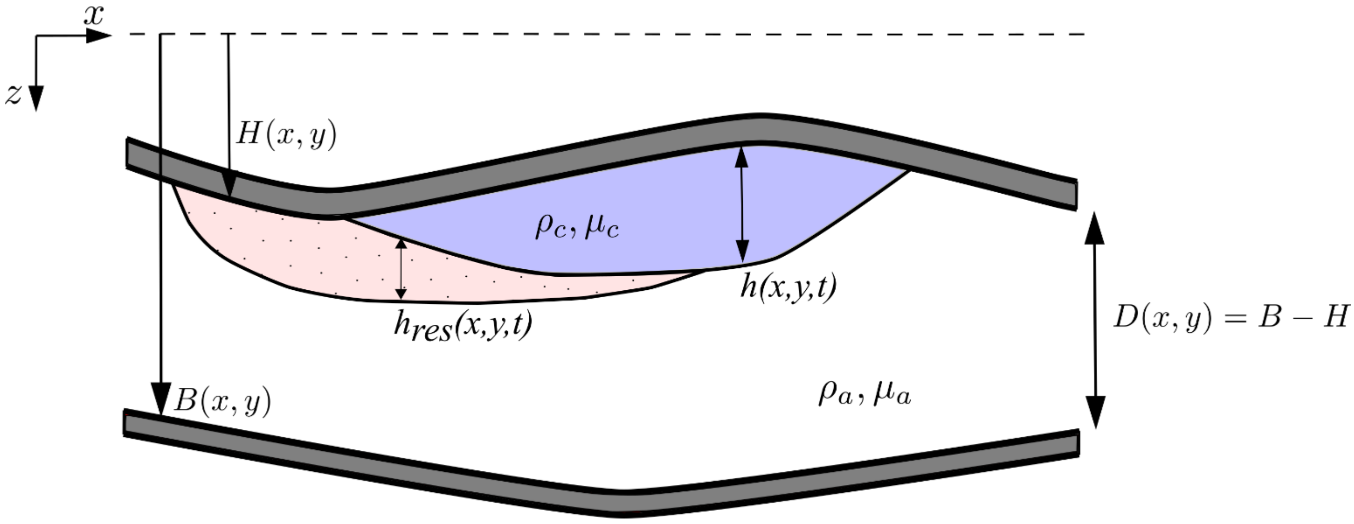


Figure 4: Schematic of the reservoir and flow setup used in the mathematical model. The reservoir is divided into regions of mobile CO2 (purple), residually trapped CO2 (spotted, light red), and pure ambient fluid (the remainder of the reservoir).

Model parameters

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

The topography of the upper impermeable seal, or caprock, is described by $z = H(x, y)$, while the lower impermeable seal, or basement, is given by $z = B(x, y)$. The local vertical extent of the storage interval is then $D(x, y) = B(x, y) - H(x, y)$. The mobile region has thickness $h(x, y, t)$ and the trapping region $h_{res}(x, y, t)$; these are calculated over time from the governing equations described below.

The injected CO2 has density ρ_c and dynamic viscosity μ_c, while for the ambient water these are ρ_a and μ_a. These parameters are constants that remain fixed throughout the simulation.

Each flow region has corresponding saturations s_c and s_a for the CO2 and ambient water, and relative permeability parameters k_{rn} and k_{rw} for the non-wetting phase (CO2) and the wetting phase (ambient water). These are displayed in Table 1. These parameters vary spatially and temporarily as the flow regions develop over time, but are fixed constants for each flow region.

Region	**Mobile CO2**	**Trapped CO2**	**Ambient Water**
Extent	$H \rightarrow H + h$	$H + h \rightarrow H + h + h_{res}$	$H + h + h_{res} \rightarrow B$
Saturation (s_c, s_a)	$(1 - s_{ai},\ s_{ai})$	$(s_{cr}, 1 - s_{cr})$	$(0, 1)$
Rel. Perm. (k_{rn}, k_{rw})	$(k_{rn}, 0)$	$(0, k_{rw})$	$(0, 1)$

Table 1: The saturation and relative permeability parameters for each of the three flow regions in the reduced-physics model.

The remaining reservoir properties are the porosity $\phi(x, y, z)$ and the absolute horizontal permeability $k(x, y, z)$, which are fixed in time but can vary in all three spatial directions.

Finally, the model includes the following dissolution parameters: the molecular diffusivity of CO2 into the ambient brine, D_{mol}; the volume fraction of CO2 that can dissolve into the ambient brine, C_{sat}; and an anisotropy ratio between the vertical and horizontal absolute permeability. These are fixed values, both spatially and temporally.

Governing equations

The flow of the two fluids in the reservoir – the injected CO2 and the ambient water – is governed by Darcy's equation:

$$\boldsymbol{u}_i = -\frac{k}{\mu_i}(\nabla p - \rho_i g \hat{\boldsymbol{z}}) \,.$$

Here $\boldsymbol{u}_i$ is the Darcy flux, k the absolute permeability, μ the dynamic viscosity, p the pore pressure, and ρ the fluid density, and z points in the direction of gravity, increasing with depth. The index i then refers to either the CO2 ($i = c$) or the ambient water ($i = a$).

With the assumptions described above, the vertical variation in the pore pressure is hydrostatic at leading order, and we can express it as

$$p_i = \begin{cases} P_a(x,y) + \Delta\rho g(H+h) + \rho_c g z, & (i = c) \\ P_a(x,y) + \rho_a g z, & (i = a) \end{cases}$$

where $\Delta\rho = \rho_a - \rho_c$ is the density difference between the two fluids and P_a is the dynamic pore pressure in the ambient phase.

With the flow as pictured in Figure 1, we can integrate Darcy's equation across

12. The CO2 region, both mobile and trapped ($H \le z \le H + h + h_{res}$)
13. The entire storage interval ($H \le z \le B$).
14. This results in two equations: one governing conservation of volume for the CO2 phase,

$$\phi C_s \frac{\partial h}{\partial t} + \tilde{\nabla} \cdot \left\{ -\frac{k_0}{\mu_c} h \kappa_c \tilde{\nabla}[P_a + \Delta\rho g H] \right\} = \tilde{\nabla} \cdot \left\{ \frac{k_0 \Delta\rho g}{\mu_c} h \kappa_c \tilde{\nabla} h \right\} + Q(x,y,t) - q_d(x,y,t) \,,$$

15. and a second governing conservation of total fluid volume,

$$\tilde{\nabla} \cdot \left\{ \frac{k_0}{\mu_c} [h\kappa_c + M(D-h)\kappa_a] \tilde{\nabla} P_a \right\} = -\tilde{\nabla} \cdot \left\{ \frac{k_0 \Delta\rho g}{\mu_c} h \kappa_c \tilde{\nabla}(H+h) \right\} - Q(x,y,t) \,.$$

Here $\tilde{\nabla} = (\partial_x, \partial_y)$ is the horizontal gradient operator; k_0 is a representative permeability value; $Q(x,y,t)$ is the local volume flux from injection; $M = \mu_c/\mu_a$ is the viscosity ratio between the two fluids; C_s and q_d incorporate the effects of saturation and dissolution; and κ_c and κ_a are the vertical permeability averages over the mobile CO2 and ambient water regions, respectively:

$$\kappa_c = \frac{1}{h} \int_H^{H+h} k_{rn} \frac{k}{k_0} \, dz \;, \qquad \kappa_a = \frac{1}{(D-h)} \int_{H+h}^{B} k_{rw} \frac{k}{k_0} \, dz$$

These are the vertical average permeabilities seen by the CO2 and the ambient water at each location, and evolve over time as the fluid regions develop.

As a result of this vertical integration, the governing equations above are now two-dimensional, only involving spatial derivatives in terms of the horizontal directions (x and y), and no longer in the vertical direction (z). The order of the governing equations has thus been reduced, but the key physical mechanisms governing the behaviour of the CO2 have been retained, e.g. saturation; heterogeneity in topography, porosity, and permeability; and dissolution.

This offers two main advantages over traditional simulation approaches that involve solving the fully-3D governing equations. Firstly, these reduced-order equations can be solved numerically much more rapidly, allowing a greater number of simulations to be performed in a given amount of time. Secondly, the calculation of the extent of the CO2 plume (given by h and h_{res}) is now limited only by numerically precision, rather than being limited by the vertical grid spacing of the original reservoir data.

Software

CO2GraVISim, which implements the mathematical model described above, is open source and publicly available on GitHub: https://github.com/ajobutler/CO2GraVISim. This software can be compiled and used on Windows, Linux, and Unix systems, with further details available in the documentation provided in the GitHub repository. This software comprises:

- Fortran files that make up the main solver
- Python scripts that
    - generate simple reservoir topographies
    - preview the reservoir structure before a simulation
    - visualise the results of a simulation
    - analyse the ensemble behaviour of a batch run
- Batch scripts for performing a batch of runs, and for doing so in parallel.

The numerical implementation of the mathematical model described in the previous section uses a Finite Differences approach and is built for a regular Cartesian grid with $n_x \times n_y$ points and regular grid spacings dx and dy.

Input data is provided in two forms. Spatial arrays (such as topography, porosity, and permeability) are provided in the form of text files following the grid structure described above. The remaining input parameters, such as density values or injection parameters, are specified together as part of a single input XML file. To read this input file, CO2GraVISim utilises FoX, a Fortran XML Library: https://fortranwiki.org/fortran/show/FoX.

Co2GraVISim can be run in two modes: Unconfined and Confined. In Unconfined mode the injection of the CO2 is assumed to have a negligible effect on the ambient water, so we take $P_a = 0$ and solve for h and h_{res}. In Confined mode, h, h_{res}, and P_a are calculated together using the governing equations described above. The unconfined approximation simplifies the governing equations further, allowing them to be solved more quickly. This approximation is generally applicable when the CO2 plume occupies a small fraction of the vertical extent of the reservoir – for more details, see *Pegler et al., J. Fluid Mech., 2014* (https://doi.org/10.1017/jfm.2014.76).

Work Package 3: Case Study Applications

In this work package, the numerical upscaling toolkit from WP1 and the simplified physics models from WP2 were applied to case studies comprising models of North Sea sites of interest, the Endurance, East Mey, and Sleipner CO2 storage locations.

Open-source data repository of upscaled reservoir simulations

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

Models demonstrating the use of the StrataTrapper upscaling approach have been made publicly available from the StrataTrapper GitHub site:

https://imperialcollegelondon.github.io/StrataTrapper/

From the main site, there is a link to a site focused on the publication of the models at

https://imperialcollegelondon.github.io/StrataTrapper-models/

The repository itself can be directly accessed at

https://github.com/ImperialCollegeLondon/StrataTrapper-models

The following information on this report recreates information published on the repository websites. Key Knowledge Deliverable report 3.2 provides further descriptive detail of the models and their use in various scenarios.

Endurance models

Endurance CCS site sector models in PFLOTRAN-OGS's input deck format are in the endurance/ directory:

one-well-base.in

one-well-upsc.in

four-wells-base.in

four-wells-upsc.in

one-/four- stands for the number of injection wells in the model. -base stands for reference viscous-limit upscaling with zero capillary pressure. -upsc stands for capillary-limit upscaling conducted by StrataTrapper toolkit.

In detail, specifications can be found in [1].

East Mey models

The East Mey models in this repository are based on a model developed by the ACT (Accelerating CCS Technologies) Acorn consortium. This simulation was constructed using that model as the starting point.

East Mey CCS site models in PFLOTRAN-OGS's input deck format are in the east-mey/ directory:

- 1-base.in
- 1-base-pc.in
- 1-upsc.in
- 2-base.in
- 2-base-pc.in
- 2-upsc.in

1-/2- stands for two particular well placements and respective injection scenarios.

-base stands for base coarse dynamic models (directly based on the base model from the ACT Acorn consortium).

-base-pc stands for the -base model with added capillary pressure model.

-upsc stands for capillary-limit upscaling conducted by StrataTrapper toolkit

Running PFLOTRAN-OGS reservoir simulations

To run the supplied models, PFLOTRAN-OGS-1.8 installed on Ubuntu 22.04 is required. A dedicated Docker image can be used instead, which is covered in the next section.

For a model folder <model_folder> containing .in files:

Unarchive large files with characteristic curves chc[xyz].data from chc[xyz].zip located at <model_folder>/include/.
Go to a model directory. Using the command line from repository root:
cd <model_folder>

Start a simulation using the run.sh shell script:
bash ./run.sh <model_name> [number_of_processes]
where <model_name> is an input file name with .in omitted
[number_of_processes] is optional. It is responsible for MPI-based parallelization and equals 4 by default.
Visualize simulation results using ResInsight or equivalents.

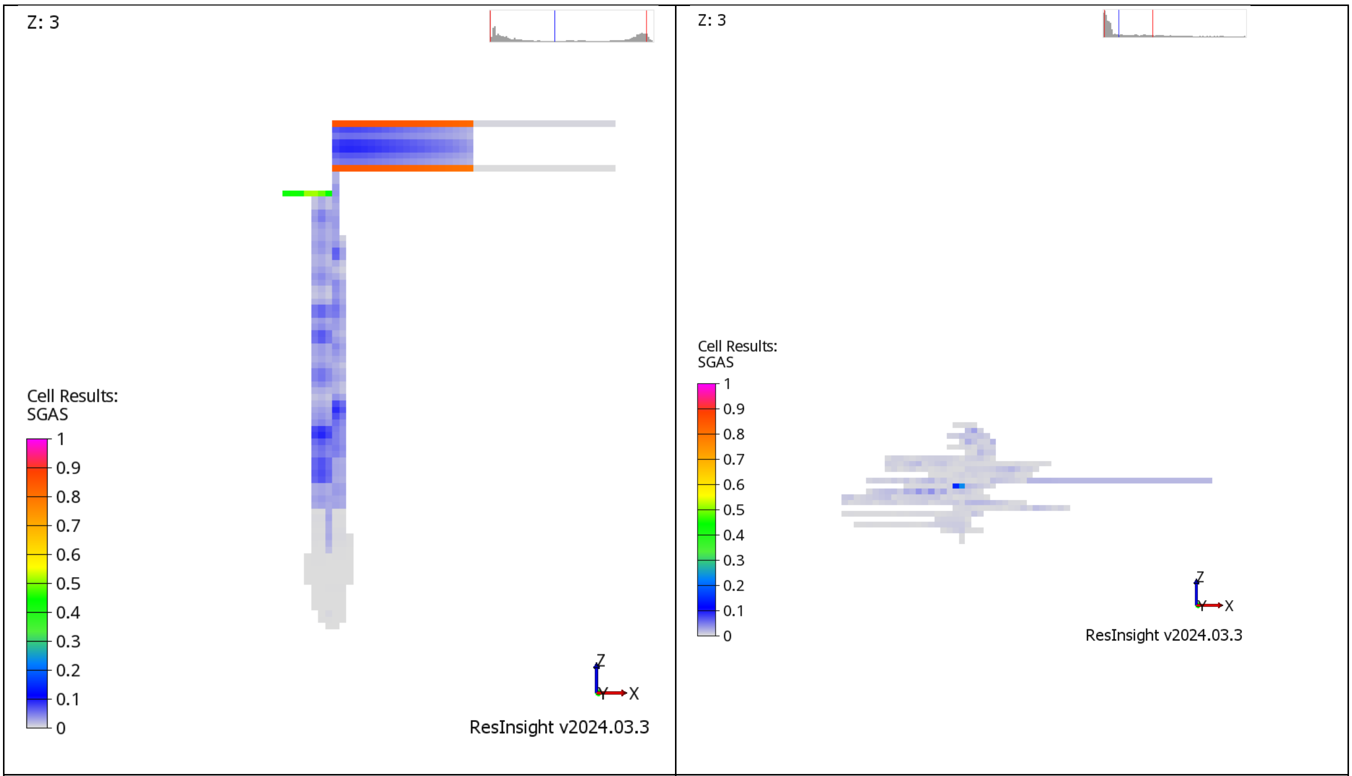


Figure 5. a. CO2 released at the bottom of a reservoir moves directly upwards if the (conventional) viscous limit upscaling is used to represent flow properties.

b. The upward migration of CO2 is baffled and the plume spreads beneath heterogeneities when the StrataTrapper upscaling approach is used to generate flow properties.

Numerical experiments with StrataTrapper: summary

16. We used the StrataTraper 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.

17. 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.

18. StrataTrapper upscaling yields different simulation results for the wide range of relevant inputs, particularly injection rate, capillary pressure curve shape, and layered heterogeneity strength.

19. 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.

20. 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.

In more detail, the results of case studies are available at [1], [2], and the latest Key Knowledge Deliverables. For example, Figure 6 shows the summary of the sensitivity analysis conducted within the framework of a factorial experiment.

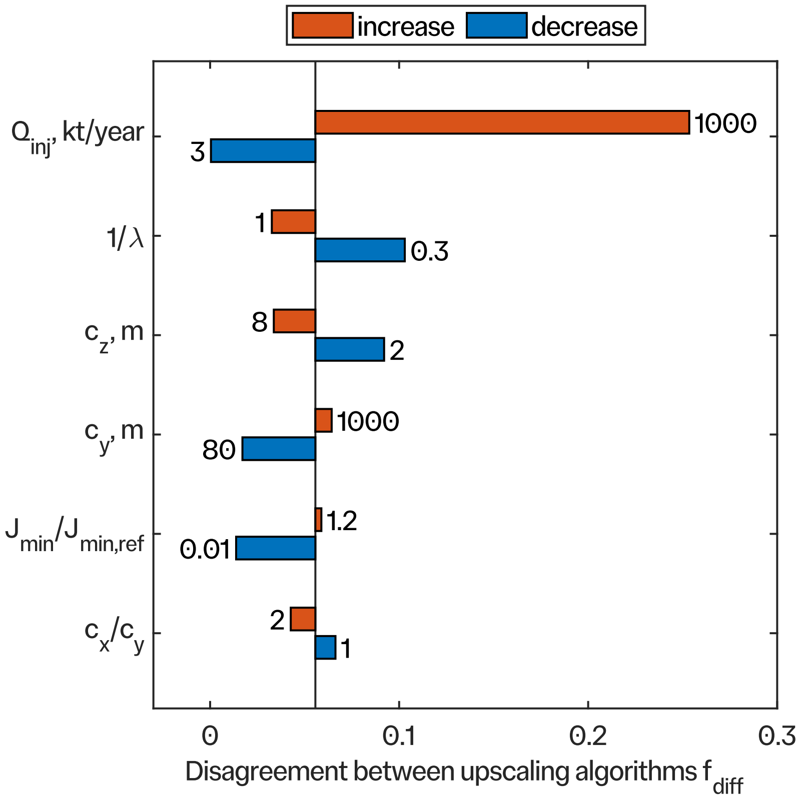


Figure 6. Sensitivity analysis of the difference in boundary CO2 saturation at the Endurance site predicted with different upscaling algorithms. Estimates are made by the trained polynomial proxy model. The vertical baseline corresponds to the base estimates of rock-fluid properties [1]. In each row, only the respective parameter is changed to one of the edge cases. For more details, see the latest Key Knowledge Deliverable.

Simplified Physics Simulations using CO2GraVISim

University of Cambridge: Adam Butler and Jerome Neufeld

A more detailed discussion of the application of CO2GraVISim to real-world reservoir data can be found in the Knowledge Deliverable documentation for WP3. Here we provide a summary of some of those applications.

As a demonstration of CO2GraVISim, we consider Layer 1 from a modified version of the Sleipner 2019 Benchmark Model, publicly available on the CO2DataShare website: https://co2datashare.org/dataset/sleipner-2019-benchmark-model.

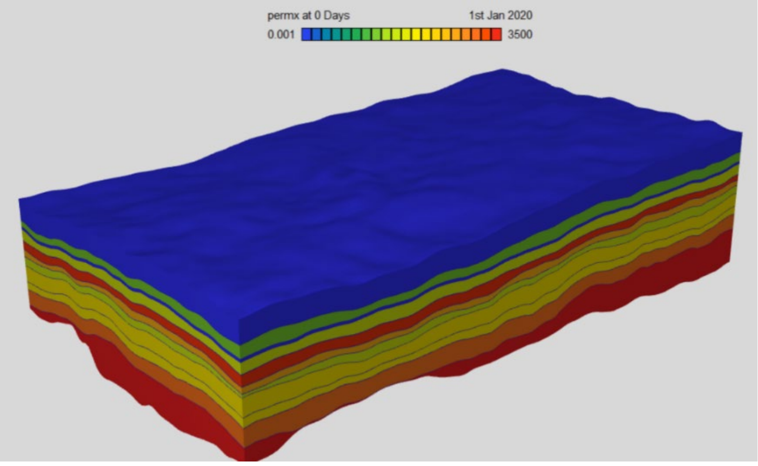


Figure 7: The permeability structure of the Sleipner geomodel, with Layer 1 shown in red at the bottom.

This section of the geomodel corresponds to a storage interval with $64 \times 128 \times 58$ grid points in x, y, and z; grid spacings $dx = dy = 50m$; a horizontal absolute permeability of $3483.09\ mD$; and a porosity of 0.36. The mean distance between the caprock and basement for this storage interval is $85m$, so the following simulations were run in Unconfined mode.

A base-case simulation of injection at $0.2\ Mt/yr$ for 3 years and a total simulation period of 270 years took $\approx 90\ s$ on a standard laptop[1]. This brief total runtime lends itself well to being part of an ensemble of variations of this simulation, to study the sensitivity of the CO2 plume to the input parameters. These can be classified into two categories: those that can be controlled by the site operator (e.g. injection strategy), and those that cannot (e.g. uncertainty in topography).

Sensitivity to Injection Strategy

For the controlled kind, we considered 30 variants of the base case – the same total mass of $0.6\ Mt$ was injected in each, with injection rates varying from $0.02\ Mt/yr$ to $2\ Mt/yr$ ($0.1 \times$ to $10 \times$ the base case value) and the injection period adjusted appropriately.

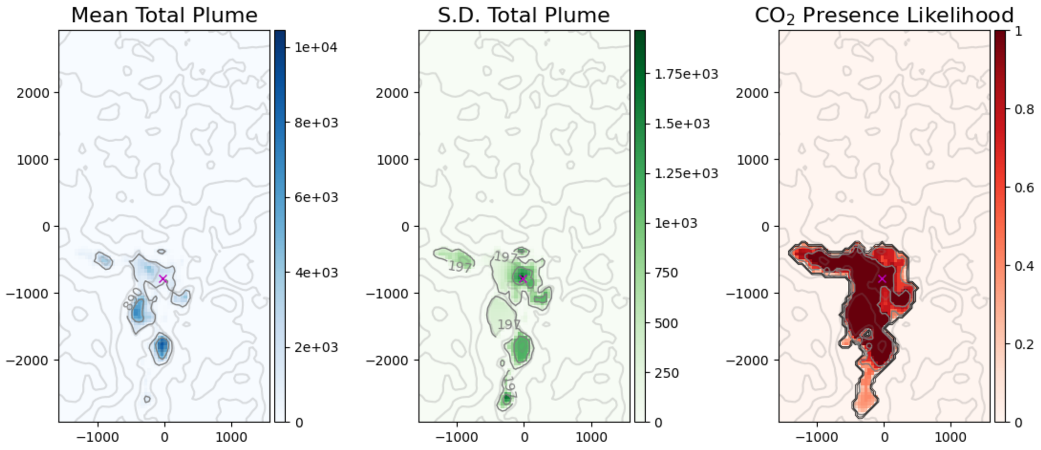


Figure 8: The ensemble plume behaviour for varying injection rate with fixed total volume. The first and second panels show the mean and standard deviation, respectively, of the volume of free-phase CO2 (i.e. mobile and

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

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 8 shows the ensemble behaviour of the CO2 plume at the end of the simulation period for this batch of runs. The likelihood plot on the right of Figure 9 shows that there is an appreciable degree of variability in the final plume profile, with the plume approaching the southern boundary of the domain in some runs, which may be of concern for site operators and regulators. The runs where this occurred were those with lower injection rates over longer injection periods.

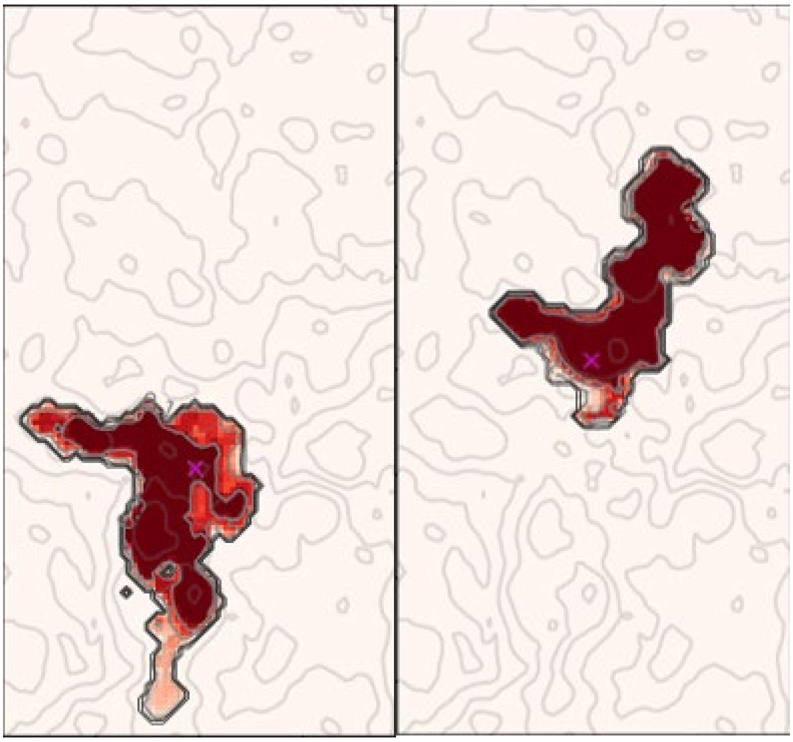


Figure 9: A comparison of the likelihood maps for the same injection-variation ensemble runs carried out at two neighbouring injection locations

This process can be repeated for other injection locations. Figure 4 shows a comparison of the likelihood plots for two injection locations: the one discussed above, and a neighbouring location that lies only 850 m away. Despite this, they have significantly different storage basins and degree of variability, due to the local caprock topography.

Sensitivity to Uncertainty to Topography

The same simulation process can be performed to investigate the influence of measurement uncertainty, such as for the caprock topography for this storage interval.

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 on the standard laptop. In series this would take $1hr\ 15mins$, but run in 4 parallel batches we are able to reduce this to $18\ mins$, ¼ of the series time.

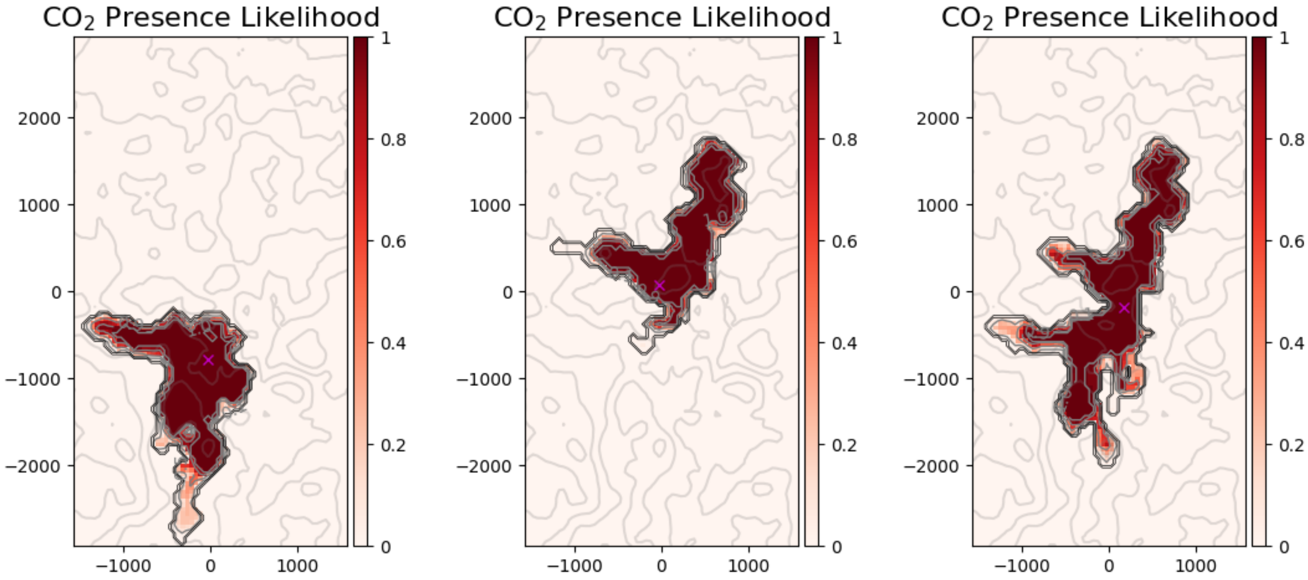


Figure 10: The likelihood maps for the topographic variation simulations at three different injection location.

Figure 10 shows the resulting likelihood maps for applying this ensemble study – using the same topography variants in each case – at three injection locations. The first two are those discussed in figure 9, and we see similar results when compared to the injection variation study. The third injection location lies between these two, on the watershed dividing their respective drainage basins.

These results highlight the importance of caprock topography in the ultimate behaviour of the CO2 plume, and how the sensitivity of the plume to variations in inputs (either injection strategy or caprock topography) can differ significantly for different injection locations.

Work Package 4: Commercialisation of StrataTrapper tools within OpenGoSim

OpenGoSim: Paolo Orsini and David Ponting

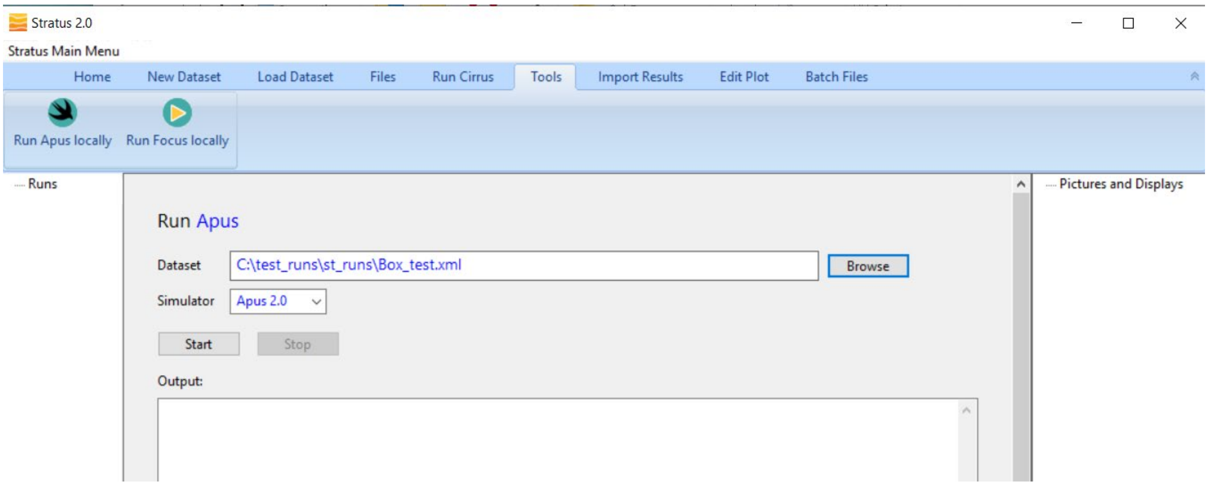
Within StrataTrapper, OpenGoSim (OGS) had the main goal to commercialise two technologies developed by Imperial College and Cambridge University in the field of geological CO2 storage, in addition to advance one of their core reservoir simulation technologies. The company worked on three main areas:

A commercial implementation of the upscaling technique developed by the Sam Krevor group at Imperial College (the numerical upscaling toolkit described above). This provides a means to include small-scale capillary pressure heterogeneities into full field reservoir models, to predict more accurately the migration of CO2 post-injection.

Development of an interface around CO2GraviSim, the reduced-physics simulator developed by Cambridge university, for the fast prediction of CO2 migration. The OGS interface gives CO2GraviSim the possibility to access real geological model in industry standard format.

Development of a new reservoir simulator tailored to Carbon Capture Sequestration applications, with support for modern computer architectures, including Graphic Processing Units (GPU) acceleration. (An OGS in-house technology).

The project produced two new products, Focus, from the upscaling technique, and Apus, from CO2GraviSim. Both tools have been integrated into Stratus, the OGS software platform for reservoir modelling of CO2 storage in the subsurface:



Dataset C:\test_runs\st_runs\Box_test.xml

Simulator Apus 2.0

Both software are installed together with Stratus on Windows 10 and 11 PCs.

Apus and Focus have been released in beta version to the project partners and few other selected users for early testing. A full commercialisation will start later in 2025, showcasing the products at trade shows, such as the EAGE-2025 annual meeting where OGS has a booth and submitted a technical paper on the work done during this project.

In addition, the core of the new-technology high-performance reservoir simulation (Nimbus), was also developed, with promising results when compared to the simulator OGS is currently providing to their clients (PFLOTRAN-OGS). Beta testing is expected to take place later in 2025, with commercialisation planned for 2026.

Below a short description that highlight some of the key feature of each product.

Focus

From Stratus, the user loads and view the go-model to upscale, in a format compatible with industry standard (grdecl). After setting up the input parameters needed to define the upscaling (coarsening level, etc.), Focus can be run directly from Stratus to produce the data needed for the upscaled reservoir model: the coarse static model and the pseudo relative permeability functions. These can be readily visualised in Stratus:

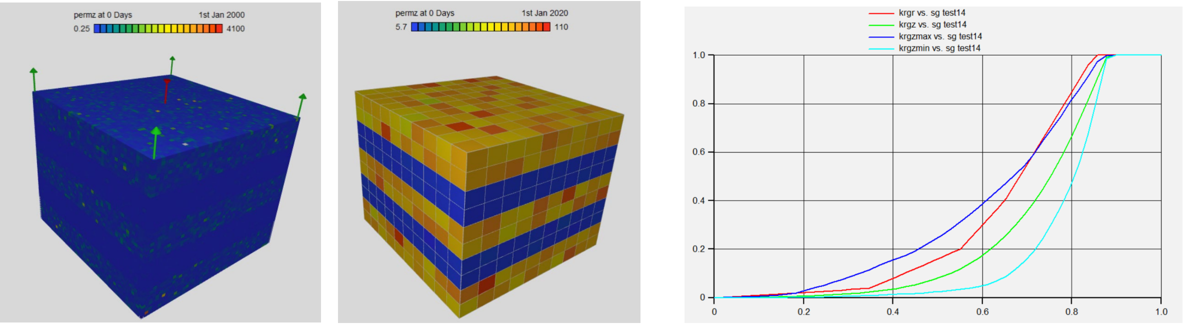


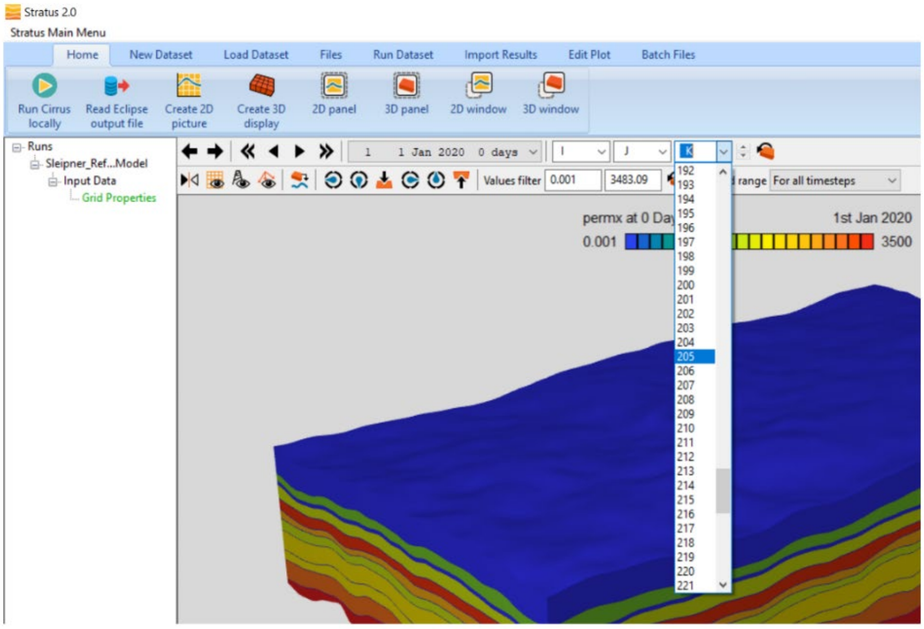
Fig. 11. From left to right: geo-model to upscale: upscaled static model; initial rel. perm curves, min, max and average pseudo rel. perm curves.

The upscaling algorithm produces a larger number of pseudo relative permeability functions (up to 12 for each grid block), and Focus helps the user to visualise them displaying minimum, maximum and average curves. It also has option to compress these functions, discarding those that are very similar to each other, to lighten the input of the reservoir simulators, not normally designed to handle such a large number of relative permeability functions.

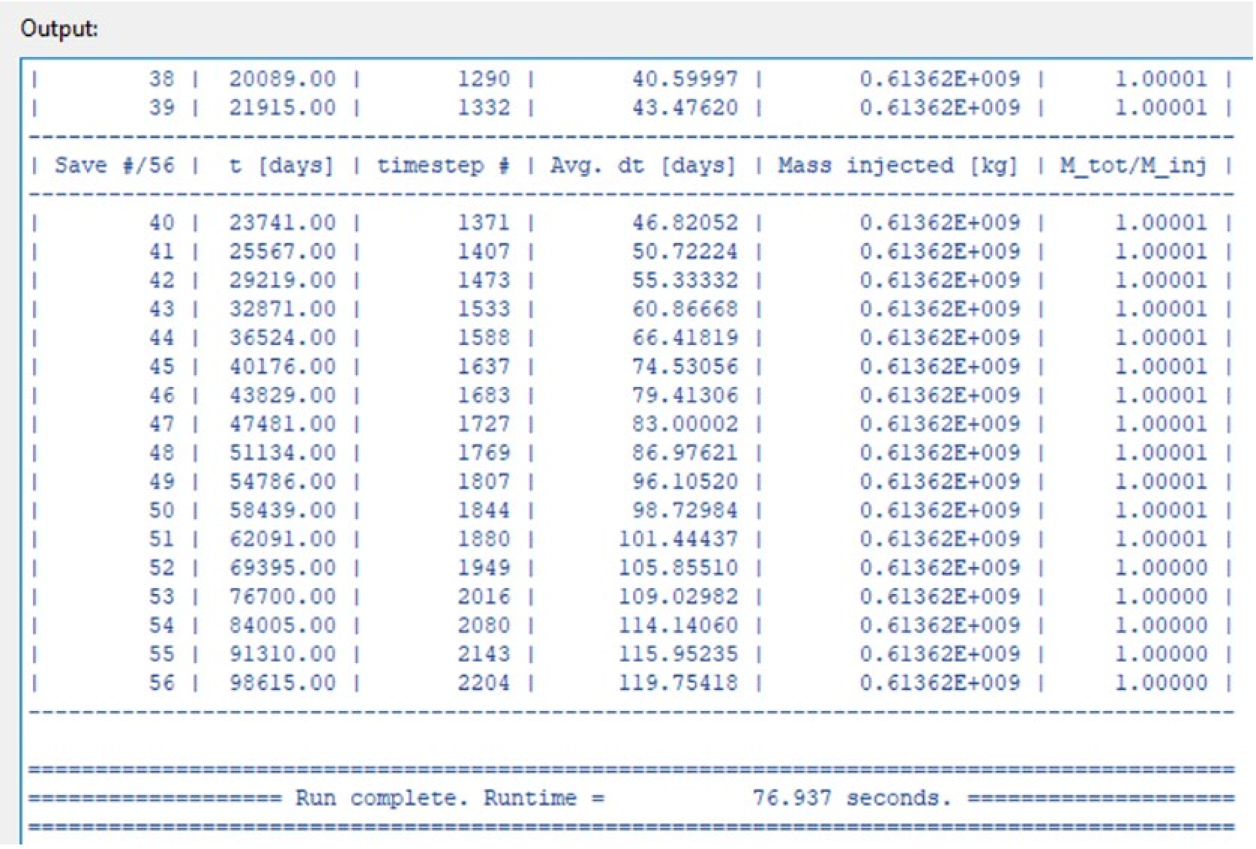
With the data provided by Focus, the user can set up and run a dynamic simulation of the upscaled model, directly within Stratus using the OGS reservoir simulator. Alternatively, the user can export Focus output for other simulators, in industry standard format.

Apus

From Stratus, the user loads and view the go-model of the storage site to be analysed with 2D flow simulations, for fast assessment of the CO2 migration. In the first inspection of the geo-model, the user selects the vertical interval where CO2 will be injected and layer that will act as caprock:



The user will then edit Apus input (fluid properties, well locations and injections rates, simulation reporting times, etc.) and start the simulation within Stratus:



Output:

```
|        38 |  20089.00 |        1290 |     40.59997 |      0.61362E+009 |     1.00001 |
|        39 |  21915.00 |        1332 |     43.47620 |      0.61362E+009 |     1.00001 |
-----------------------------------------------------------------------------------------
| Save #/56 |  t [days] | timestep # | Avg. dt [days] | Mass injected [kg] | M_tot/M_inj |
-----------------------------------------------------------------------------------------
|        40 |  23741.00 |        1371 |     46.82052 |      0.61362E+009 |     1.00001 |
|        41 |  25567.00 |        1407 |     50.72224 |      0.61362E+009 |     1.00001 |
|        42 |  29219.00 |        1473 |     55.33332 |      0.61362E+009 |     1.00001 |
|        43 |  32871.00 |        1533 |     60.86668 |      0.61362E+009 |     1.00001 |
|        44 |  36524.00 |        1588 |     66.41819 |      0.61362E+009 |     1.00001 |
|        45 |  40176.00 |        1637 |     74.53056 |      0.61362E+009 |     1.00001 |
|        46 |  43829.00 |        1683 |     79.41306 |      0.61362E+009 |     1.00001 |
|        47 |  47481.00 |        1727 |     83.00002 |      0.61362E+009 |     1.00001 |
|        48 |  51134.00 |        1769 |     86.97621 |      0.61362E+009 |     1.00001 |
|        49 |  54786.00 |        1807 |     96.10520 |      0.61362E+009 |     1.00001 |
|        50 |  58439.00 |        1844 |     98.72984 |      0.61362E+009 |     1.00001 |
|        51 |  62091.00 |        1880 |    101.44437 |      0.61362E+009 |     1.00001 |
|        52 |  69395.00 |        1949 |    105.85510 |      0.61362E+009 |     1.00000 |
|        53 |  76700.00 |        2016 |    109.02982 |      0.61362E+009 |     1.00000 |
|        54 |  84005.00 |        2080 |    114.14060 |      0.61362E+009 |     1.00000 |
|        55 |  91310.00 |        2143 |    115.95235 |      0.61362E+009 |     1.00000 |
|        56 |  98615.00 |        2204 |    119.75418 |      0.61362E+009 |     1.00000 |
-----------------------------------------------------------------------------------------


=========================================================================================
================== Run complete. Runtime =          76.937 seconds. ====================
=========================================================================================
```

Apus maps the 2D flow solution into the original 3D geo-model, so that the reservoir engineers can easily visualise results (e.g. gas saturation distribution) on the real geometry. A number of key outputs important for CO2 storage, such as total amount of CO2 residually trapped and dissolved in brine are also made available for visualisation in the 2D plotter of Stratus:

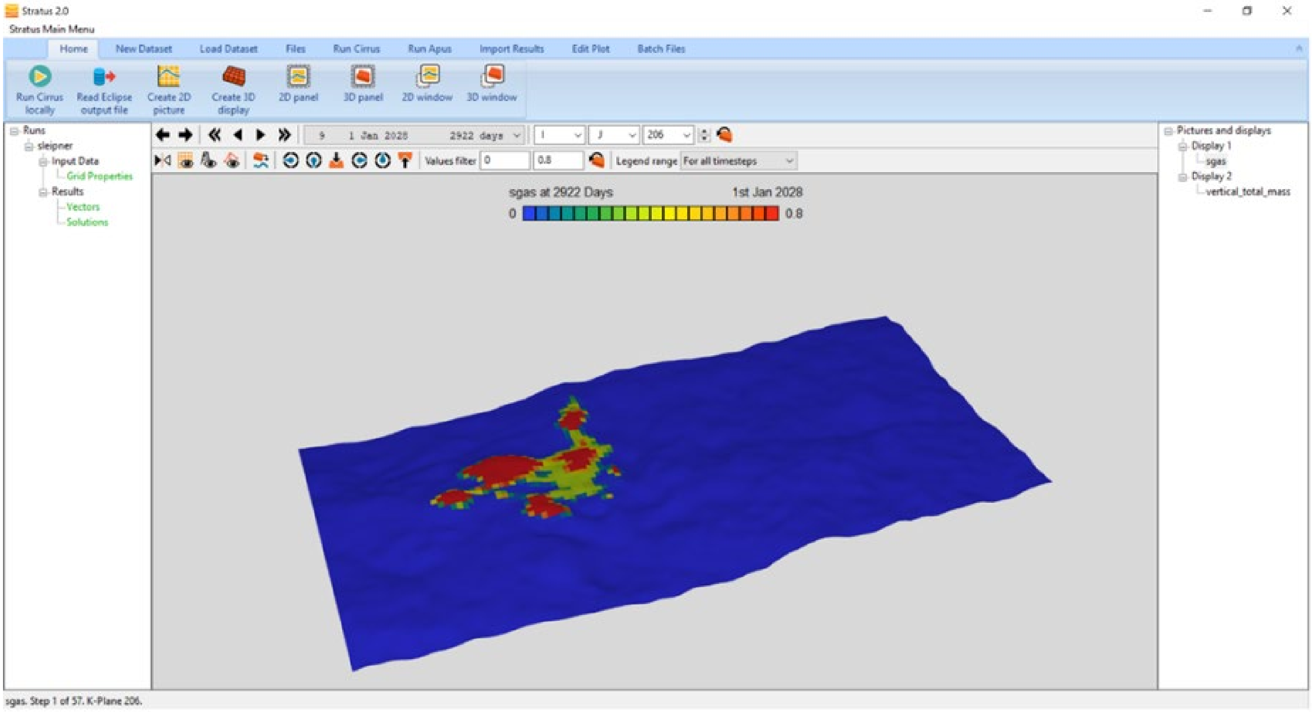


Fig 12. Gas Saturation plot, mapped into the original 3D model.

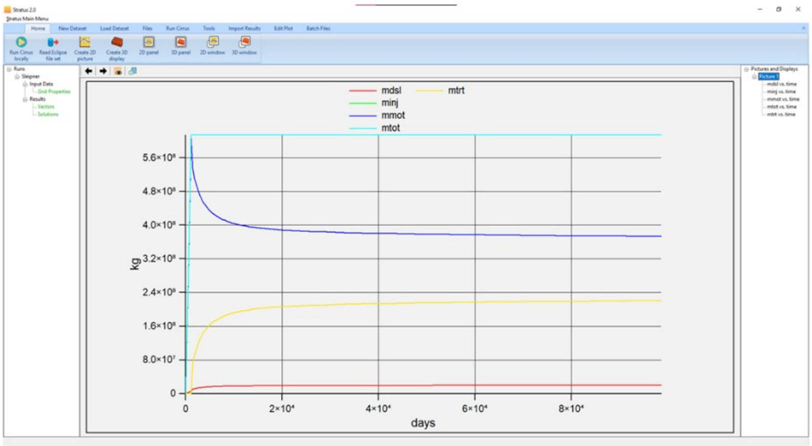


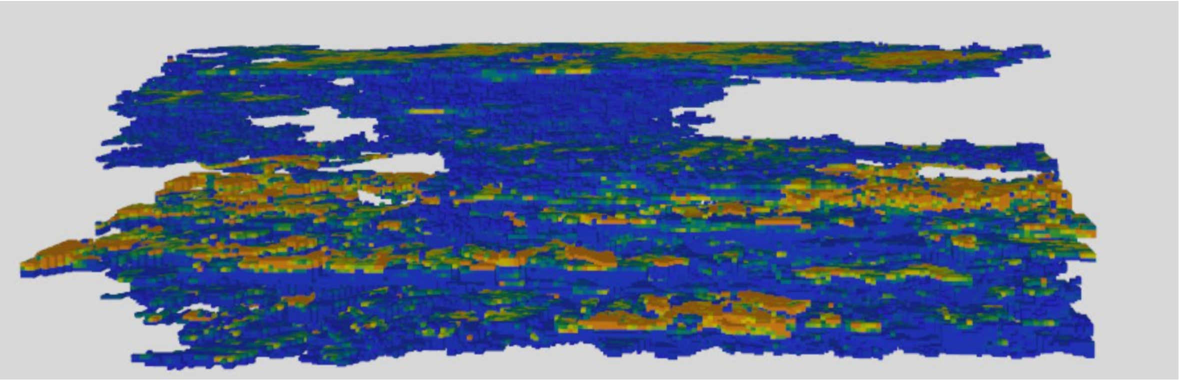
Fig. 13. Example of 2D plot, with time evolution of total mass of CO2 residually trapped, dissolved, mobile, etc.

Nimbus

Nimbus is a new-technology high-performance reservoir simulation code capable of thermal simulation of gas-water to model CO2 storage into saline aquifers. It supports multi-level parallel processing on both CPU and GPU hardware. The GPU support is in CUDA. Testing on the SPE10 industry benchmark has shown that on the Nvidia A30 GPU Nimbus outperforms PFLOTRAN-OGS simulations on top-end CPUs. The A30 is a mid-range GPU, therefore more gain are expected from more powerful models (e.g. A100 or H100).

After the initial effort in the development of an efficient linear solver for Nimbus, the focus has now shifted in adding capabilities to model CO2 storage into saline aquifers. One of the first realistic CCS model used for testing was built readapting the SPE10 industry benchmark mentioned earlier, setting up a challenging CO2 migration scenario. Starting from the original set up, the top layer was moved to a depth of 2000 m, and the reservoir was considered to be initially filled with brine (instead of oil) at 100 C. A pressure of 200 Bar was fixed at the top, and the 4 producers of the original case were kept to stabilise the pressure, while injecting gas at 20000 sm3/d for 1000 days. After injection, the simulation was let run to model the gas rising through the formation. CO2 dissolution in brine was turned off. The case was named CCS10, to reflect the geology of the SPE10 case, and its readaptation to CCS (Carbon Capture Storage).

Below the 3D gas saturation contour at the end of the simulation, after removing all grid blocks that do not contain any CO2:



The CO2 rises to the top through tortuous paths, and part of it gets trapped on the way up. The model, which has about 1 Million active cells, is very challenging, due to the fine scale heterogeneity in permeability, and the continuous move of the extended CO2/brine front during the migration, which limit the time step the simulator can take.

Benefits and Dissemination activities

The StrataTrapper public workshop took place on March 21, 2025 at Imperial College London. There were 100 participants in total with 80 online and 20 in person. This included participation from stakeholders from many sectors including CO2 storage project operators and service companies, startups and consulting companies, academic and research organisations, and government.

Figure 14: The StrataTrapper public workshop at Imperial College London

Dissemination has also taken place through journal publication and conference presentation and exhibition: WCCUS 2025, EAGE 2025, Interpore2025, APS 2024, GHGT-17, CCUS Houston 2024

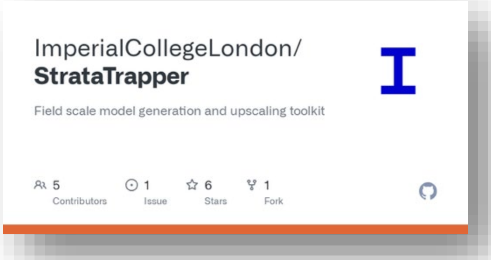
See references:

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

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, 3(1), geoenergy2024-029

Figure 15: Apus being demonstrated at the OpenGoSim booth in the exhibition of the 2025 EAGE Annual 86th Conference & Exhibition in Toulouse.

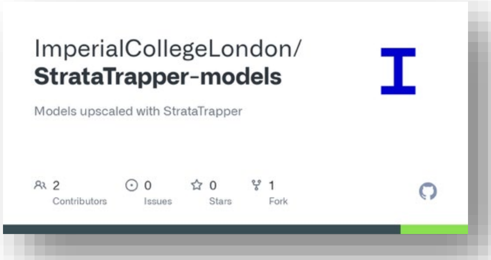
Finally, the upscaling, simplified physics toolkits, and reservoir simulations are publicly available on the StrataTrapper GitHub pages.



ImperialCollegeLondon/
StrataTrapper

Field scale model generation and upscaling toolkit

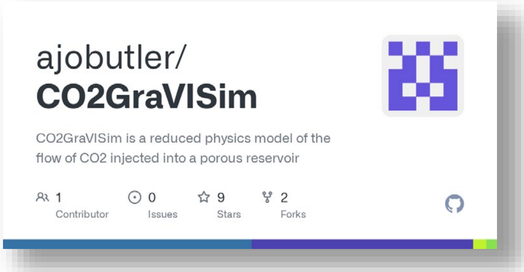
5 Contributors
1 Issue
6 Stars
1 Fork



ImperialCollegeLondon/
StrataTrapper-models

Models upscaled with StrataTrapper

2 Contributors
0 Issues
0 Stars
1 Fork



ajobutler/
CO2GraVISim

CO2GraVISim is a reduced physics model of the flow of CO2 injected into a porous reservoir

1 Contributor
0 Issues
9 Stars
2 Forks

Lessons learnt and barriers

The main technical barrier and lesson learned concerned the identification of the commercial workflow for the upscaling step. The challenge was that reservoir engineers usually already receive a coarse grid model, and the fine scale model is unavailable.

The solution we developed was to create a component of the toolset to generate a downscaled model from the coarse grid model, i.e., two variations for the workflow are now available, one for the scenario where a high resolution (fine-scale) model is provided, and one in which only the coarse-grid model is available.

Project Impact and follow on/route to commercialisation

As anticipated, several elements of the work have achieved commercialisation (TRL 8) through the project. This includes the implementation of Apus, Focus, and Nimbus, which provides commercial support for the use of the tools developed by StrataTrapper through OpenGoSim.

Several elements of the work are also publicly available as proofs of concept (TRL 5) including upscaling, simplified physics toolkits, and reservoir simulations, through the StrataTrapper GitHub page.

Exhibition and demonstration continues at major conferences, e.g., the EAGE 2025 Annual meeting. The StrataTrapper project leads are organizing a short course in association with major conferences

There is already ongoing leverage and follow-on activity, including funded research on expansion of the technique to sites offshore Norway, and the UK; through funding from two industry sponsors, these support two postdoctoral researchers and a PhD student for the coming 4 years. Another project supported by an industry partner is implementing StrataTrapper tools to analyse underground hydrogen storage, with research carried out by an MSc student.