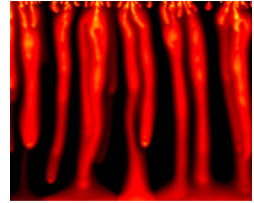# Sinking inside the box

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Convection in a closed porous domain is a temporally and spatially complex flow which evolves over long time scales as the driving buoyancy contrasts are eliminated by mixing. In a contribution that combines numerical, experimental and asymptotic approaches, Hewitt, Neufeld & Lister (*J. Fluid Mech.*, vol. 719, 2013, pp. 551–586) demonstrate that the essential dynamics can be captured by simple 'box' models, both when the buoyancy supply is imposed at the upper boundary and when the domain contains a moving interface between different fluids. This work provides insights into the dynamics and viability of schemes for the geological sequestration of CO_2.

Key words: convection in porous media, geophysical and geological flows, mixing and dispersion

1. Introduction

In recent years, proposals for carbon capture and storage in deep geological formations (Metz *et al.* 2005) have encouraged a resurgence of interest in buoyancy-driven flow through porous media. Although this topic has a substantial history, the focus on processes typical of injected CO_2 rather than of groundwater or oil has prompted new and interesting questions. As well as investigating the many site-specific issues connected with individual injection schemes, it is also essential to develop a fundamental understanding of the processes that control the dispersal of injected CO_2, and in particular of the time scales over which they occur – time scales that may vary from the decades presumed typical of injection schemes and of climate change to the thousands or millions of years more commonly associated with geological processes.

CO_2 is typically injected at pressures and temperatures under which it forms a supercritical fluid that is less dense than the water or oil already to be found in the formation. Consequently, the injectate spreads laterally along impermeable upper boundaries, as has been observed from seismic surveys (Boait *et al.* 2012). However, CO_2 is also somewhat soluble in water, and the solution is denser than either component. In order to understand the fate of injected CO_2, it is therefore necessary to consider vertical flow and mixing driven by negative buoyancy supplied from above. This is a variation on the classical Rayleigh–Bénard convection problem in a porous

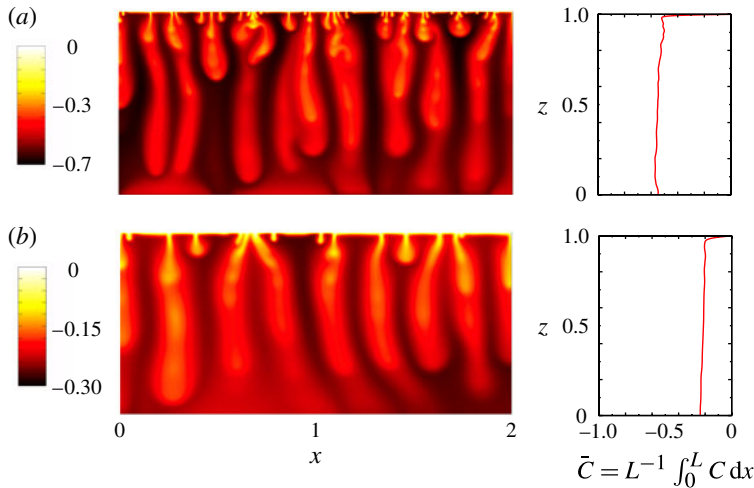† Email address for correspondence: david.pritchard@strath.ac.uk

FIGURE 1. Results from Hewitt *et al.*'s numerical simulations at (*a*) an earlier and (*b*) a later stage of the shutdown process (their figure 4*c*,*d*). Left side: snapshots of the rescaled concentration. Right side: corresponding horizontally averaged concentration profiles.

medium, first investigated by Horton & Rogers (1945). Modern research has focused mainly on the onset of convection following a change in the conditions at a horizontal boundary (e.g. Riaz *et al.* 2006), and on characterizing the complex flow that results at high Rayleigh number, when the buoyancy contrasts are large (e.g. Otero *et al.* 2004). In their contribution, Hewitt, Neufeld & Lister (2013) deploy new insights into this latter question in order to develop a surprisingly simple but effective model of a convective 'filling box' with direct relevance to CO_2 sequestration.

2. Overview

The model system considered by Hewitt *et al.* (2013) consists of a box with impermeable walls, in which a layer of liquid CO_2 overlies a layer of water. CO_2 diffuses across the interface and dissolves into the water, forming a layer of dense fluid at the interface, which drives convection in the underlying water. The Rayleigh number *Ra* associated with this convection is large, and the structure of the convection closely resembles that seen in high-*Ra* convection in a porous Rayleigh–Bénard cell, with small plumes of dense fluid forming in the unstable upper boundary layer and merging into larger 'megaplumes', which descend to the base of the box (figure 1, left side). This convective flow is both spatially and temporally complex, but over long time scales it acts to mix CO_2 fairly evenly through the water layer; thus the average CO_2 content of the water layer gradually increases (figure 1, right side), reducing both the diffusive flux across the interface and the density differences that drive convection. Consequently, over long time scales, the convection gradually shuts down: the key question is how rapidly this occurs.

Three versions of the problem are considered, in increasing order of complexity. In the first, the box initially contains only water, but a constant concentration of dissolved CO_2 is imposed at the upper boundary, so the system represents a 'one-sided' version of the classical Rayleigh–Bénard cell. This allows the dynamics of mixing and shutdown to be investigated independently of the motion of the interface. In the second version, a two-layer 'immiscible' system is considered, in which a pure CO_2

layer overlies the water layer. The interface remains sharp, because the maximum concentration of dissolved CO_2 in the water is lower than that in the pure CO_2 layer, but it is now free to move as mass is transferred across it, so the convection in the water layer is now coupled to a Stefan problem. In the third version, the two fluids are fully miscible, so the sharp interface is replaced by a localized region of steep concentration gradients; the 'interface' may now be identified with the maximum density contour (isopycnal), and it is only below this isopycnal that convection occurs.

The key idea in Hewitt *et al.*'s treatment of these problems is to develop a 'box' model of the evolution of the lower layer. Detailed numerical simulations of the first problem show that the horizontally averaged concentration of dissolved CO_2 is almost constant throughout this region, except in a narrow boundary layer at the top (figure 1, right side). The mass transfer across this boundary layer depends on the convective flow, and may be represented by positing a relationship between the Nusselt number Nu and the Rayleigh number. Assuming a separation between the time scale of mixing and that over which shutdown occurs, this relationship is obtained from the statistically steady behaviour in a Rayleigh–Bénard cell (Hewitt, Neufeld & Lister 2012). A simple parametrization $Nu = \alpha Ra + \beta$ is shown to fit these data well, and is used to close the box model for the evolution of the averaged concentration. The box-model results show convincing agreement with the full numerical simulations.

To tackle the second ('immiscible') problem, assuming that the interface remains horizontal it is necessary only to supplement the box model with a global mass conservation condition to determine the interface location. Again, the box model does a convincing job and, in particular, it captures the gradual ascent of the interface as mass is lost from the upper layer. The third, fully miscible, problem requires further extension of the box model since, although the upper layer of CO_2 is stably stratified, its density evolves through mass diffusion. This is represented in the numerics explicitly, and in the box model by a simplified description of the diffusive boundary layer, still assuming the 'interface' to be flat. Now, the 'interface' first ascends as before, but at long times descends again as the convective flux of CO_2 downwards from the interface is overwhelmed by the diffusive flux above the interface. Even this substantially augmented box model is shown to capture the numerical results well.

However, this is not quite the full story. In systems where the interface is sharp, it resists deformation because of the strongly stabilizing density jump across it. Without a sharp interface, however, the stabilizing density gradient is not able to keep the isopycnals perfectly horizontal, and the 'interface' region may deform. To investigate the miscible problem including deformation, Hewitt *et al.* (2013) combine numerical simulations and experiments carried out using an analogue system. Surprisingly, the deformation of the interface increases the solute flux across it by a factor of up to two or three, and so accelerates the shutdown of convection. This feature cannot be captured quantitatively by the box model, although the qualitative behaviour is unchanged.

3. Future

Hewitt *et al.*'s work bears on the outstanding fundamental question of the structure of convective flow at high Ra. Although scaling relationships between Nu and Ra are now fairly well constrained, it is not entirely clear how they arise. In particular, it is uncertain what controls the size of the megaplumes that dominate the flow field, and how this relates to net heat and mass transfer across the cell (Hewitt *et al.* 2012). This is a natural target for further research.

More specifically, this work provides insight into the dynamics and time scales of vertical CO_2 dispersal, complementing that offered by studies of the lateral

migration of injected fluid and its leakage through the cap rock (e.g. Nordbotten *et al.* 2005). These insights should help extend recent work on the interaction of vertical and horizontal dispersal: how, for example, do mixing and buoyant instability affect the rate at which a current of injected CO_2 intrudes into an aquifer (MacMinn, Szulczewski & Juanes 2011)?

Even for flows dominated at the macroscale by buoyancy forces, the difference between miscible and immiscible fluids may be critical. The trapping of fluid by capillary forces at the pore scale is known to be important (Farcas & Woods 2009), and the unexpectedly large increase in the flux across the interface when it can deform even slightly suggests another key difference, since diffuse miscible interfaces may be more readily deformed than sharp immiscible interfaces. This indicates a potentially serious drawback of the miscible experimental systems that are most readily used as analogues for CO_2 sequestration problems (e.g. Backhaus, Turitsyn & Ecke 2011).

Although many aspects of CO_2 injection have been clarified, the full picture comprising both pore- and formation-scale processes remains to be drawn. It would clearly be valuable to develop laboratory analogues in which capillarity and dissolution play roles more directly comparable with those in CO_2–water systems. Similarly, it is essential that efforts continue to incorporate fundamental insights into field-scale modelling (e.g. Mykkeltvedt & Nordbotten 2012), and to benchmark models such as Hewitt *et al.*'s against field observations. Nevertheless, the encouraging agreement between detailed numerical simulations and the box-model predictions illustrates the ability of physically informed asymptotic descriptions to capture the behaviour of such complex flows.

References

BACKHAUS, S., TURITSYN, K. & ECKE, R. E. 2011 Convective instability and mass transport of diffusion layers in a Hele-Shaw geometry. *Phys. Rev. Lett.* **106**, 104501.

BOAIT, F. C., WHITE, N. J., BICKLE, M. J., CHADWICK, R. A., NEUFELD, J. A. & HUPPERT, H. E. 2012 Spatial and temporal evolution of injected CO_2 at the Sleipner Field, North Sea. *J. Geophys. Res.* **117**, B03309.

FARCAS, A. & WOODS, A. W. 2009 The effect of drainage on the capillary retention of CO_2 in a layered permeable rock. *J. Fluid Mech.* **618**, 349–359.

HEWITT, D. R., NEUFELD, J. A. & LISTER, J. R. 2012 Ultimate regime of high Rayleigh number convection in a porous medium. *Phys. Rev. Lett.* **108**, 224503.

HEWITT, D. R., NEUFELD, J. A. & LISTER, J. R. 2013 Convective shutdown in a porous medium at high Rayleigh number. *J. Fluid Mech.* **719**, 551–586.

HORTON, C. W. & ROGERS, F. T. 1945 Convection currents in a porous medium. *J. Appl. Phys.* **16**, 367–370.

MACMINN, C. W., SZULCZEWSKI, M. L. & JUANES, R. 2011 CO_2 migration in saline aquifers. Part 2. Capillary and solubility trapping. *J. Fluid Mech.* **688**, 321–351.

METZ, B., DAVIDSON, O., DE CONINCK, H. C., LOOS, M. & & MEYER, L. 2005 *IPCC Special Report on Carbon Dioxide Capture and Storage*. Cambridge University Press.

MYKKELTVEDT, T. S. & NORDBOTTEN, J. M. 2012 Estimating effective rates of convective mixing from commercial-scale injection. *Environ. Earth Sci.* **67**, 527–535.

NORDBOTTEN, J. M., CELIA, M. A., BACHU, S. & DAHLE, H. K. 2005 Semianalytical solution for CO_2 leakage through an abandoned well. *Environ. Sci. Technol.* **39**, 602–611.

OTERO, J., DONTCHEVA, L. A., JOHNSTON, H., WORTHING, R. A., KURGANOV, A., PETROVA, G. & DOERING, C. R. 2004 High-Rayleigh-number convection in a fluid-saturated porous layer. *J. Fluid Mech.* **500**, 263–281.

RIAZ, A., HESSE, M., TCHELEPI, H. A. & ORR, F. M. 2006 Onset of convection in a gravitationally unstable diffusive boundary layer in porous media. *J. Fluid Mech.* **548**, 87–111.