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OpenGoSim

Reduced Physics Models of Fluid Flow and Trapping

CCUS Innovation 2.0

Key Knowledge Deliverable 2.1

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Key Knowledge Deliverable Cover Sheet

This Key Knowledge Deliverable (KKD) has been produced by University of Cambridge 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 contains key knowledge deliverable 2.1, open-source research codes for the rapid estimate of the impacts of heterogeneity on lateral plume migration, residual and dissolution trapping.

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

KKD4.3 StrataTrapper Workshop to CCS project developers

KKD5.1 Annual reports

KKD5.2 Project final report

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Contents

The mathematical model developed as part of WP2 describes the field-scale behaviour of CO2 injected into a subsurface, fluid-saturated reservoir. The model incorporates spatially variable porosity, permeability, and upper- and lower-caprock topography, as well as residual trapping and dissolution. By leveraging some widely applicable assumptions about the flow of the CO2, the resulting reservoir simulations can be run quickly on a standard laptop.

Description of the Mathematical Model

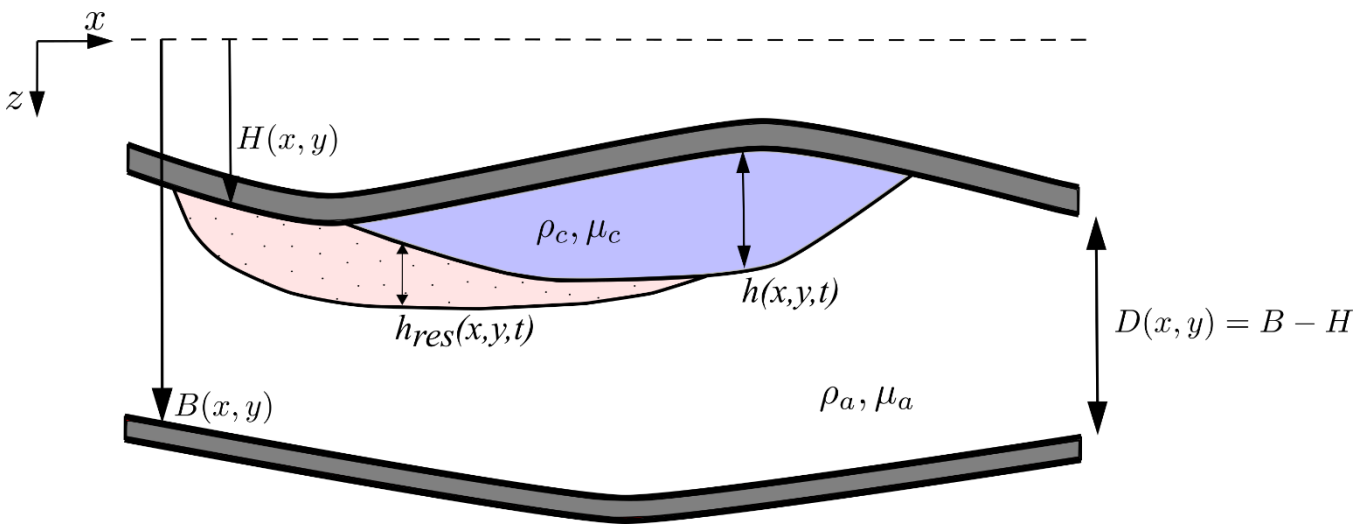

Figure 1: Schematic of the reservoir and flow setup used in the mathematical model. The reservoir is divided into regions of mobile CO2 (purple), residually trapped CO2 (spotted, light red), and pure ambient fluid (the remainder of the reservoir).

Subsurface storage of CO2 typically consists of injecting CO2, in a supercritical fluid state, into a porous formation of rock that is bounded above and below by low-permeability sealing layers, such as mudstones. The pore space of the rock is pervaded by brine (referred to as the ambient fluid), prior to injection. The general flow of fluids through porous media is governed by Darcy's law. Here, we consider the flow of both the injected CO2 and the ambient.

This model combines Darcy's law with two key assumptions, which are applicable in a wide range of settings for field-scale modelling of CO2 sequestration:

1. The flow of fluid in the reservoir is predominantly horizontal,
2. Buoyancy drives the CO2 to build up beneath the upper caprock a short distance from the injection site.

As a result of this, the vertical variation of the pore pressure in the reservoir is primarily due to gravity (i.e. hydrostatic), and we are able to vertically integrate the governing equations to reduce the full 3D system of equations to a simpler 2D system.

The structure of the flow assumed for the model is shown in Figure 1. This consists of

- a region of mobile CO2 and immobile brine, of thickness h,
- a region of trapped CO2 and mobile brine, of thickness h_{res},
- the remaining part of the reservoir, filled purely with the ambient fluid, brine.

By vertically integrating first across the mobile and trapped CO2 regions, and then across the entire reservoir, we arrive at a pair of equations that determine how the thickness of the CO2 current evolves, and how the pore pressure is constrained by volume conservation:

$$\phi \mathcal{C}_s \frac{\partial h}{\partial t} - \widetilde{\nabla} \cdot \left\{ \frac{h\kappa_c}{\mu_c} \widetilde{\nabla}[P_a + \Delta\rho g H] \right\} = \widetilde{\nabla} \cdot \left\{ \frac{h\kappa_c \, \Delta\rho g}{\mu_c} \widetilde{\nabla} h \right\} + Q(x,y,t) - q_d \mathbb{I}_{(h>0, \mathrm{h_{res}}=0)} ,$$

$$\widetilde{\nabla} \cdot \left\{ \frac{1}{\mu_c} [h\kappa_c + M(D-h)\kappa_a] \widetilde{\nabla} P_a \right\} = -\widetilde{\nabla} \cdot \left\{ \frac{h\kappa_c \, \Delta\rho g}{\mu_c} \widetilde{\nabla}(H+h) \right\} - Q(x,y,t) \ .$$

In the above

- t is time, x, y, and z are spatial variables with z pointing vertically downwards, and $\widetilde{\nabla} = (\partial_x, \partial_y)$ is the horizontal gradient operator,
- $H(x,y)$ is the depth to the upper caprock, $B(x,y)$ the depth to the basement layer, and $D(x,y) = B - H$ the thickness of the reservoir.
- $\phi(x,y,z)$ is the porosity, while κ_c and κ_a are vertical averages of the permeability $k(x,y,z)$ across the mobile CO2 current and the ambient fluid, respectively,
- μ_c is the viscosity of the CO2, μ_a that of the ambient, and $M = \mu_c/\mu_a$ the viscosity ratio,
- $\widetilde{\nabla} P_a$ is the horizontal pressure gradient in the ambient,
- $Q(x,y,t)$ is the vertically integrated injection profile for the CO2,
- $\Delta\rho = \rho_a - \rho_c$ is the density difference between the ambient and the CO2,
- $\mathcal{C}_s$ is a prefactor due to saturation and dissolution, involving:
    - the irreducible saturation of water, s_{ai} in the mobile region of CO2,
    - the residual saturation s_{cr} of CO2 in the trapped region of CO2,
    - and the volume fraction C_{sat} of CO2 that can be dissolved in the ambient,
- $q_d \mathbb{I}_{(h>0, \mathrm{h_{res}}=0)}$ is a loss term due to convective dissolution acting on the interface between mobile CO2 and the ambient. The effect of convective dissolution on the residually trapped region is incorporated into $\mathcal{C}_s$.

The spatial variability of the reservoir is incorporated through $\phi(x,y,z)$, $k(x,y,z)$, $H(x,y)$, and $D(x,y)$. In particular, the vertical integration of the governing equations incorporates the vertical structure of the permeability into the two vertical averages κ_c and κ_a. These

correspond respectively to the average permeability across the region of mobile CO2, and that across the remainder of the reservoir:

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

Model Derivation

Here we provide an overview of the derivation of the mathematical model. For further details, see the provided documentation at https://github.com/ajobutler/CO2GraVISim.

We consider the setup as shown in Figure 1. There is a region of mobile CO2 lying between $z = H$ and $z = H + h$. This region is predominantly filled with CO2, but with a small fraction of the pore space still occupied by ambient fluid that cannot be removed due to surface tension, as the ambient fluid preferentially wets to the rock. In this region we assume that the saturation of CO2 is constant and set by the irreducible saturation of the ambient, $s_a = s_{ai}$.

Similarly, there is a region of residually trapped CO2 lying between $z = H + h$ and $z = H + h + h_{res}$ (allowing $h = 0$ and $h_{res} = 0$), where the CO2 saturation is at its residual value, i.e. $s_c = s_{cr}$, $s_a = 1 - s_{cr}$. The remainder of the pore space, below these two regions, consists purely of ambient fluid. The fluid saturations used in this model are thus given by:

$s_c = 1 - s_{ai}$	$s_a = s_{ai}$	mobile CO2	$(H \le z \le H + h)$
$s_c = s_{cr}$	$s_a = 1 - s_{ai}$	trapped CO2	$(H + h \le z \le H + h + h_{res})$
$s_c = 0$	$s_a = 1$	pure ambient	$(H + h + h_{res} \le z \le B)$

The fluid flow in the reservoir is governed by Darcy's law,

$$\boldsymbol{u} = -\frac{k}{\mu}\nabla(p - \rho g z)\,.$$

The assumption that vertical flow is negligible means that the pore fluid pressure p is hydrostatic in the vertical direction, at leading order, and so can be written as

$$p = \begin{cases} P_a + \Delta\rho g(H+h) + \rho_c g z, & CO2 \\ P_a + \rho_a g z, & ambient \end{cases}$$

where $\Delta\rho = \rho_a - \rho_c$ and the pressure is made to be continuous at the interface $z = H + h$. Thus the horizontal Darcy velocities $\tilde{\boldsymbol{u}} = (u, v)$ for the two mobiles phases are

$$\tilde{\boldsymbol{u}}_c = -\frac{k}{\mu_c}\tilde{\nabla}[P_a + \Delta\rho g(H+h)]\,, \qquad \tilde{\boldsymbol{u}}_a = -\frac{k}{\mu_a}\tilde{\nabla}P_a\ .$$

Dissolution

We incorporate dissolution of the CO2 in two forms – invasive dissolution, and convective dissolution. Since the time for dissolution to occur over the pore scale is comparatively fast, we assume that a volume fraction C_{sat} of CO2 dissolves instantaneously into fresh ambient when they come into contact. This 'invasive' dissolution, along with the saturation structure described above, is taken into account when considering the total amount of CO2 within a vertical column. The effect of these is ultimately incorporated into a prefactor $\mathcal{C}_s$ that multiplies the time derivative $\partial h/\partial t$.

Over a much longer time scale, the density difference between CO2-saturated and unsaturated ambient generates convective circulation that introduces unsaturated ambient into the CO2 regions. We model this convective dissolution as a loss term, $-q_d$, acting on the interface between the CO2 and the ambient fluid beneath. This interface is either that for the residually trapped region ($z = H + h + h_{res},\ h_{res} > 0$) or for the exposed mobile region ($z = H + h,\ h_{res} = 0$). Following (Neufeld, 2010) and (MacMinn, 2012), this loss term is given by

$$q_d = 0.12\left(\frac{\phi_0 C_{sat} D_{mol}}{\mathcal{L}}\right)\left(\frac{\Delta\rho_a^{sat} g k_v \mathcal{L}}{\phi_0 \mu_a D_{mol}}\right)^{0.84}\ ,$$

where D_{mol} is the molecular diffusivity of the CO2 in the ambient, and $\Delta\rho_a^{sat}$ is the density difference between the saturated and unsaturated ambient.

Total conservation of volume

In the region $H \le z \le H + h$, CO2 is the mobile phase and the ambient fluid that could not be expelled is immobile. In contrast, in the remaining section $H + h \le z \le B$ the ambient fluid is mobile, and any CO2 is residually trapped and immobile. Vertically integrating the governing equations across the entire reservoir gives an equation governing the conservation of fluid volume within a vertical column:

$$\tilde{\nabla}\cdot\left\{\int_H^{H+h}\tilde{\boldsymbol{u}}_c\,dz\right\} + \tilde{\nabla}\cdot\left\{\int_{H+h}^{B}\tilde{\boldsymbol{u}}_a\,dz\right\} = Q(x,y,t)\,.$$

Combined this with the expressions for the Darcy velocities $\tilde{\boldsymbol{u}}_c$, $\tilde{\boldsymbol{u}}_a$ and rearranging, we get

$$\tilde{\nabla}\cdot\left\{\frac{1}{\mu_c}[h\kappa_c + M(D-h)\kappa_a]\tilde{\nabla}P_a\right\} = -\tilde{\nabla}\cdot\left\{\frac{h\kappa_c\Delta\rho g}{\mu_c}\tilde{\nabla}(H+h)\right\} - Q(x,y,t)$$

where $M = \mu_c/\mu_a$, and κ_c and κ_a are the vertically averaged permeabilities given by

$$h\kappa_c = \int_H^{H+h} k\ dz\ , \qquad (D-h)\kappa_a = \int_{H+h}^{B} k\ dz\ .$$

Governing Equations

Together, the governing equations for the mobile current thickness h and the ambient pressure P_a are

$$\phi\mathcal{C}_s\frac{\partial h}{\partial t} - \widetilde{\nabla}\cdot\left\{\frac{h\kappa_c}{\mu_c}\widetilde{\nabla}[P_a + \Delta\rho g H]\right\} = \widetilde{\nabla}\cdot\left\{\frac{h\kappa_c\,\Delta\rho g}{\mu_c}\widetilde{\nabla}\,h\right\} + Q(x,y,t) - q_d\mathbb{I}_{(h>0,\mathrm{h_{res}}=0)}\ ,$$

$$\widetilde{\nabla}\cdot\left\{\frac{1}{\mu_c}[h\kappa_c + M(D-h)\kappa_a]\,\widetilde{\nabla}P_a\right\} = -\widetilde{\nabla}\cdot\left\{\frac{h\kappa_c\,\Delta\rho g}{\mu_c}\widetilde{\nabla}(H+h)\right\} - Q(x,y,t)\ .$$

Nondimensional Form

The software developed here solves the nondimensional form of these governing equations, based on a characteristic injection flux, $\mathcal{Q}$.

To perform this nondimensionalisation, we choose:

- the length scale $\mathcal{L}$ in both the vertical and horizontal directions to be the characteristic thickness of the reservoir,
- a characteristic flux scale $\mathcal{Q}$,
- a characteristic porosity value ϕ_0,
- a characteristic permeability k_0.

The dimensional scaling behaviours of the terms in the governing equations above are then

$$\phi_0\frac{\mathcal{L}}{\mathcal{T}}\ , \qquad \frac{\mathcal{L}k_0\mathcal{P}}{\mu_c\mathcal{L}^2}\ , \qquad \frac{k_0\Delta\rho g\mathcal{L}^2}{\mu_c\mathcal{L}^2}\ , \qquad \frac{k_0\Delta\rho g\mathcal{L}^2}{\mu_c\mathcal{L}^2}\ , \qquad \frac{\mathcal{Q}}{\mathcal{L}^2}\ , \qquad \frac{\mathcal{Q}}{\mathcal{L}^2}\ ,$$

where $\mathcal{T}$ and $\mathcal{P}$ are as-yet-unspecified time and pressure scales, respectively. We choose to scale by the injection velocity scale $u_Q = \mathcal{Q}/\mathcal{L}^2$, giving

$$\mathcal{T} = \frac{\phi_0 \mathcal{L}^3}{\mathcal{Q}}, \qquad \mathcal{P} = \frac{\mu_c}{k_0}\frac{\mathcal{Q}}{\mathcal{L}},$$

along with the nondimensional governing equations

$$\phi^* \mathcal{C}_s \frac{\partial h^*}{\partial t^*} - \widetilde{\nabla}^* \cdot \left\{ h^* \kappa_c^* \widetilde{\nabla}^* [P_a^* + \Gamma H^*] \right\} = \widetilde{\nabla}^* \cdot \left\{ \Gamma h^* \kappa_c^* \widetilde{\nabla}^* h^* \right\} + Q^*(x^*, y^*, t^*) - q_d^* \mathbb{I}_{(h^*>0, h_{\mathrm{res}}^*=0)},$$

$$\widetilde{\nabla}^* \cdot \left\{ [h^* \kappa_c^* + M(D^* - h^*)\kappa_a^*] \widetilde{\nabla}^* P_a^* \right\} = -\widetilde{\nabla}^* \cdot \left\{ \Gamma h^* \kappa_c^* \widetilde{\nabla}^* (H^* + h^*) \right\} - Q^*(x, y, t).$$

where * denotes nondimensional/scaled terms, and Γ is the ratio between the buoyancy velocity u_b and the injection velocity u_Q, given by

$$\Gamma = \frac{u_b}{u_Q} = \frac{(\Delta \rho g k_0 / \mu_C)}{(\mathcal{Q}/\mathcal{L}^2)}.$$

The nondimensional convective dissolution term is given by $q_d^* = q_d / u_Q$.

Description of the Software

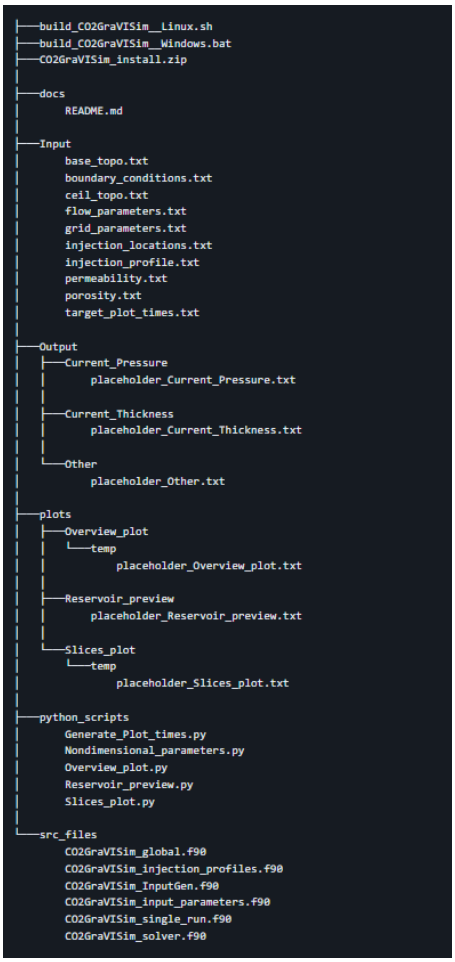

Figure 2: File structure for the Reservoir Simulator codes provided.

The code produced to solve equations the nondimensional governing equations for h and P_a has been written in Fortran 90, in order to take advantage of the computational efficiencies of a compiled language, and to aid future interface with other sections of the StrataTrapper project.

The equations for h and P_a are solved in tandem. The elliptic equation for P_a is solved via a successive-overrelaxation (SOR) method, while the advection--diffusion equation for h is discretised using the Il'in scheme, in order to accommodate advection and diffusion terms correctly, and solved using the Alternating-Direction Implicit (ADI) method. The residual current thickness, h_{res}, is updated concurrently via an explicit method. This is all wrapped within a Predictor-Corrector approach in order to deal with nonlinearities. On top of this, an adaptive time-stepping routine is used to minimise overall runtime while still maintaining the desired level of numerical accuracy.

The code can be found at https://github.com/ajobutler/CO2GraVISim. The file structure for the code is shown in Figure 2. Accompanying the main solver are codes and python scripts for generating example input files, running the solver, and producing plots of the calculated outputs. Further details about the code are provided in the documentation included there.

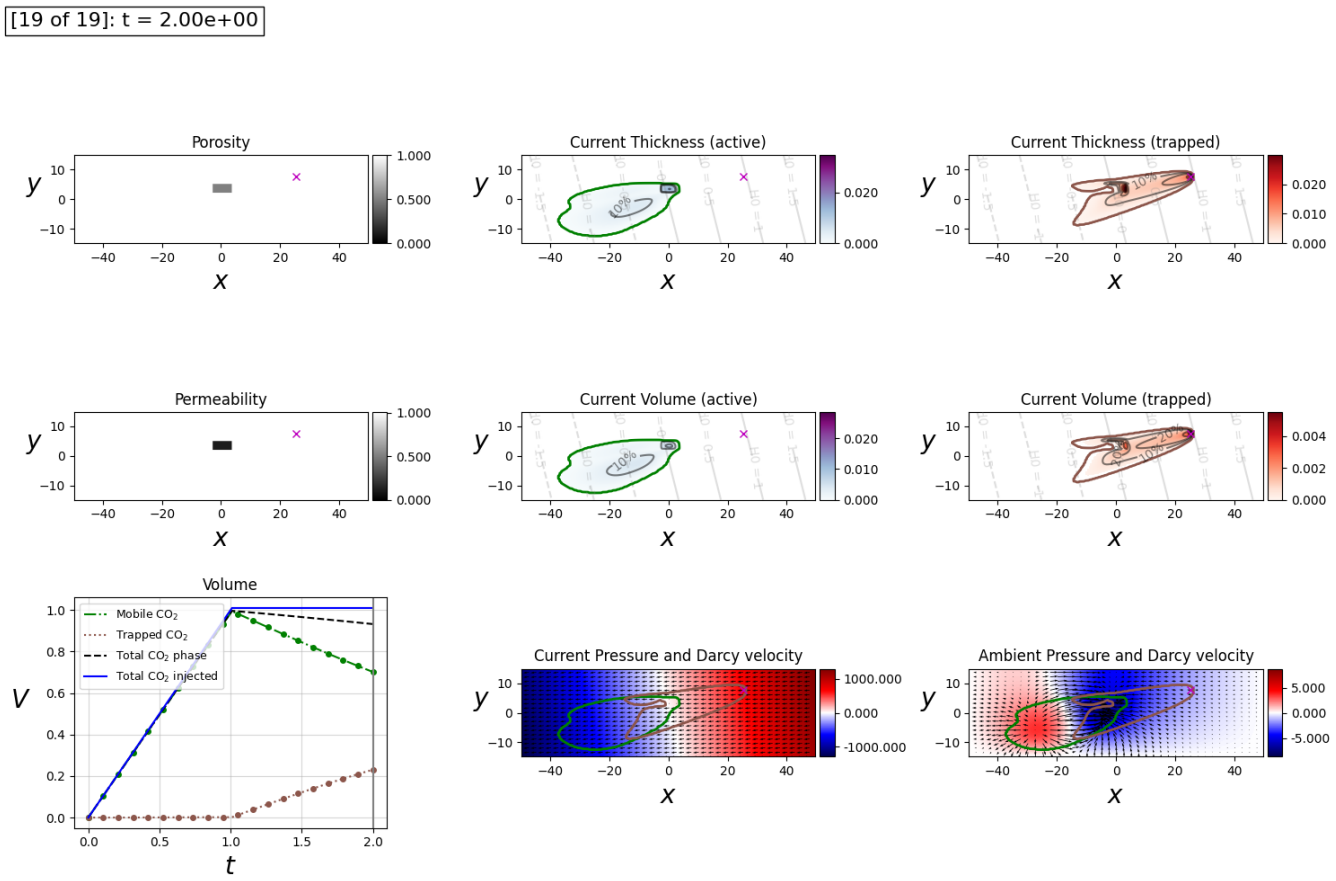

Figure 3: Plot of the mobile current thickness, $h(x, y, t)$, the trapped current thickness , $h_{res}(x, y, t)$, the corresponding local volumes in those regions, and the respective pressures and Darcy velocities for the mobile CO2 and ambient phases.

Results from an example calculation are shown in Figure 3. Here, CO2 is injected into a reservoir with a shallow upward slope to the South West, and a low-porosity, low-permeability region just to the West of the injection well. For this calculation, the permeability is linked to the porosity via the Kozeny-Carman equation. Using typical parameter values, the dimensional timescale for this simulation is $\mathcal{T} \approx 181$ days. A 200×100 grid with nondimensional grid spacings $dx = 0.5, dy = 0.3$ was used, and the full simulation took ≈ 4 minutes to run on a standard laptop.

Future Work

The code described here is a stand-alone version that can be used to simulate the behaviour of CO2 injected into an ambient-filled porous reservoir. As part of WP4, a version of this code

is also being developed to interface with the Stratus software from OpenGoSim. This will allow Stratus to pass input data (e.g. reservoir topography, permeability, etc.) provided in industry-standard formats such as for ECLIPSE to this solver, and then display the calculated results via a user-friendly interface.

References

MacMinn, C. W. (2012). Spreading and convective dissolution of carbon dioxide in vertically confined, horizontal aquifers. *Water Resources Research*.

Neufeld, J. A. (2010). Convective dissolution of carbon dioxide in saline aquifers. *Geophysical research letters*.

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