Simulating CO_2 Injection and Storage in the Cloud

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OpenGoSim

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CO_2 Storage

The process of CO_2 storage in aquifers is broadly understood.

CO_2 can be stored in disused gas reservoirs or in saline aquifers. DECC estimates the total oil and gas reservoir capacity in the UK North Sea to be 7.3 Gt (Giga-tonnes), whilst the aquifer capacity is in the range 4 to 46 Gt. CO_2 can also be used in enhanced oil recovery processes, which may finally result in some CO_2 storage.

Example of CO_2 storage in saline aquifers:

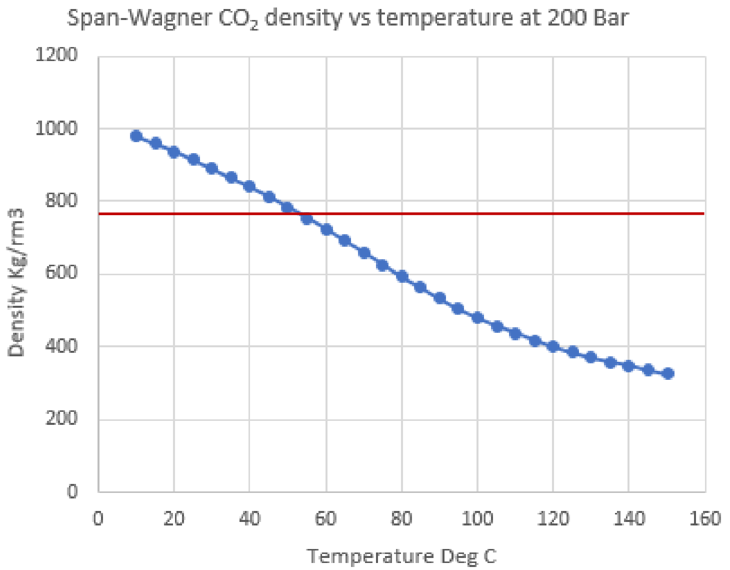
- Sleipner is the first commercial project (Norway).
- The UK is assessing several potential sites for storage.

CO_2-EOR has been used for years in the US, mainly in the Permian Basin.

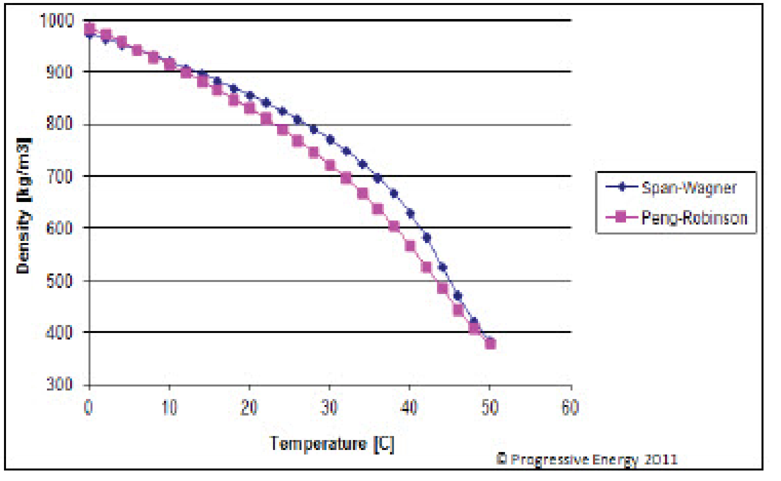
1. *CO_2 Storage in the UK - Industry Potentia.* Senior, Bill. Senior CCS Solutions Ltd. https://ukccsrc.ac.uk/system/files/publications/ccs-reports/DECC_Gas_156.pdf
2. Progressing Development of the UK's Strategic Carbon Dioxide Storage Resource. Constain, ETI, Pale Blue Dot, Axis Well Technology. April 2016.

Characterising - CO_2 – EOR

CO_2 is quite dense at reservoir conditions (e.g. 2000 m depth): not denser than water, but can be denser than oil. The density is a sensitive function of temperature. At a pressure of 200 Bar, using Span & Wagner (values from http://www.energy.psu.edu/tools/CO2-EOS).



ρ_o =748.5 at 200 bar, ρ_o^{surf}=750 Kg/sm^3, C_o=10^{-5} 1/bar



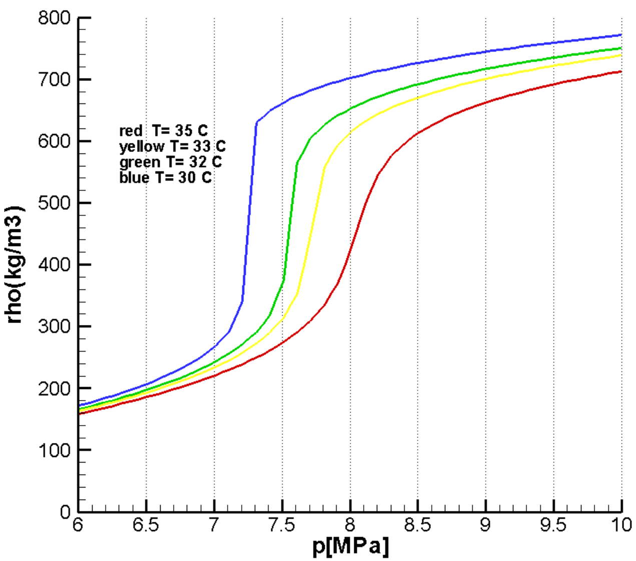
Span-Wagner vs PR at 100 bar

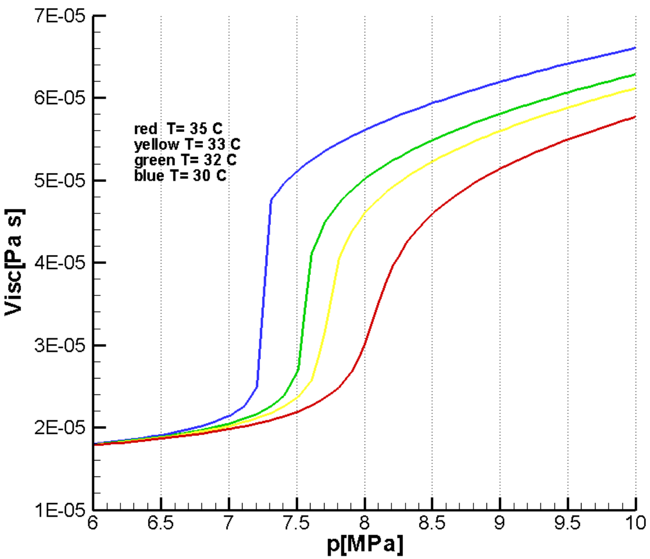
1. 'Composition Swing Injection for CO_2 Storage and EOR' B. Nazarian, SPE; A. Cavanagh, SPE; P.S. Ringrose, SPE; and B. Paasch, Statoil, 2014

2. 'Span and Wagner (1996), A new equation of state for carbon dioxide covering the fluid region from the triple-point temperature to 1100K at pressures up to 800 Mpa', *J. Phys. Chem. Ref. Data*., **25**, 1509-1596.

Characterising - CO_2 Storage

Reservoirs for storage must ensure conditions for CO_2 to be dense ($P > P_{cr}$ = 73.4 Bar) to guarantee capacity, but not too deep to avoid high drilling costs. Typical storage site at a depth between 800-1000 m.

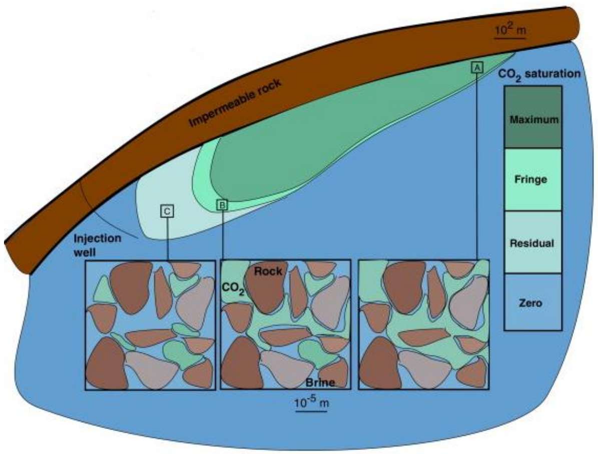




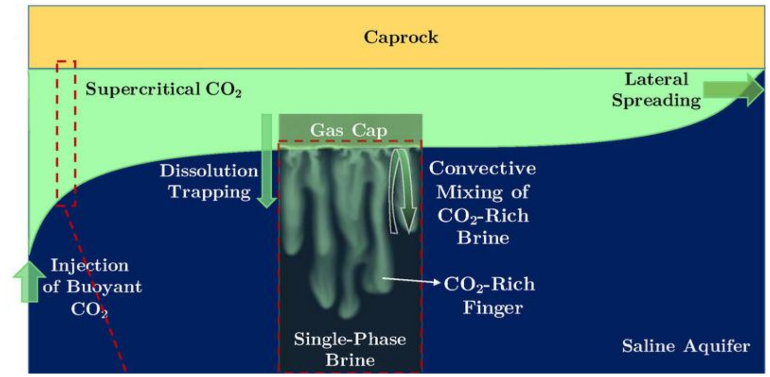
For typical reservoir storage pressures (75-85 Bar), CO_2 density and viscosity are very sensitive to temperature variations, as close to the critical point (T_{cr} =31 C).

CO_2 Properties: 'Span and Wagner (1996), A new equation of state for carbon dioxide covering the fluid region from the triple-point temperature to 1100K at pressures up to 800 Mpa', *J. Phys. Chem. Ref. Data*., 25, 1509-1596.

The CO_2 Storage In Saline Aquifers



1. Inject CO_2, which rises to form a plume at the top of the aquifer[1]. Structural & Residual trapping.

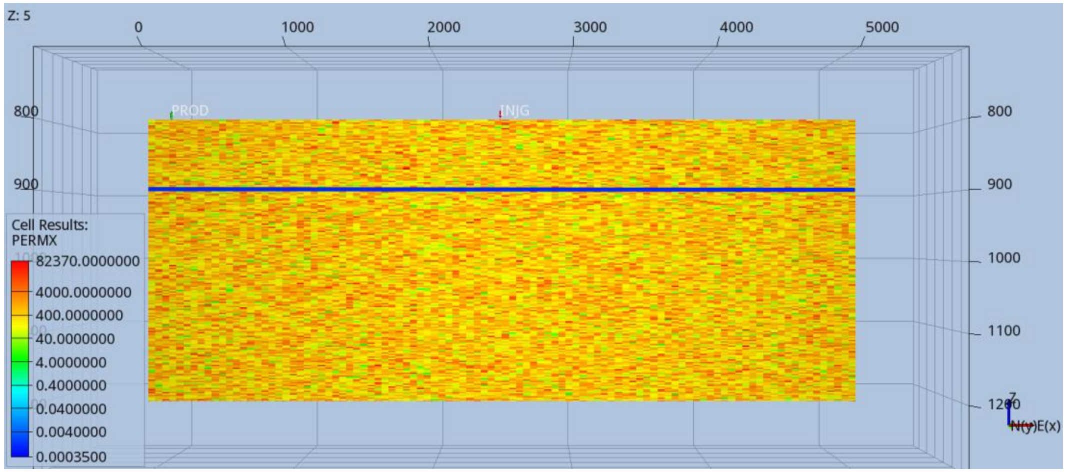


2. CO_2 dissolves, heavier saturated brine falls back down into aquifer[2]. Solution trapping, hundreds to thousands of years.

3. Reaction with metallic ions leads to mineralisation trapping. Tens to hundreds of thousands of years.

1. Capillary trapping for geologic carbon dioxide storage – From pore scale physics to field scale implications. Krevor, Samuel, et al. 2015, International Journal of Greenhouse Gas Control, Vol. 40, p. 221-237.
2. Solutal convection in porous media: Comparison between boundary conditions of constant concentration and constant flux. Amooie, Mohammad Amin, Soltanian, Mohamad Reza e Moortgat, Joachim. 3, 2018, PHYSICAL REVIEW E, Vol. 98, p. 033118.

Model To Discuss Storage Process



Generic sector study: 100x10x200 regular grid. Perm~500 mD, except layer 50 perm~0.05 mD, heterogeneity added. 50 m spacing in x, 500 m in y, 2 m in z.
Injection for 2500 d (6.85 years), run to 5000 years.
Bhp-controlled producer in deepest layer to simulate water zone below model.

Condition typical of reservoir storage sites (e.g. Sleipner):

- Top of reservoir at 800 m depth, pressure ranges from 80 to 120 Bar.
- Residual gas saturation, two values tested: 0 and 0.3.
- Temperature:
  - Isothermal studies: T = 33°C.
  - Thermal study: T= 29°C at the top, and a gradient of 3°C/100 m.
- Brine at 10% wt salinity (CO_2 solubility decreases with salt concentration)

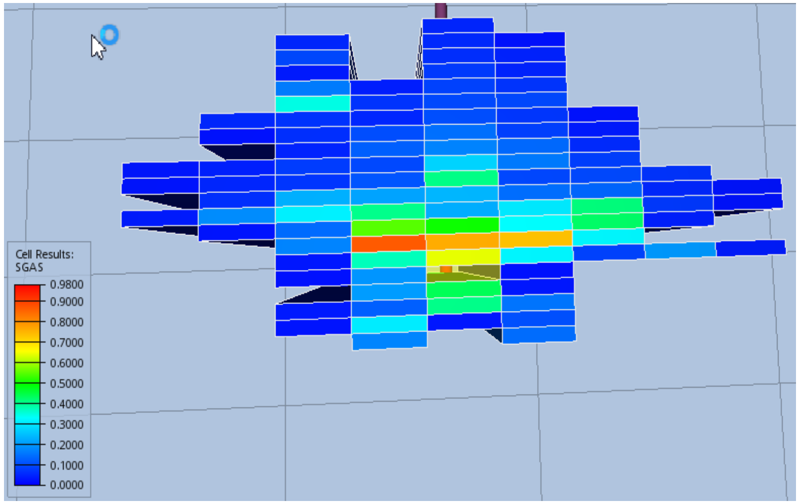
Injection

The first step is rather like engineering a reservoir, in the sense of creating one.

CO_2 is more mobile than brine: this is an adverse mobility ratio injection – the front will be unstable and tend to finger.

Some gain in not injecting at the top of the aquifer: avoids large pressure rises near the caprock, and maximises the swept path over which the CO_2 will travel (increases solution and residual trapping).

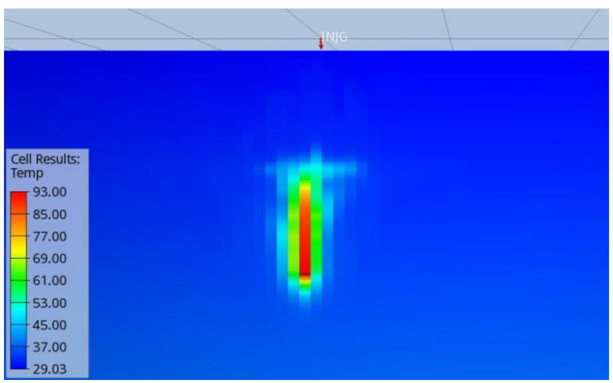
The injection process is viscous dominated – pressure and mobility.



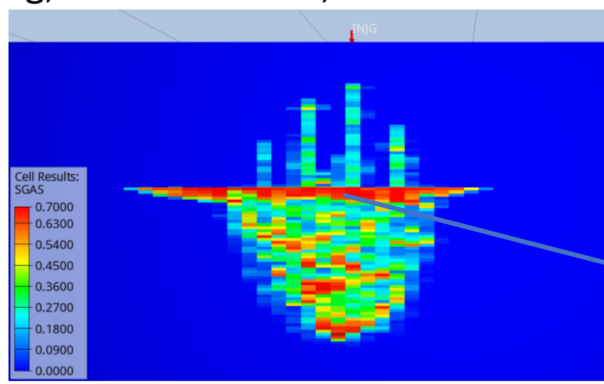
Injection – thermal effect

CO_2 will usually warm-up under injection; the result is some local heating or cooling. Given a certain CO_2 mass rate to inject at surface, the biggest thermal effect is the bottom hole density variation, which changes the reservoir injected volume. Near-well effect.

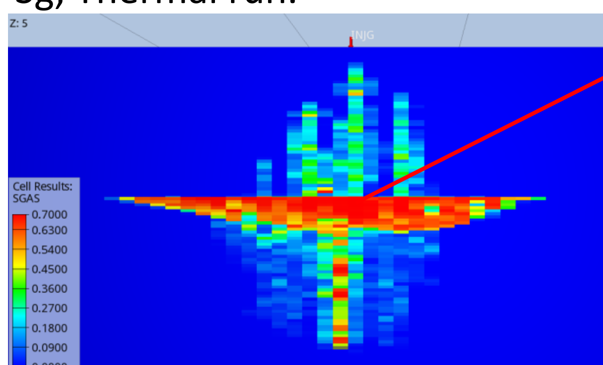
Extreme CO_2 compression from 6 to 100 Bars, T_{inj} = 93 C vs a T_{res} = [29-44] C.



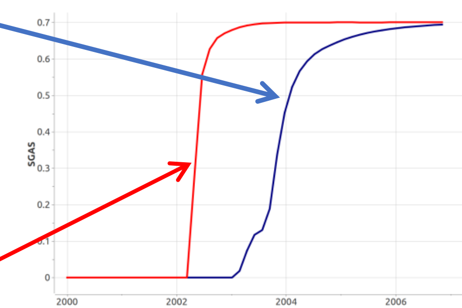
Sg, Isothermal run, T = 33°C.



Sg, Thermal run.



Sg vs time
Arrival time to mid layer difference about 1 year.



All plots at the end of the injection period (6.85 y).

Migration

The migration process is gravity dominated. Gravity and density.

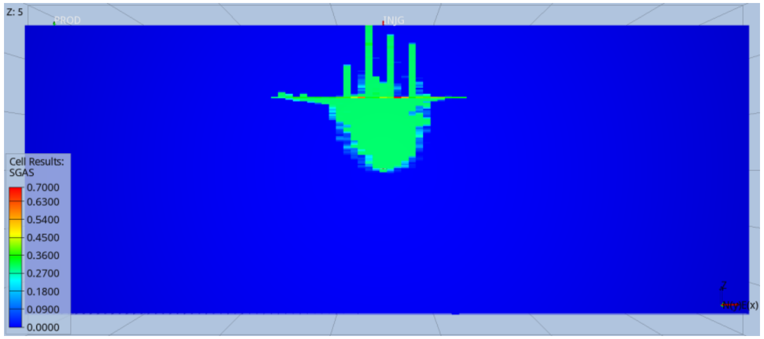
As the CO_2 is lighter than the brine, will move upwards from the injection region.

Switch to an imbibition process, and will generally leave a trapped gas saturation.

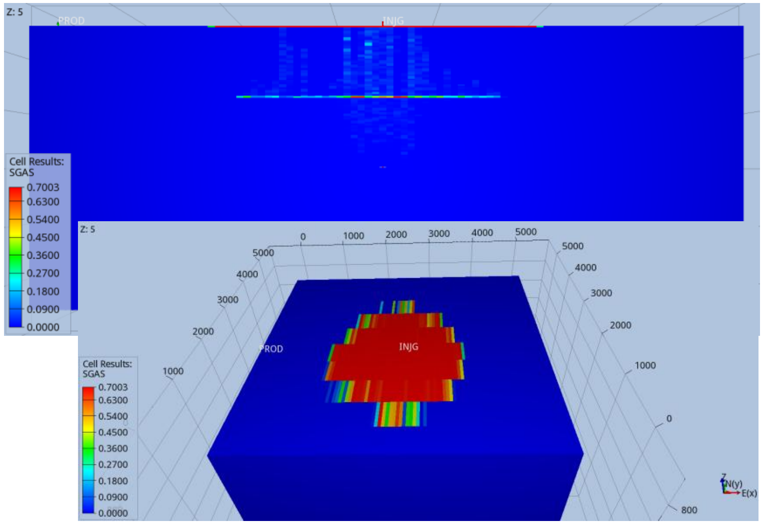
Brine is undersaturated with respect to CO_2, and as the CO_2 moves into new brine it must dissolve to saturate the brine.

So leave two trails: trapped gas saturation and saturated brine.

In permeable rock like a sandstone, CO_2 can flow at a saturation not too far above critical. When it meets a barrier to vertical flow, gas will build up, and will eventually flow round or through.



Sg at 100 years, Sgr = 0.3.



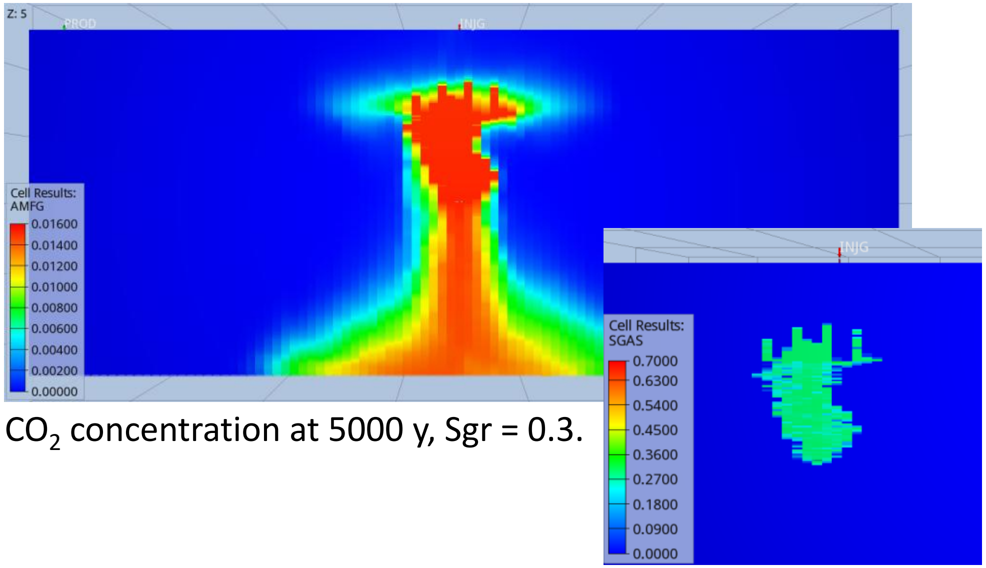
Sg at 100 years, Sgr = 0.

Dispersal

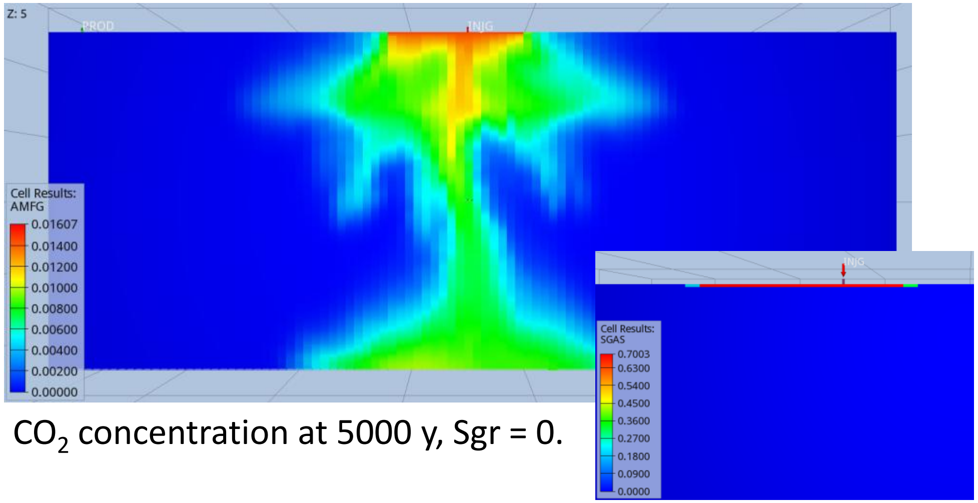
The dissolved CO_2 will sink.

In the section study at 5000 years:

- Dissolved gas that didn't make it to the top falls back, allowing undersaturated brine to move in above it.
- Dissolved gas around the old injection region falls back, forming fingers as it goes.
- Sgr = 0.3 case: all CO_2 is trapped, part of it solved, part is trapped by the rock pores.
- Sgr = 0 case: a thin layer of free gas remains at the top.



CO_2 concentration at 5000 y, Sgr = 0.3.



CO_2 concentration at 5000 y, Sgr = 0.

Dispersal: Molecular Diffusion effects

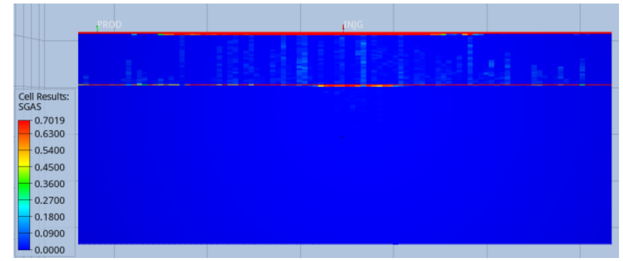
The molecular diffusion plays a role in the long term runs, when the fluid is dominated by density instabilities due to CO_2-rich brine.

The example presented is a cross section study built from the sector model, J=5, all other setting unchanged. Scenario with Sgr = 0.

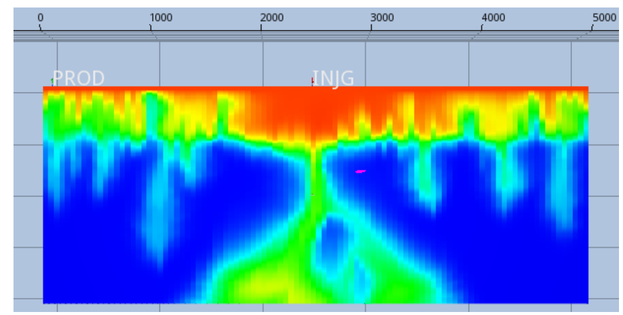
Numerical dispersion not generated when the gas is no moving. The molecular diffusion enhances significanlty solution in brine.

Molecular diffusion $D = 4 \times 10^{-9}\ m^2/s$[1].

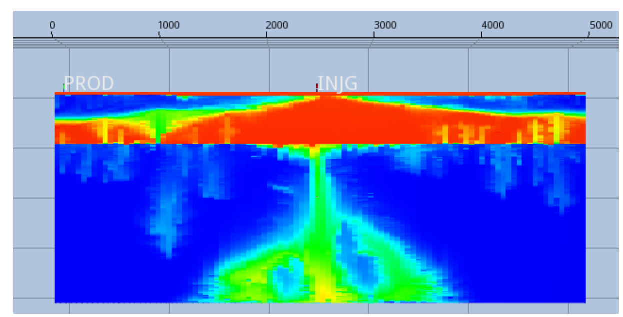
The CO_2 concentration plots at 5000 years, show how molecular diffusion enhanced density-driven fingering and solution trapping.



Sg at 250 years.



CO_2 conc. at 5000 y, $D= 4\times10^{-9}\ m^2/s$.



CO_2 concentration at 5000 years, D= 0.

1. Tamimi, A., Rinker, E. B., and Sandall, O.C. Diffusion Coefficient for Hydrogen Sulfide, Carbon Dioxide, and Nitrous Oxide in Water over the Temperature Range 293-368 K. J. Chem. Eng. Data, 1994, 39(2), 330-332.

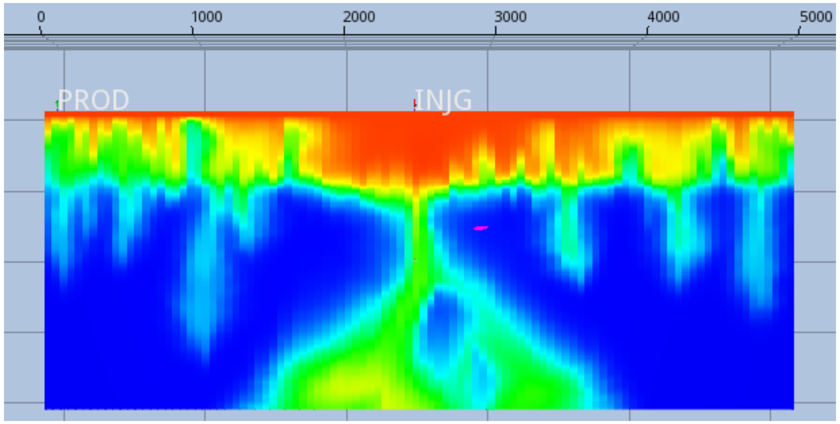
Dispersal: Salinity effects

As the salinity of brine increases, the solubility of CO_2 decreases (salting-out).

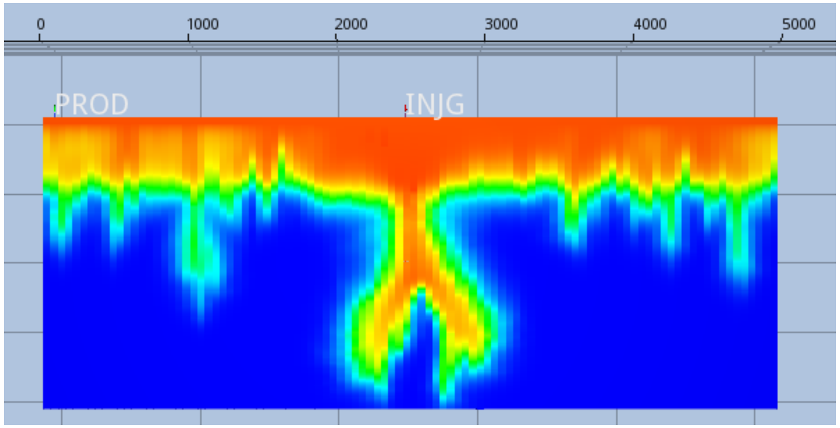
Lower CO_2 concentration in brine results in reduced solution trapping and a smaller density difference between CO_2-saturated brine and fresh brine.

The resulting density-driven fingers have a different shape as less CO_2 is transported downward.

The CO_2 concentration plots at 5000 years, show that in the higher salinity case, fingers don't make it to the bottom.



Psat at 5000 years, D= 4 x 10^{-9} m^2/s, Sgr = 0
Salt wt = 10%



Psat at 5000 years, D= 4 x 10^{-9} m^2/s, Sgr = 0
Salt wt = 20%

Parallel Simulation in the Cloud

The Pflotran **P**arallel **Flo**w **Tran**sport Simulator is an Open Source project started by US labs and held on BitBucket. OpenGoSim have developed, with Equinor's support, an initial oil and gas simulation capability within Pflotran. And a specific CO_2 Storage module.

Built over Petsc, Hypre, PtScotch, HDF5…mixture of C, C++ and Fortran.

The background of Pflotran is environmental science, groundwater flow. Vast range of capabilities and options, not all available in all modes.

The black oil mode can run SPE1, SPE5, SPE10 etc.

Kept on BitBucket, easy to install on Linux, possible to install on Windows.

Parallel Simulation in the Cloud

Fully implicit in time with an Algebraic Multigrid (AMG) linear solver.
The variable-switch technique is used to detect phase states.
Thermal mode is the default. A stack of PVT tables, one for each temperature, can be entered.

The CO_2 storage module has internal implementations of:

- Span & Wagner to compute CO_2 properties
- Duan & Sun for CO_2 solubility and density of CO_2-enriched brine[1,2]

To define CO_2 and brine, the user simply enters:

```
#========================== EOSs ============
BRINE 4.28 MOLAL

EOS WATER
  SURFACE_DENSITY 1077 kg/m^3  !10% Salt
  DENSITY IF97
END

EOS GAS
 SURFACE_DENSITY 1.867 kg/m^3
 CO2_DATABASE ../include_files/co2_db.dat
END
```


1. Zhenhao Duan, Rui Sun. An improved model calculating CO2 solubility in pure water and aqueous NaCl solutions from 273 to 533 K and from 0 to 2000 bar. Chemical Geology, Volume 193, Issues 3–4, 2003, Pages 257-271, ISSN 0009-2541.
2. 2 Duan, Z., Hu, J., Li, D., and Mao, S. Densities of the CO2-H2O and CO2-H2O-NaCl Systems up to 647 K and 100 MPa, Energy & Fuels, 2008, 22, 1666–1674.

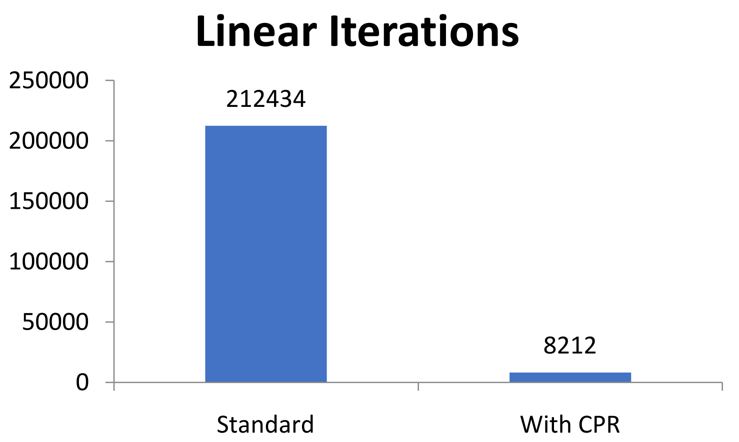
Parallel Simulation in the Cloud

Compressed Pressure Residual (CPR) is a two-stage preconditioner:

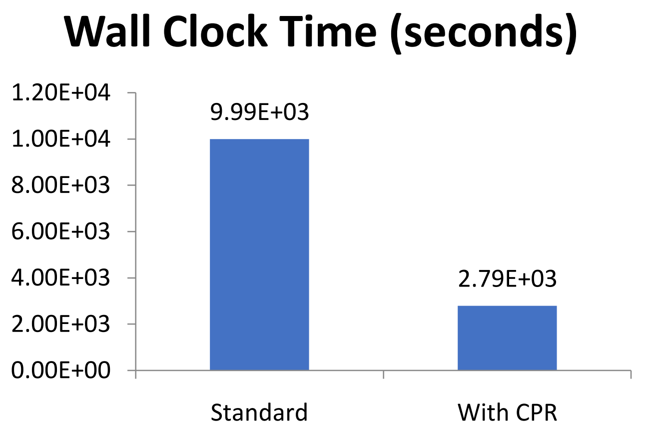
- Stage 1 extracts a pressure equation from the multiphase system, then uses Algebraic Multigrid (AMG) to approximate the pressure.
- Stage 2 uses Block-Jacobi to approximate all variables.

The AMG solves the pressure on coarser & finer meshes, using variable interpolation, to reduce both low and high frequency errors.
CPR seems to also work for thermal problems.

Large CO_2 Injection model results:



Decrease factor = 25.



Decrease factor = 3.6.

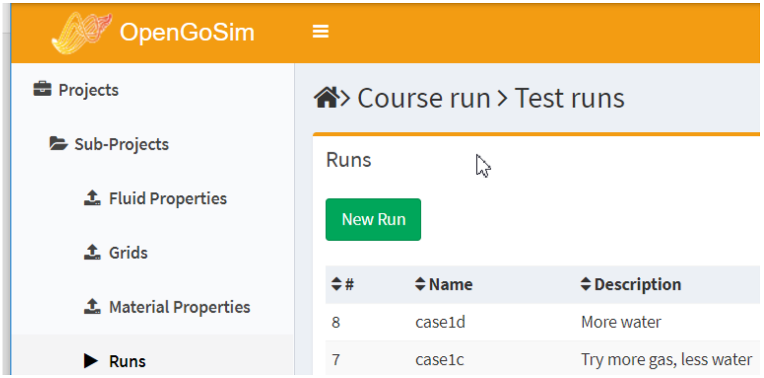
Parallel Simulation in the Cloud

The majority of the runs pictured here are run in the AWS cloud environment, using a new Web-based interface[1]. Graphics is ResInSight.

It is possible to do a Linux install from source on AWS – not easy – and the Web interface is generally much simpler.

Positive aspects:

- Real hundred-core firepower from laptop from any location without need to own or maintain a big cluster.
- Can share runs and data in the cloud.



Negative aspects:

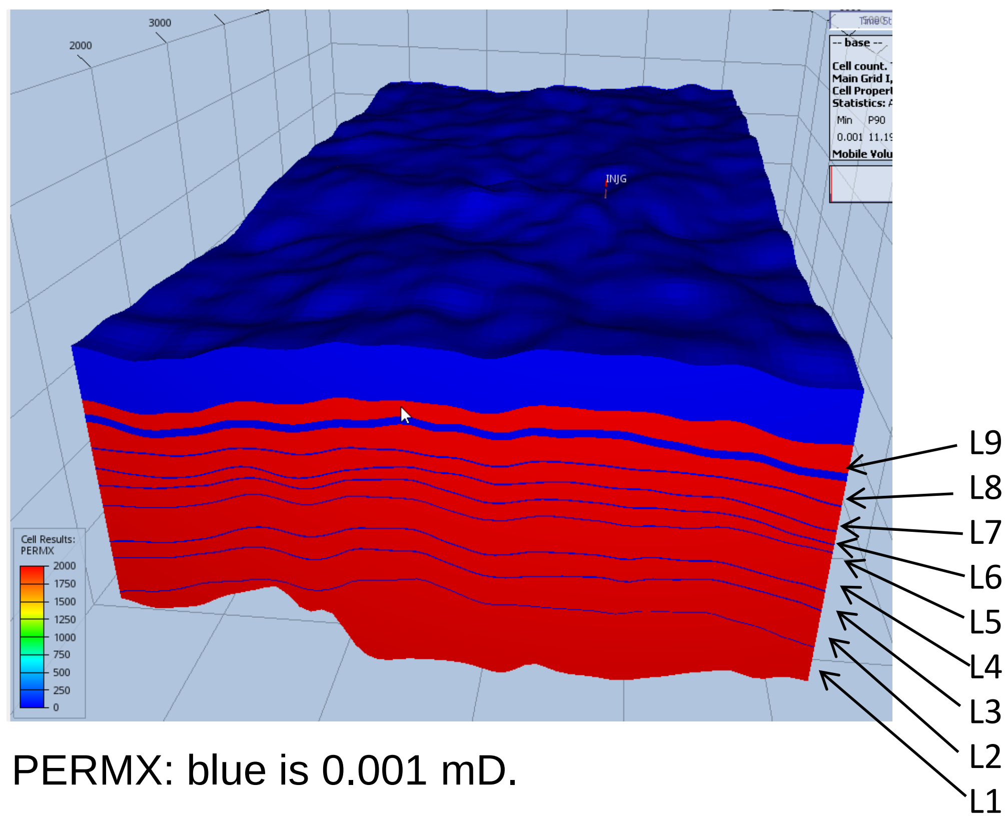
- Upload/download still a nuisance and delay.
- Security still a concern for many.

1. www.opengosim.com

Example I: Sleipner (Oct 2019 data)

Data available from: https://portal.co2.sigma2.no/
Accurate horizon data, currently low and high permeability layers.

Pressure[1]: 105 bar at injection depth of 1012 m.
Temp: 29°C to 35.5°C.
Injection temp: 48°C.



PERMX: blue is 0.001 mD.

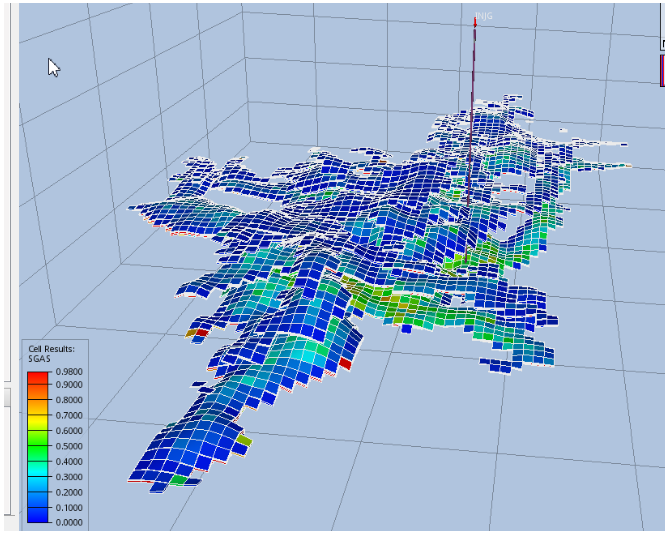
1. Chadwick and Eiken, 'Offshore CO2 Storage: Sleipner natural gas field beneath the North Sea'.
Map from BGS, https://www.bgs.ac.uk/science/CO2/home.html

Example I: Sleipner (Oct 2019 data)

Simulation grid is:
64 x 118 x 263
(about 2M grid blocks)
Run on 36 cores,
~ 2 days simulation time
Gas saturations at
15 years:

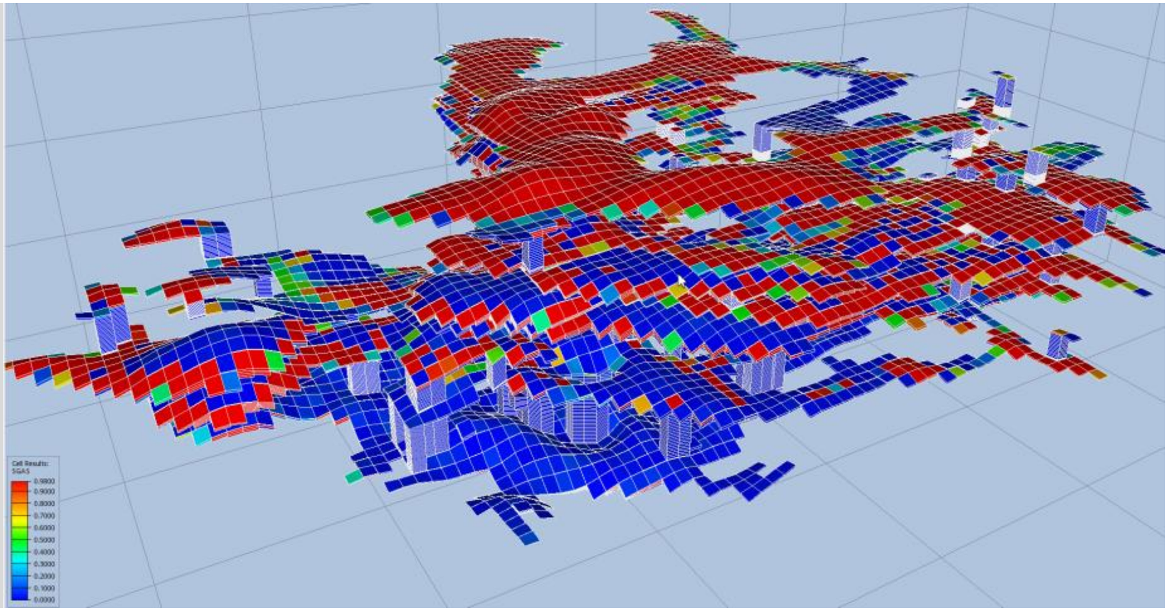
Original perms + Dykstra-Parsons heterogeneity

Saturations below S_{gcr} have been removed for clarity. The gas is into the L5 cycle and about to enter the L6 one, but is some way off getting to the L9 cycle. This is a poor match to the observed appearance of the gas in L9 at around 3 years.



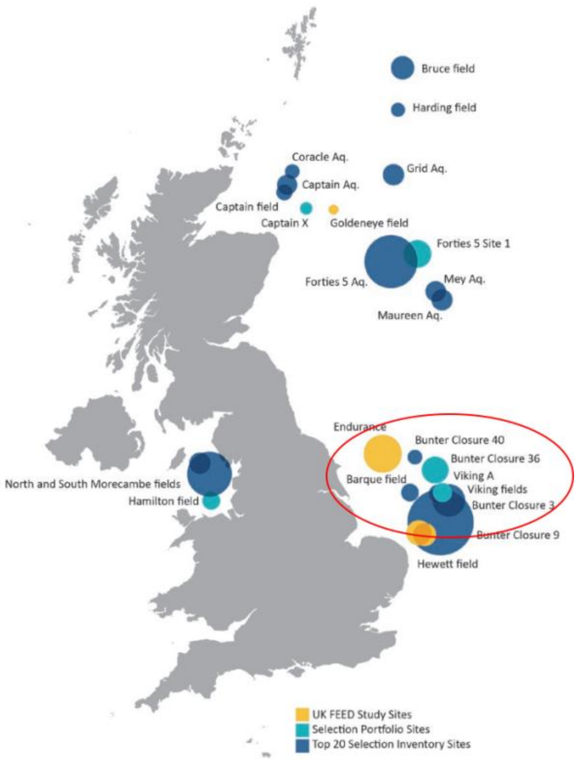
250 random single column holes in each shale

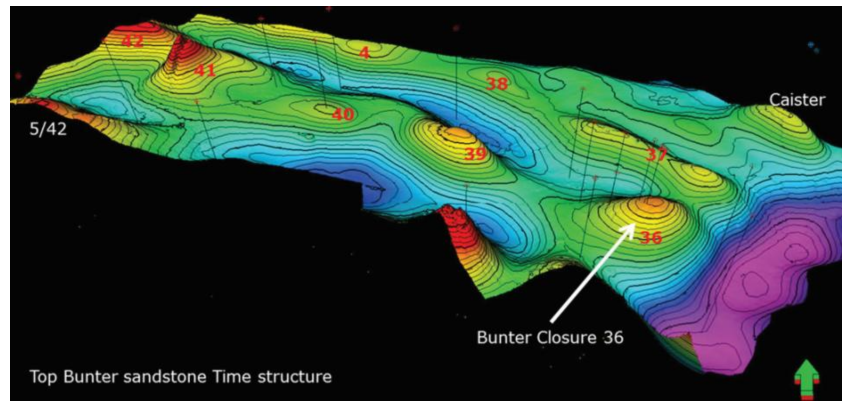
The predicted gas saturation at 15 years is a series of stacked plumes of similar size, connected by low-saturation gas chimneys above the breaches in the tight layers.
Size and arrival of L9 plume similar to observed, not the same shape – observed has greater NS extension.



Example II: Bunter Closure 36 model

Data available from: https://www.eti.co.uk/programmes/carbon-capture-storage/strategic-uk-ccs-storage-appraisal



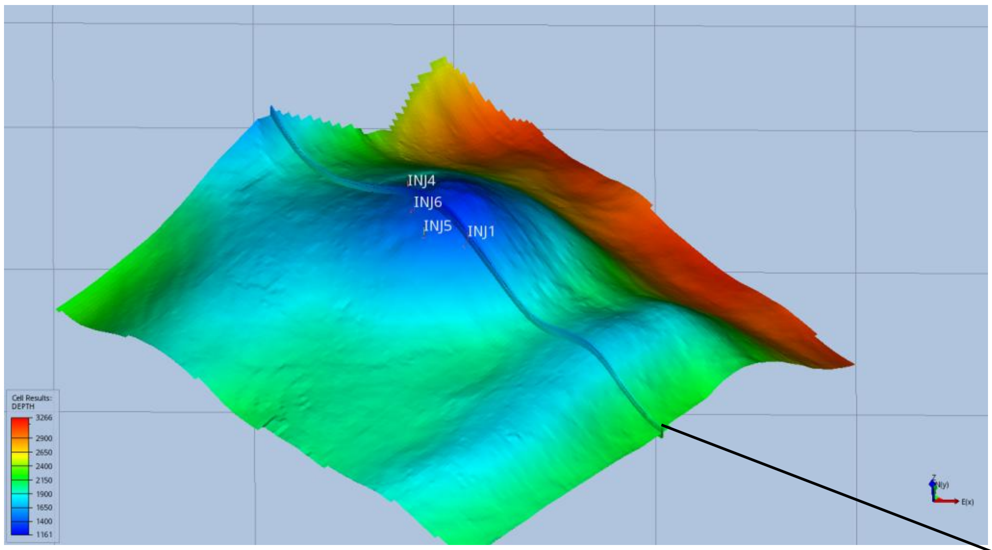


Reservoir top Pressure: 116 bar Reservoir.
top: 1117 m.
Temp: 45°C.
Salinity: 20 wt%.
Injection of 7 Mt/Year for 56 years (base scenario of ETI development report)[1].
Aquifer attached: 270 x 10^9 m^3.

1. Strategic UK CCS Storage Appraisal Project, funded by DECC - ETI Open Licence for Materials.
D10: WP5A – Bunter Storage Development Plan.

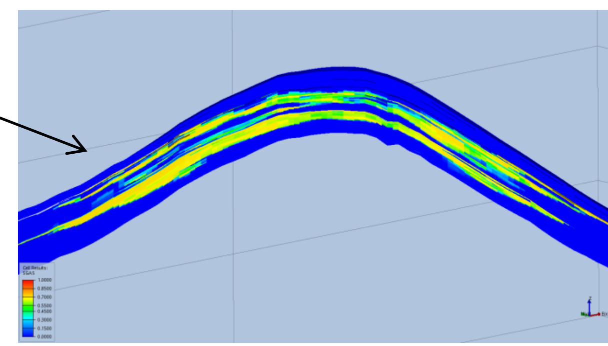
Example II: Bunter Closure 36 model

Wells placed in a way to maximise injectivity and capacity while keeping the pressure below a fracture value[1]. 4 wells located at the western side of the closure, to minimise pressure build up.



The injectivity is limited by the maximum allowed pressure, taken as 90% of the fracture pressure (0.168bar/m)

At 1170 m, max allowed pressure 177 bars.



The wells penetrate both available permeable layers, which are nearly-isolated by an intra shale layer.

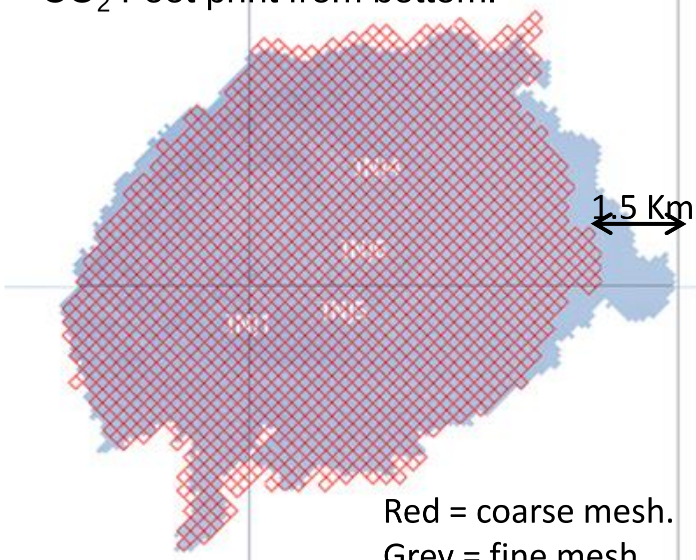
1. Strategic UK CCS Storage Appraisal Project, funded by DECC - ETI Open Licence for Materials. D10: WP5A – Bunter Storage Development Plan.

Example II: Bunter Closure Model

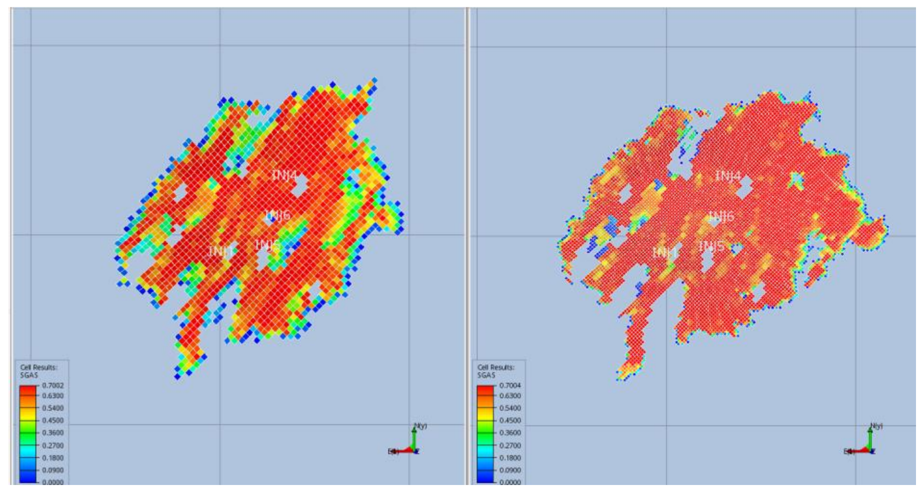
OpenGoSim

Original model is discretised with 200 m x 200 m in the horizontal directions, and about dz = 4 m vertically (600 k cells). Refined model [100 x 100 x 1] m (10 M cells), runs in about 8 hours on 180 cores.

CO_2 Foot print from bottom.



Red = coarse mesh.
Grey = fine mesh.

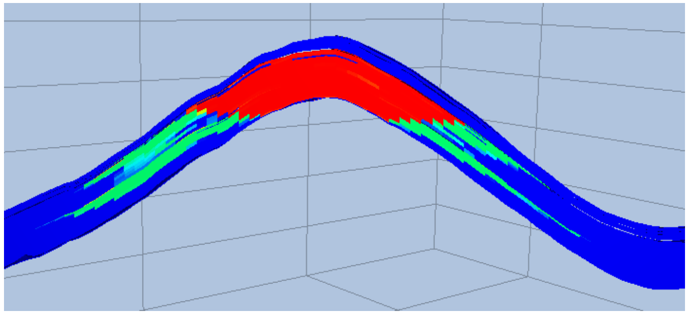


Gas saturation map in the layer at the top of the deeper permeable layer.

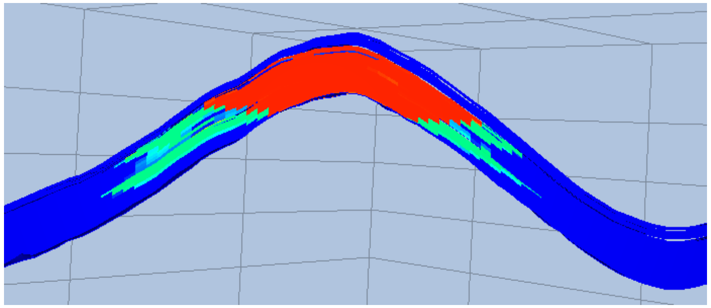
The finer mesh returns a larger foot print. In general finer vertical resolution tends to predict larger spreads until mesh-independent results are obtained. The foot print is a very important parameter, as authorities give permission for a restricted area.

Example II: Bunter Closure Model

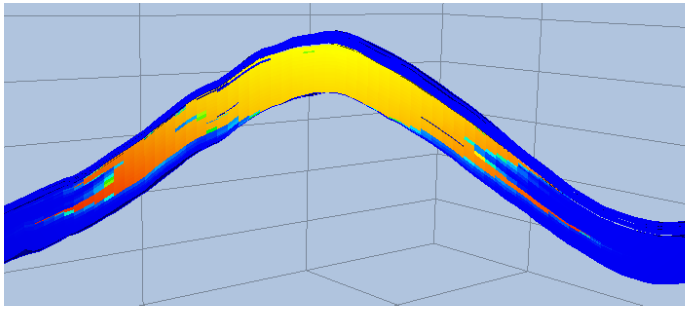
5000 years after the injection – coarse mesh – cross section along the closure



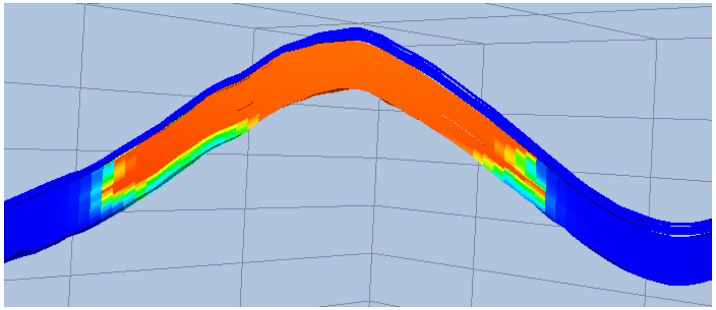
Sg, min =0.3, Max =0.7. No diffusion.



Sg, min =0.3, Max =0.7. Diffusion on.



CO_2 concentration. No diffusion.

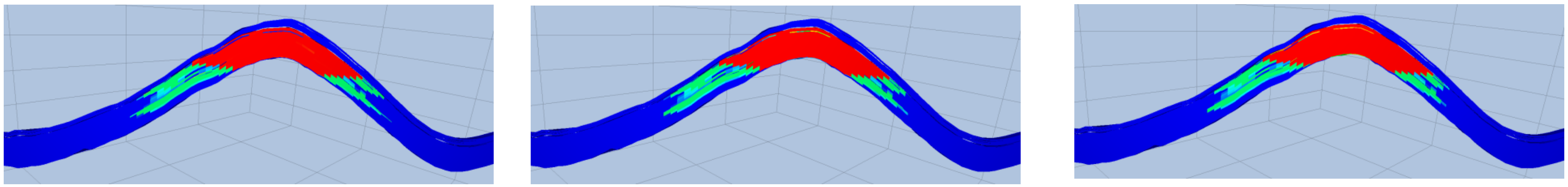


CO_2 concentration. Diffusion on.

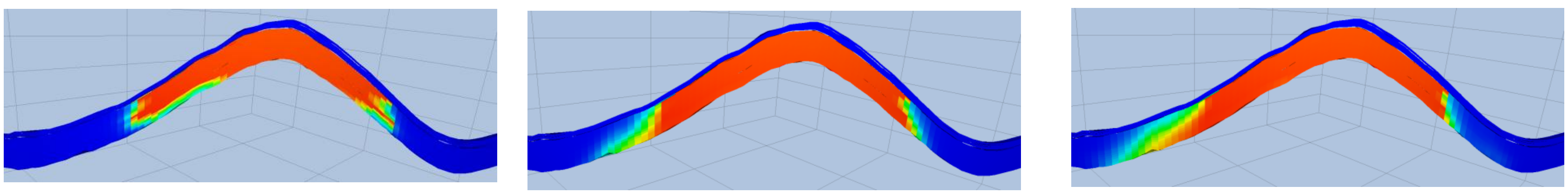
The molecular diffusion tends to smooth high concentration regions and help dissolving thin free gas layers. It also enhances the gravity-driven flow of CO_2-enriched brine.

Example II: Bunter Closure Model

Solution trapping of CO_2 seems to occur over a long time for this model.
Coarse mesh – cross section along the closure:



Sg, min =0.3, Max =0.7. From left to right: 5000 y, 50000 y, 100000 y.



CO_2 concentration. From left to right: 5000 y, 50000 y, 100000 y.

Solution trapping in this case is dominated by diffusion and density-driven flow.

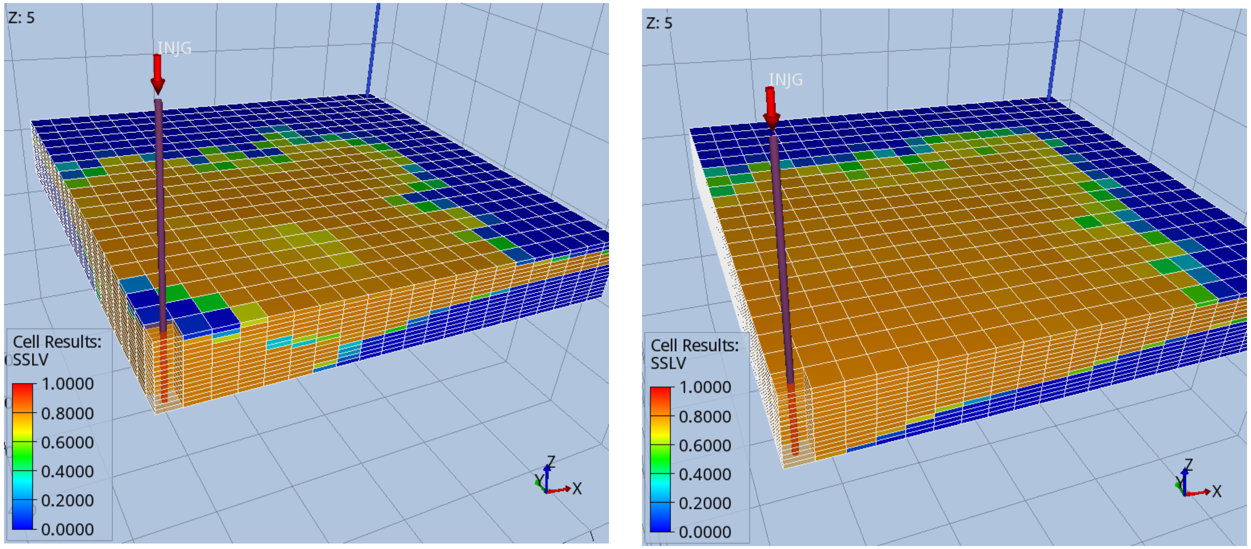
Effects of mesh refinement in the long term runs have not been investigated.

Mineralisation might also play an important role at this time scale, and was ignored in the simulation to 100,000 years.

Thermal Swing CO_2 Injection

In a lot of studies, the main effect is that of the temperature background on fluid properties. However cases do exist in which injection temperature can affect the dynamics. CO_2 can be heavier or lighter than oil, depending on temperature.

Example: inject hot and cold CO_2 in an CO_2-EOR case[1] based on heterogeneous and extended version of SPE5 with 4-phase Todd-Longstaff:



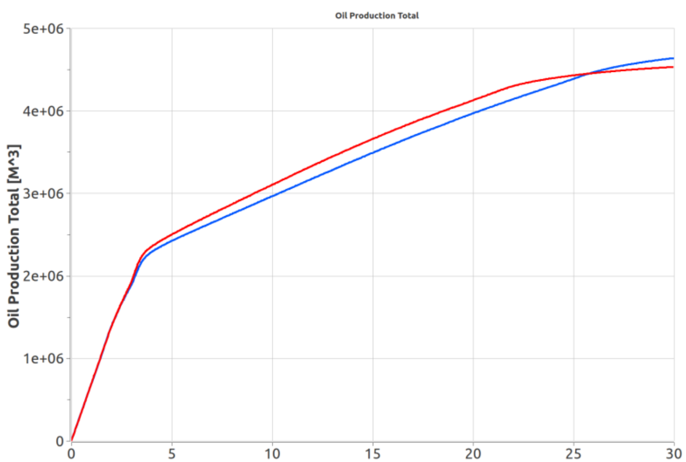
Solvent saturation at 12 years: left 5°C injection, right 70°C injection.

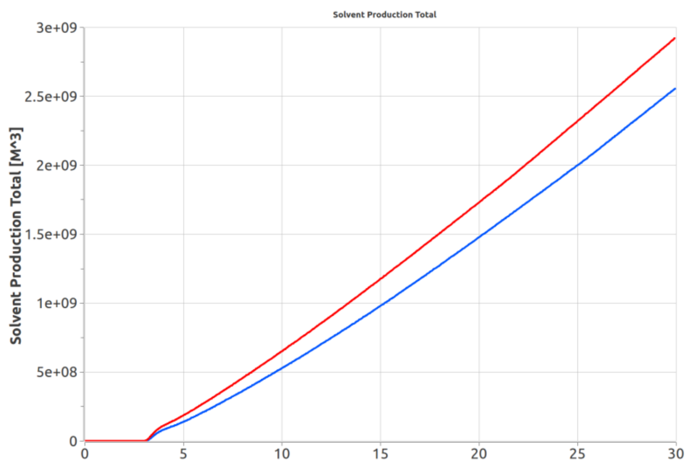
1 https://opengosim.com/blog/post.php?s=2019-09-14-thermal-solvent-model-todd-longstaff-case-study

Thermal Swing CO_2 Injection

The cooler CO_2 is effective in recovery terms – it occupies reservoir volume and displaces oil into the producers, without (at first) getting produced itself – i.e. improves the overall sweep efficiency.

The result is a better gas efficiently in the low temperature case: i.e. the cumulative oil recovery is similar in the two cases, but less CO_2 is produced in the cold injection case as less CO_2 arrives at the producer:





Oil and solvent production in sm3 vs. Time in years, red hot, blue cool injection case.

Conclusions

The CO_2/brine system is well-modelled with Span-Wagner and Duan models, this can be also represented using a stack of black-oil type tables at multiple temperatures.

The effects of temperature variation and molecular diffusion may be significant.

Cloud simulation enables large scale computer resources to be accessed at a reasonable cost and without maintaining a cluster.

Large scale storage simulation requires high resolution and much longer (10^6 day) time scales than hydrocarbon recovery simulation.

Thank you

OpenGoSim