

# StrataTrapper - WP2 Reduced Physics Models of Fluid Flow and Trapping

Adam Butler, Jerome Neufeld

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The mathematical model developed as part of WP2 describes the field-scale behaviour of  $\text{CO}_2$  injected into a subsurface, fluid-saturated reservoir, incorporating 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  $\text{CO}_2$ , the resulting reservoir simulations can be run quickly on a standard laptop.

## Description of the Mathematical Model

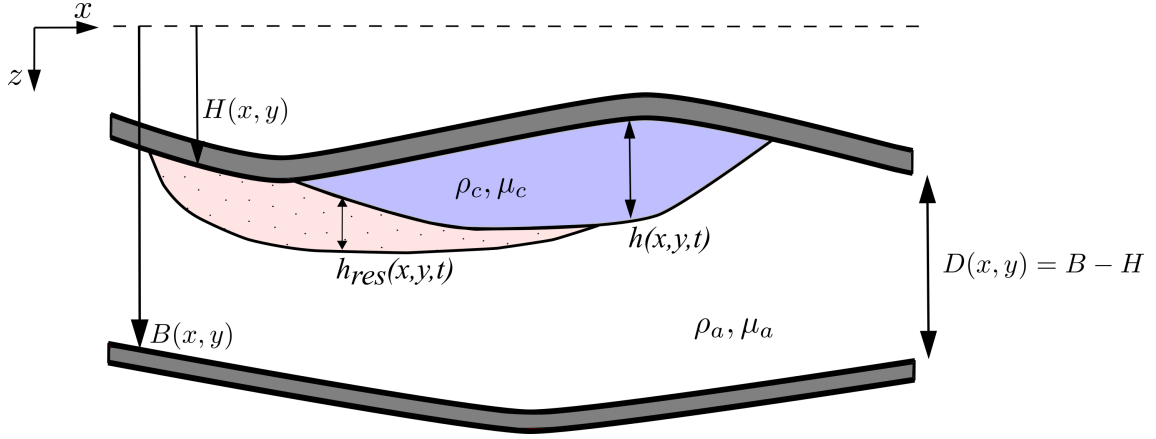


Figure 1: Schematic of the reservoir and flow setup used in the mathematical model.

The general flow of fluids through porous media is governed by Darcy's law. This model combines this with two key assumptions, which are applicable in a wide range of settings for field-scale modelling of  $\text{CO}_2$  sequestration:

1. The flow of fluid in the reservoir is predominantly horizontal,
2. Buoyancy drives the  $\text{CO}_2$  to build up beneath the upper caprock a short distance from the injection site.

As a result of this, the pore pressure in the reservoir is hydrostatic at leading order, and we are able to vertically integrate the governing equations to reduce the full, 3D system of equations to a simpler, 2D system. Vertically integrating across the regions of mobile and trapped  $\text{CO}_2$ , i.e.  $H \leq z \leq H + h + h_{res}$ , we get

$$\frac{\partial}{\partial t} \left( \int_H^{H+h} [(1 - s_{ai}) + C_{sat}s_{ai}] \, dz \right) \quad (1)$$

By vertically integrating first across the  $\text{CO}_2$  current, and then across the entire reservoir, we arrive at a pair of equations that determine how the thickness of the  $\text{CO}_2$  current evolves, and how the pore pressure is constrained by volume conservation:

$$\begin{aligned}
\phi \mathcal{C}_s \frac{\partial h}{\partial t} - \tilde{\nabla} \cdot \left\{ \frac{h \kappa_c}{\mu_c} \tilde{\nabla} [P_a + \Delta \rho g H] \right\} &= \tilde{\nabla} \cdot \left\{ \frac{h \kappa_c \Delta \rho g}{\mu_c} \tilde{\nabla} h \right\} \\
&\quad + Q(x, y, t) - q_d \mathbf{1}_{(h>0, h_{res}=0)} \tag{2} \\
\tilde{\nabla} \cdot \left\{ \frac{1}{\mu_c} [h \kappa_c + M (D - h) \kappa_a] \tilde{\nabla} P_a \right\} &= -\tilde{\nabla} \cdot \left\{ \frac{h \kappa_c \Delta \rho g}{\mu_c} \tilde{\nabla} (H + h) \right\} - Q(x, y, t). \tag{3}
\end{aligned}$$

In the above

- $t$  is time,  $x$ ,  $y$ , and  $z$  are spatial variables with  $z$  pointing vertically downwards, and  $\tilde{\nabla} = (\partial_x, \partial_y)$  is the horizontal gradient operator,
- $H(x, y)$  is the depth to the upper caprock and  $D(x, y)$  the thickness of the reservoir. The thickness of the region of mobile  $\text{CO}_2$  is  $h(x, y, t)$  and that of the residually trapped  $\text{CO}_2$  is  $h_{res}(x, y, t)$ ,
- $\phi(x, y, z)$  is the porosity, while  $\kappa_c$  and  $\kappa_a$  are the vertical averages of the permeability  $k(x, y, z)$  across the mobile  $\text{CO}_2$  current and the ambient fluid, respectively,
- $\mu_c$  is the viscosity of the  $\text{CO}_2$ ,  $\mu_a$  that of the ambient, and  $M = \mu_c/\mu_a$  the viscosity ratio,
- $\tilde{\nabla} P_a$  is the horizontal pressure gradient in the ambient,
- $Q(x, y, t)$  is the vertically integrated injection profile for the  $\text{CO}_2$ ,
- $\Delta \rho = \rho_a - \rho_c$  is the density difference between the ambient and the  $\text{CO}_2$ ,
- $\mathcal{C}_s$  is a saturation and dissolution prefactor involving:
  1. the irreducible saturation of water,  $s_{ai}$  in the mobile region of  $\text{CO}_2$ ,
  2. the residual saturation of  $\text{CO}_2$  in the trapped region of  $\text{CO}_2$ ,
  3. and the volume fraction  $C_{sat}$  of  $\text{CO}_2$  that can be dissolved in the ambient,
- $q_d(x, y, t) \mathbf{1}_{(h>0, h_{res}=0)}$  is a loss term due to convective dissolution acting on the interface between mobile  $\text{CO}_2$  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  $D(x, y)$ .

## Model derivation

We consider the setup as shown in Figure 1. There is a region of mobile  $\text{CO}_2$  lying between  $z = H$  and  $z = H + h$ . In this region we assume that the saturation of  $\text{CO}_2$  is constant and set by the irreducible saturation of the ambient, i.e.  $s_c = 1 - s_{ai}$ ,  $s_a = s_{ai}$ . Similarly, there is also a region of residually trapped  $\text{CO}_2$  lying between  $z = H + h$  and  $z = H + h + h_{res}$  (allowing  $h = 0$  and  $h_{res} = 0$ ), where the  $\text{CO}_2$  saturation is at its residual value, i.e.  $s_c = s_{cr}$ ,  $s_a = 1 - s_{cr}$ . Beneath this lies pure ambient fluid, where  $s_c = 0$  and  $s_a = 1$ .

We also incorporate dissolution of the  $\text{CO}_2$  in two forms. Since the time for dissolution to occur over the pore scale is comparatively fast, we assume that this occurs instantaneously, with a volume fraction  $C_{sat}$  of  $\text{CO}_2$  dissolving into fresh ambient when they come into contact. Over a much longer time scale, the density difference between  $\text{CO}_2$ -saturated and unsaturated ambient generates convective circulation that introduces unsaturated ambient into the  $\text{CO}_2$  regions. We model this convective dissolution as a loss term,  $-q_d$ , acting on the interface between the  $\text{CO}_2$  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 ( $z = H + h$ ,  $h_{res} = 0$ ).

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

$$\mathbf{u} = -\frac{k}{\mu} \nabla (p - \rho g z). \tag{4}$$

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

$$p = \begin{cases} P_a + \Delta\rho g (H + h) + \rho_c g z & \text{CO}_2 \\ P_a + \rho_a g z & \text{ambient} \end{cases}, \quad (5)$$

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  $\tilde{\mathbf{u}} = (u, v)$  for the two mobile phases are

$$\tilde{\mathbf{u}}_c = -\frac{k}{\mu_c} \tilde{\nabla} [P_a + \Delta\rho g (H + h)], \quad \tilde{\mathbf{u}}_a = -\frac{k}{\mu_a} \tilde{\nabla} P_a. \quad (6)$$

### Equations governing $h$ and $h_{res}$

Vertically integrating the governing equations of the two CO<sub>2</sub> regions, i.e. over  $H \leq z \leq H + h + h_{res}$ , gives

$$\begin{aligned} \frac{\partial}{\partial t} \left( \int_H^{H+h} \phi [(1 - s_{ai}) + C_{sat} s_{ai}] dz + \int_{H+h}^{H+h+h_{res}} \phi [s_{cr} + C_{sat} (1 - s_{cr})] dz \right) \\ + \tilde{\nabla} \cdot \left\{ \int_H^{H+h} \tilde{\mathbf{u}}_c dz \right\} = Q(x, y, t) - q_d. \end{aligned} \quad (7)$$

Applying the derivative to the two integrals in the first term, this becomes

$$\begin{aligned} \phi [(1 - s_{ai}) + C_{sat} s_{ai}] \frac{\partial h}{\partial t} + \phi [s_{cr} + C_{sat} (1 - s_{cr})] \frac{\partial h_{res}}{\partial t} + \tilde{\nabla} \cdot \left\{ \int_H^{H+h} \tilde{\mathbf{u}}_c dz \right\} \\ = Q(x, y, t) - q_d. \end{aligned} \quad (8)$$

To determine  $h$ , which is our ultimate aim, we need to know how  $h_{res}$  behaves.

### The residually trapped region

First consider regions where the amount of mobile CO<sub>2</sub> in a vertical column is increasing or remaining the same, i.e. where  $\frac{\partial h}{\partial t} \geq 0$ . If there is no residually trapped CO<sub>2</sub> already, then  $h_{res}$  will remain 0. If however  $h_{res} > 0$ , then will the interface at  $z = H + h$  advances, the interface at  $z = H + h + h_{res}$  remains fixed as previously trapped CO<sub>2</sub> is remobilised. Thus the thickness of the trapped region decreases at the same rate as the thickness of the mobile region increases. If we then include convective dissolution in the regions where  $h_{res} > 0$ , we find that

$$\frac{\partial h_{res}}{\partial t} = \begin{cases} -\frac{\partial h}{\partial t} - \frac{q_d}{\phi[s_{cr} + C_{sat}(1 - s_{cr})]} & h_{res} > 0 \\ 0 & h_{res} = 0 \end{cases} \quad \text{for } \frac{\partial h}{\partial t} \geq 0. \quad (9)$$

In regions where the amount of mobile CO<sub>2</sub> in a vertical column is decreasing, i.e. where  $\frac{\partial h}{\partial t} < 0$ , then either a residually trapped region will be created if  $h_{res} = 0$  initially, or it will be extended. As mobile CO<sub>2</sub> is withdrawn, unsaturated ambient will be drawn in across  $z = H + h + h_{res}$ , dissolving residually trapped CO<sub>2</sub>. If  $h \mapsto h - \Delta h$ , then the CO<sub>2</sub> saturation in this region changes from  $1 - s_{ai}$  to  $s_{cr}$ . Thus  $\phi[1 - s_{ai} - s_{cr}] \Delta h$  of unsaturated water is drawn in, dissolving  $\phi C_{sat} [1 - s_{ai} - s_{cr}] \Delta h$  of residually trapped CO<sub>2</sub>. The corresponding volume of fluid in the residually trapped region that is ‘lost’ to the ambient below as  $z = H + h + h_{res}$  decreases to  $z = H + (h - \Delta h) + (h_{res} - \Delta h_{res})$  is given by  $\phi[s_{cr} + C_{sat}(1 - s_{cr})] (\Delta h + \Delta h_{res})$ . Equating these, and incorporating convective dissolution as before, we find that

$$\frac{\partial h_{res}}{\partial t} = \begin{cases} \left[ \frac{C_{sat}(1 - s_{ai} - s_{cr})}{s_{cr} + C_{sat}(1 - s_{cr})} - 1 \right] \frac{\partial h}{\partial t} - \frac{q_d}{\phi[s_{cr} + C_{sat}(1 - s_{cr})]} & h_{res} > 0, \\ \left[ \frac{C_{sat}(1 - s_{ai} - s_{cr})}{s_{cr} + C_{sat}(1 - s_{cr})} - 1 \right] \frac{\partial h}{\partial t} & h_{res} = 0 \end{cases} \quad \text{for } \frac{\partial h}{\partial t} < 0. \quad (10)$$

The two of these can be combined as

$$\frac{\partial h_{res}}{\partial t} = C_{res} \frac{\partial h}{\partial t} - \frac{q_d}{\phi[s_{cr} + C_{sat}(1 - s_{cr})]} \mathbf{1}_{(h_{res} > 0)}, \quad (11)$$

where the latter term indicates that convective dissolution only acts on the residual trapping region where residually trapped CO<sub>2</sub> is present, i.e. where  $h_{res} > 0$ .

### Governing equation for $h$

Substituting this expression for  $\frac{\partial h_{res}}{\partial t}$  into (8), we arrive at

$$\phi \mathcal{C}_s \frac{\partial h}{\partial t} + \tilde{\nabla} \cdot \left\{ \int_H^{H+h} \tilde{\mathbf{u}}_c dz \right\} = Q(x, y, t) - q_d \mathbf{1}_{h>0, h_{res}=0}, \quad (12)$$

where  $\mathcal{C}_s$  is a prefactor incorporating  $s_{ai}$ ,  $s_{cr}$ , and  $C_{sat}$ , and is given by

$$\mathcal{C}_s = \begin{cases} (1 - s_{ai} - s_{cr}) & \frac{\partial h}{\partial t} < 0 \\ (1 - C_{sat})(1 - s_{ai} - s_{cr}) & \frac{\partial h}{\partial t} \geq 0, h_{res} > 0 \\ (1 - s_{ai} - s_{cr}) & \frac{\partial h}{\partial t} \geq 0, h_{res} = 0 \end{cases}. \quad (13)$$

### Total conservation of volume

In the region  $H \leq z \leq H + h$ ,  $\text{CO}_2$  is the mobile phase and the ambient fluid that could not be expelled is immobile. In contrast, in the remaining section  $H + h \leq z \leq B$  the ambient fluid is mobile, and any  $\text{CO}_2$  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:

$$\tilde{\nabla} \cdot \left\{ \int_H^{H+h} \tilde{\mathbf{u}}_c dz \right\} + \tilde{\nabla} \cdot \left\{ \int_{H+h}^B \tilde{\mathbf{u}}_a dz \right\} = Q(x, y, t). \quad (14)$$

Combined with the Darcy velocities (6) and rearranged, this becomes

$$\tilde{\nabla} \cdot \left\{ \frac{1}{\mu_c} [h\kappa_c + M(D - h)\kappa_a] \tilde{\nabla} P_a \right\} = -\tilde{\nabla} \cdot \left\{ \frac{h\kappa_c \Delta \rho g}{\mu_c} \tilde{\nabla} (H + h) \right\} - Q(x, y, t), \quad (15)$$

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

$$h\kappa_c = \int_H^{H+h} k dz, \quad (D - h)\kappa_a = \int_{H+h}^B k dz. \quad (16)$$

### Governing equations

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

$$\phi \mathcal{C}_s \frac{\partial h}{\partial t} - \tilde{\nabla} \cdot \left\{ \frac{h\kappa_c}{\mu_c} \tilde{\nabla} [P_a + \Delta \rho g H] \right\} = \tilde{\nabla} \cdot \left\{ \frac{h\kappa_c \Delta \rho g}{\mu_c} \tilde{\nabla} h \right\} + Q(x, y, t) - q_d \mathbf{1}_{(h>0, h_{res}=0)}, \quad (17)$$

$$\tilde{\nabla} \cdot \left\{ \frac{1}{\mu_c} [h\kappa_c + M(D - h)\kappa_a] \tilde{\nabla} P_a \right\} = -\tilde{\nabla} \cdot \left\{ \frac{h\kappa_c \Delta \rho g}{\mu_c} \tilde{\nabla} (H + h) \right\} - Q(x, y, t). \quad (18)$$

### Nondimensional form

The software developed here solves the nondimensional form of these governing equations, based on an characteristic injection flux. To do this nondimensionalisation, we use: 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  $\phi_0$ ; and a characteristic permeability  $k_0$ . The dimensional scaling behaviours of the terms in (17) are then

$$\phi_0 \frac{\mathcal{L}}{\mathcal{T}}, \quad \frac{\mathcal{L} k_0 \mathcal{P}}{\mu_c \mathcal{L}^2}, \quad \frac{k_0 \Delta \rho g \mathcal{L}^2}{\mu_c \mathcal{L}^2}, \quad \frac{k_0 \Delta \rho g \mathcal{L}^2}{\mu_c \mathcal{L}^2}, \quad \frac{\mathcal{Q}}{\mathcal{L}^2}, \quad \frac{\mathcal{Q}}{\mathcal{L}^2}, \quad (19)$$

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

$$\mathcal{T} = \frac{\phi_0 \mathcal{L}^3}{\mathcal{Q}}, \quad \mathcal{P} = \frac{\mu_c}{k_0} \frac{\mathcal{Q}}{\mathcal{L}}, \quad (20)$$

along with the nondimensional governing equations

$$\phi^* \mathcal{C}_s \frac{\partial h^*}{\partial t^*} - \tilde{\nabla}^* \cdot \left\{ h^* \kappa_c^* \tilde{\nabla}^* [P_a^* + \Gamma H^*] \right\} = \tilde{\nabla}^* \cdot \left\{ \Gamma h^* \kappa_c^* \tilde{\nabla}^* h^* \right\} + Q^*(x, y, t) - q_d^* \mathbf{1}_{(h^* > 0, h_{res}^* = 0)}, \quad (21)$$

$$\tilde{\nabla}^* \cdot \left\{ [h^* \kappa_c^* + M(D^* - h^*) \kappa_a^*] \tilde{\nabla}^* P_a^* \right\} = -\tilde{\nabla}^* \cdot \left\{ \Gamma h^* \kappa_c^* \tilde{\nabla}^* (H^* + h^*) \right\} - Q^*(x, y, t), \quad (22)$$

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

$$\Gamma = \frac{u_b}{u_Q} = \frac{(\Delta \rho g k_0 / \mu_c)}{(Q / \mathcal{L}^2)}. \quad (23)$$

The nondimensional form of the governing equation for  $h_{res}$ , (11) is

$$\frac{\partial h_{res}^*}{\partial t^*} = \mathcal{C}_{res} \frac{\partial h^*}{\partial t^*} - \frac{q_d^*}{\phi^* [s_{cr} + \mathcal{C}_{sat} (1 - s_{cr})]} \mathbf{1}_{(h_{res}^* > 0)}. \quad (24)$$

## Convective Dissolution

Convective dissolution occurs due to the increased density of the ambient fluid as it becomes saturated with  $\text{CO}_2$ , leading to the development of circulation that replaces saturated ambient with unsaturated ambient within the  $\text{CO}_2$  region. We model this as acting on the interface between the pure-ambient region and either the region of residually trapped  $\text{CO}_2$  (if  $h_{res} > 0$ ) or the region of mobile  $\text{CO}_2$  (if  $h_{res} = 0$  and  $h > 0$ ), via a loss term  $-q_d$ . Following [1, 2], this is given by

$$q_d = 0.12 \left( \frac{\phi_0 \mathcal{C}_{sat} D_{mol}}{\mathcal{L}} \right) \left( \frac{\Delta \rho_a^{sat} g k_0 \mathcal{L}}{\phi_0 \mu_a D_{mol}} \right)^{0.84}, \quad (25)$$

where  $D_{mol}$  is the molecular diffusivity of the  $\text{CO}_2$  in the ambient, and  $\Delta \rho_a^{sat}$  is the density difference between the saturated and unsaturated ambient. The nondimensional convective dissolution term is then given by  $q_d^* = q_d / u_Q$ .

## Description of the Software

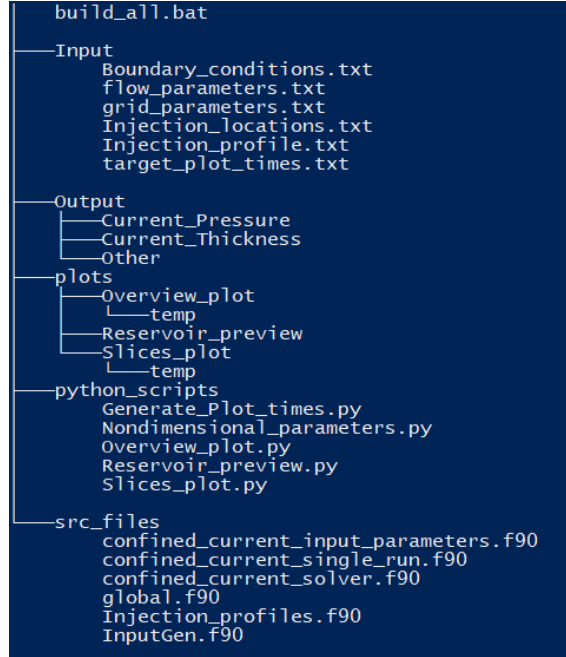


Figure 2: File structure for the Reservoir Simulator codes provided.

The code produced to solve equations (2) and (3) 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.

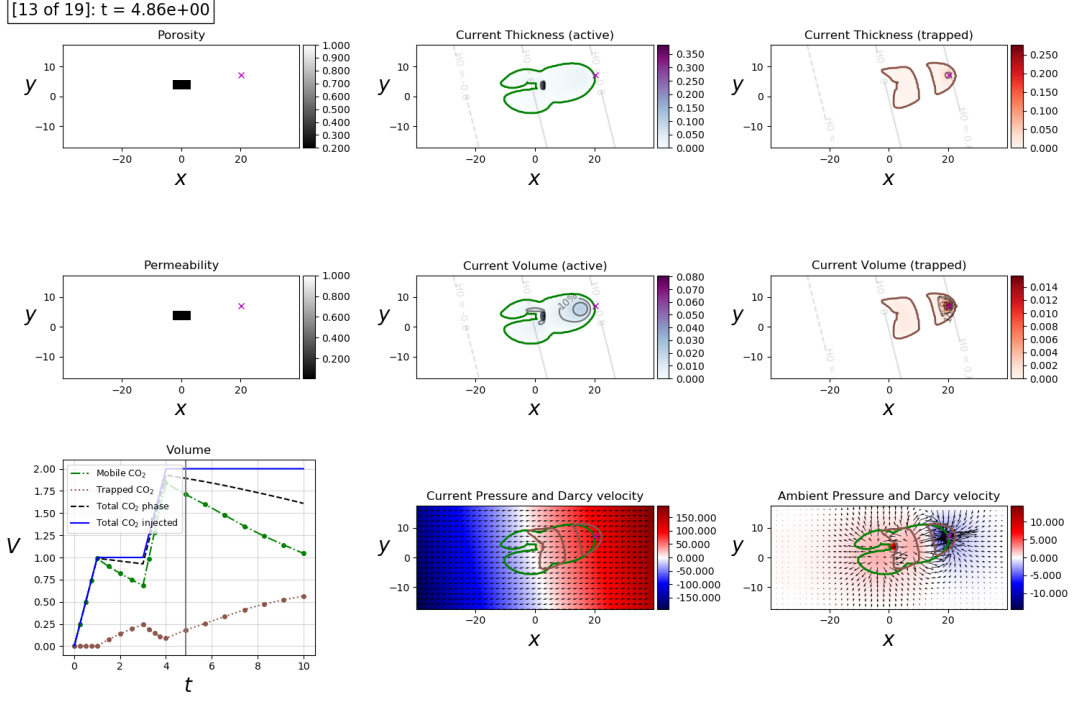


Figure 3: Plot of the mobile current thickness,  $h(x,y,t)$ , the trapped current thickness,  $h_{res}(x,y,t)$ , the corresponding local volumes in those regions, and the respective pressures and Darcy velocities for the mobile CO<sub>2</sub> and ambient phases.

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 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 [\[github url\]](#). 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.

Results from an example calculation are shown in Figure 3. Here, CO<sub>2</sub> is injected into a reservoir with a shallow upward slope to the South West, and a low-porosity region just to the West of the injection well. For this calculation, the permeability is linked to the porosity via the Kozeny-Carman equation. CO<sub>2</sub> is injected at a constant rate for one time unit, paused for two time units, and then injected again from the same location for another time unit. Using typical parameter values, the dimensional timescale for this simulation is  $\mathcal{T} \approx 23$  days, and the entire run corresponds to a physical time of  $\approx 230$  years. A  $200 \times 100$  grid with nondimensional grid spacings  $dx = 0.4, dy = 0.35$  was used, and the full simulation took  $\approx 56$  seconds 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 CO<sub>2</sub> 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

- [1] J. A. Neufeld, M. A. Hesse, A. Riaz, M. A. Hallworth, H. A. Tchelepi, and H. E. Huppert, “Convective dissolution of carbon dioxide in saline aquifers,” *Geophysical research letters*, vol. 37, no. 22, 2010.
- [2] C. W. MacMinn, J. A. Neufeld, M. A. Hesse, and H. E. Huppert, “Spreading and convective dissolution of carbon dioxide in vertically confined, horizontal aquifers,” *Water Resources Research*, vol. 48, no. 11, 2012.