High Rayleigh Number
Convection in a Porous Medium

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This thesis is the result of my own work and includes nothing which is the outcome of work done in collaboration. All the work has been carried out over the course of my doctorate under the supervision of Professor John Lister and Dr. Jerome Neufeld, at the Department of Applied Mathematics and Theoretical Physics, University of Cambridge.

The material contained in chapters 2, 3, 4, 5, 6, and 7 has been published or submitted for publication, as noted at the start of each chapter.
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“Isn’t it splendid to think of all the things there are to find out about? It just makes me feel glad to be alive - it’s such an interesting world. It wouldn’t be half so interesting if we knew all about everything, would it?”

L. M. Montgomery, *Anne of Green Gables*


“Oil poured under water is drawn up to the surface on top of the water. Water poured on top of oil sinks below the oil. They are acted on by their respective densities, they seek their own place...”

St. Augustine, *Confessions, 13* (ix)
Convection in a fluid-saturated porous medium is of widespread importance in a variety of geophysical and industrial settings. In this thesis, a range of porous convective systems are investigated at high Rayleigh number $Ra$, using numerical, theoretical, and experimental techniques. The thesis begins with an introductory chapter in which the relevance of this work to the long-term geological storage of CO$_2$ is discussed.

In chapter 2, well resolved direct numerical simulations of two-dimensional Rayleigh–Bénard convection in a porous medium (‘Rayleigh–Darcy convection’) are presented for Rayleigh numbers $Ra \leq 4 \times 10^4$. Measurements of the convective flux, as described by the Nusselt number $Nu$, for $1300 \leq Ra \leq 4 \times 10^4$ are extremely well fitted by $Nu = \alpha Ra + \beta$, for $\alpha = 6.9 \times 10^{-3}$ and $\beta = 2.75$, which indicates that the linear classical scaling $Nu \sim Ra$ is attained asymptotically. The flow dynamics are analysed, and the interior of the vigorously convecting system is shown to be increasingly well-described as $Ra \to \infty$ by a steady columnar ‘heat-exchanger’ model with a single horizontal wavenumber $k$ and a linear background temperature field. Numerical measurements are approximately fitted by $k \sim Ra^{0.4}$.

In chapter 3, the stability of this heat-exchanger flow is examined, with the aim of uncovering the mechanism that controls the columnar wavelength. A Floquet linear-stability analysis and a matched asymptotic expansion reveal that the flow is always unstable in an unbounded domain. The results are applied to the columnar flow in a Rayleigh–Darcy cell at high $Ra$: a balance of time scales for growth and propagation suggests that the flow is unstable for horizontal wavenumbers $k$ greater than $k \sim Ra^{5/14}$ as $Ra \to \infty$. This stability criterion is consistent with the numerical measurements of $k$ presented in chapter 2.

Geological porous formations are commonly interspersed with thin low-permeability layers. In chapter 4, statistically steady high-$Ra$ porous convection in the presence of a thin, low-permeability, horizontal layer is investigated. The flow is found to depend only on the ratio of the height and relative permeability of the interior layer, given by the impedance $\Omega$. As $\Omega$ is increased, the dominant
horizontal lengthscale of the flow increases, and, surprisingly, $Nu$ can increase before decreasing markedly for larger values of $\Omega$. The dependence of the flow on $Ra$ is explored, and simple one-dimensional models are developed to describe some of the observed behaviour.

Convection in a closed domain, driven by a dense buoyancy source along the upper boundary, soon starts to wane due to the increase in the average interior density. In chapters 5 and 6, theoretical and numerical models are developed of the subsequent long period of shutdown of convection. The relationship between this slowly evolving ‘one-sided’ system and statistically steady ‘two-sided’ Rayleigh–Darcy convection is investigated. Measurements of $Nu(Ra)$ from chapter 2 are used in simple box models of the one-sided shutdown system, which give excellent agreement with numerical simulations of the system. The dynamical structure of shutdown is also accurately predicted by measurements from a Rayleigh-Darcy cell. These ideas are extended to model the shutdown of convection in systems that comprise two fluid layers, with an equation of state such that the solution that forms at the (moving) interface is more dense than either layer. The two fluids are either immiscible or miscible. Theoretical box models compare well with numerical simulations in the case of a flat interface between the fluids. Experimental results from a Hele–Shaw cell and numerical simulations both show that interfacial deformation can dramatically enhance the convective flux for miscible fluids.

In chapter 7, well resolved direct numerical simulations of three-dimensional Rayleigh–Darcy convection are presented, and measurements of $Nu$ for $1750 \lesssim Ra \lesssim 2 \times 10^4$ are very well described by the relationship $Nu = \alpha_3 Ra + \beta_3$, for $\alpha_3 = 9.6 \times 10^{-3}$ and $\beta_3 = 4.6$. The magnitude of the flux is roughly 40% higher than in two dimensions. The flow dynamics are analysed, and the interior flow is again found to be increasingly well described by a heat-exchanger model. Measurements of the dominant wavenumber $k$ are approximately fitted by $k \sim Ra^{0.52}$, which is a distinctly stronger scaling than in two dimensions.

This work is summarized in chapter 8, and the applicability of the results to the convective dissolution of geologically sequestered CO$_2$ in a saline aquifer is discussed.
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Chapter 1

Introduction

Convection plays a central role in an enormous range of environmental processes (Linden, 2000). It is responsible for much of the Earth’s weather: on a large scale, convection drives atmospheric and oceanic circulation; on a smaller scale, the formation of clouds and storms. Flow in the Earth’s mantle, which fuels the geodynamo and the motion of tectonic plates, is driven by convection. The freezing of the polar oceans, the motion of volcanic plumes, and the rate at which a kettle boils or a radiator heats a room are all controlled by convection. In addition, from a mathematical viewpoint, convection is a complex nonlinear process that provides an archetypal fluid-dynamical setting for the study of chaotic and turbulent dynamics, bifurcations, and emergent patterns (Cross & Hohenberg, 1993; Kadanoff, 2001).

Convection can be broadly defined as the motion of fluid due to gravity acting on an unstable density profile. The density of a fluid is determined by the distribution of internal energy, which is typically set by differences in temperature or in the concentration of a solute. If dense fluid lies above less dense fluid, such that the fluid is unstably stratified, then, under the action of gravitational forces, the dense fluid sinks and the less dense fluid rises; potential energy is converted into kinetic energy, and convection ensues.

In this thesis, we explore in detail a range of physically motivated problems involving convection in a fluid-saturated porous medium. Porous convection has widespread importance in a number of geophysical and industrial processes (Nield
1. INTRODUCTION

& Bejan, 2006). Heat from deep within the Earth drives underground hydrothermal convection that is crucial for the extraction of geothermal energy (Cheng, 1978), while convective currents in both the continental and the oceanic lithosphere play a major role in the heat budget of the Earth (Stein, 1995; Davis et al., 1997; Cherkaouim & Wilcock, 1999). Density differences that drive convection may also be due to variations in salinity, as in the flow of saline groundwater due to evaporation from the surface (Wooding et al., 1997a, b). The convective gravity drainage of brine from sea ice in the polar oceans has important implications for global oceanic circulation and mixing (Notz & Worster, 2009), while a similar process is responsible for the formation of freckles in industrial alloy castings (Fowler, 1985). In recent years, there has been particular interest in the effect of porous convection on the long-term storage of CO$_2$ by geological sequestration (Bachu, 2008; Orr Jr., 2009; Bickle, 2009; Huppert & Neufeld, 2014), which has been widely proposed as a technological means of stabilizing the rising concentration of atmospheric CO$_2$ (Metz et al., 2005). The importance of convection for the long-term sequestration of CO$_2$ is the primary motivation for this work, and is discussed in more detail in §1.1 below.

For the sake of clarity, throughout this thesis we refer to convection in a porous medium as ‘porous convection’, in contrast to ‘pure-fluid’ convection, not in a porous medium. Porous convection, which is governed by Darcy’s law rather than the full Navier–Stokes equations, provides a more tractable system than pure-fluid convection in which to study the nonlinear dynamics and pattern formation of convective flows (Graham & Steen, 1994), owing primarily to the absence of inertia in Darcy’s law.

The vigour of convection and the associated dynamics of the flow depend in large part on the driving strength of buoyancy and the inhibiting dissipative effects of diffusion and viscosity in the system. The ratio of driving and inhibiting effects is given by a dimensionless parameter called the Rayleigh number $Ra$. The aim of this thesis is to provide a thorough exploration of convection in a porous medium at high $Ra$, in a range of physical systems. In particular, we examine the complex nonlinear dynamics of high-$Ra$ convection, and characterize the dependence of the convective transport of buoyancy, which is perhaps the most physically important measure of convection, on the physical parameters and geometry of different sys-
tems. We also develop physically motivated reduced models of convection that can be applied to different systems.

In §1.1, we outline the details of geological CO$_2$ sequestration and the importance of convective transport for the long-term security of sequestered CO$_2$. In §1.2, we discuss the basic equations and modelling assumptions which underlie the work throughout this thesis, and in §1.3 we give a brief overview of some previous studies of porous convection. The structure of the thesis is laid out in §1.4.

1.1 Geological CO$_2$ sequestration

There has been recent resurgent interest in the subject of convection in a porous medium, owing to its relevance to the long-term storage of geologically sequestered CO$_2$ (Bachu, 2008; Orr Jr., 2009; Bickle, 2009; Huppert & Neufeld, 2014). Geological sequestration entails the storage of pressurized CO$_2$ in underground porous rock. With growing global demand for energy, it seems probable that sequestration will need to play a major role as a part of attempts to curb the rising anthropogenic emissions of CO$_2$, which are now higher than 30 gigtons a year (Metz et al., 2005; Friedlingstein et al., 2010). Estimates of the subterranean storage capacity of CO$_2$ range from 1700 to 14000 gigatons or higher (Metz et al., 2005; Orr Jr., 2009). This wide range reflects both the large uncertainty in the properties that constitute a suitable storage site, and the lack of sufficiently accurate geological data of potential sites. Sequestration has been tested on large scales in various locations around the world; the longest-running industrial example is at the offshore Sleipner gas fields in the North sea, where roughly one million tons of CO$_2$ have been sequestered in the nearby Utsira sand reservoir every year since 1996 (Kongsjorden et al., 1997; Boait et al., 2012).

After capturing and compressing CO$_2$ into a supercritical liquid at its source (e.g. a power plant), geological storage is achieved by injecting the supercritical CO$_2$ down into deep porous formations that are typically located at depths $\gtrsim 800 \text{m}$ below the Earth’s surface. The most abundant potential storage sites are deep saline aquifers (brine-saturated porous rock), and it is these that are the focus of this work. Other possible sites include depleted oil and gas reservoirs, coal beds, and seabed sediments. Under storage conditions in a saline aquifer,
supercritical CO$_2$ is significantly less dense (\(\sim 700 \text{ kg m}^{-3}\)) than the ambient brine (\(\sim 1000 \text{ kg m}^{-3}\)), and will rise through the aquifer after injection.

From the point of view of both viability and safety, it is essential that the long-term (\(\sim 10^4 \text{ years}\)) underground storage of sequestered CO$_2$ can be assured. Therefore, since the injected CO$_2$ is buoyant, the presence of a bounding impermeable caprock (typically a shale or clay layer) below which the CO$_2$ can pool and spread under gravity, is vital for any storage site. This ‘topographic’ trapping of CO$_2$ may not necessarily result in secure long-term storage, because fractures in the caprock or migration due to its topography can lead to undesired leakage of the buoyant CO$_2$ plume (Pritchard, 2007; Neufeld et al., 2011; Vella et al., 2011). There are, however, other mechanical and geochemical processes which take place over different timescales. Three main processes are: ‘residual trapping’, in which small pockets of CO$_2$ are immobilized in the brine by capillary forces; ‘mineral trapping’, in which chemical reactions with minerals in the host rock lead to the precipitation of CO$_2$; and ‘dissolution trapping’, in which CO$_2$ dissolves into the host brine (Metz et al., 2005; Huppert & Neufeld, 2014).

Residual or capillary trapping, well known to oil engineers and hydrologists (Bear, 1988), takes place whenever a porous medium is initially saturated with one fluid, which is then displaced by another immiscible fluid. Such is the case with brine and CO$_2$, where capillary forces act to trap pockets of CO$_2$ in the wake of the injected current over relatively short time scales (Hesse et al., 2008; Golding et al., 2011). Mineral trapping, on the other hand, is anticipated to take place over extremely long time scales (typically much longer than the timescales over which the injected CO$_2$ might leak to the surface), and is very dependent on the properties of the host rock (Orr Jr., 2009).

Dissolution trapping (Bolster, 2014), or convective dissolution, forms the primary motivation for this thesis. Supercritical CO$_2$ is roughly 3 – 5% soluble by weight in brine under typical storage conditions (van der Meer, 2005). Although CO$_2$ is significantly less dense than brine, this weak dissolution forms a solution that is denser than brine. The dense solution is, therefore, unstable to downwelling convection, which enhances the transport of CO$_2$ away from the injected current, and leads to more secure storage. Geochemical field observations in natural CO$_2$ reservoirs suggest that convective dissolution provides a very significant
and persistent mechanism for the transport of CO$_2$ (Gilfillan et al., 2009; Bickle & Kampman, 2013).

Typical values of the Rayleigh number (which determines the strength of convection and is more formally defined in §1.2.3 below) for convective dissolution can vary significantly, and can be very high owing to the relatively small diffusivity of CO$_2$ in brine ($\approx 10^{-9}$ m$^2$s$^{-1}$), the potentially large permeability of the rock ($10^{-15}$ to $10^{-11}$ m$^2$), and the large spatial scales of subsurface saline aquifers ($\sim 10^2$ m). These parameter values give rise to Rayleigh numbers in the range $10 < Ra < 10^5$. If $Ra$ is small, convective dissolution will not have a significant impact; for $Ra > O(10^3)$, on the other hand, convective dissolution is expected to play a major role in the long-term stability of stored CO$_2$. The range $Ra > O(10^3)$ is the focus of this thesis.

1.2 Governing equations and modelling assumptions

1.2.1 Darcy velocity and Darcy’s law

The porosity $\phi$ of a porous medium is defined as the fraction of the medium that is made up of pore space. Flow in the pore space is typically modelled by taking the average of quantities like the local velocity and pressure in each pore over a representative volume that encapsulates many pores (known as a ‘representative elementary volume’ or REV; Bear 1988). The interstitial velocity $v$ is defined to be the mean velocity over all the pore space in a REV. The average volume flux or Darcy velocity, $u$, is the average velocity over both the solid matrix and the pore space in a REV, and is therefore given by $u = \phi v$.

We assume that the porosity $\phi$ is constant and the fluid is incompressible, which gives
\[ \nabla \cdot u = 0. \tag{1.1} \]

The Darcy velocity $u$ is governed by Darcy’s law (Bear, 1988; Phillips, 2009), which relates the driving pressure and buoyancy forces to the viscous drag imparted by the medium on the pore scale. The driving forces are given by the pressure gradient

\[ \nabla \cdot u = 0. \]
1. INTRODUCTION

\[-\nabla p \text{ and buoyancy } - \rho \mathbf{g}, \]

where \( p \) is the pressure, \( \rho \) is the density, and \( \mathbf{g} \) is the gravitational acceleration. The viscous drag scales with \( \mu \nabla^2 \mathbf{v} \sim \mu \mathbf{v} / \delta_p^2 \), where \( \mu \) is the viscosity of the fluid and \( \delta_p \) is the typical lengthscale of the pores. A balance of driving and drag forces gives Darcy’s law,

\[
\mathbf{u} = - \frac{K}{\mu} (\nabla p - \rho \mathbf{g}),
\]

where \( K \sim \phi \delta_p^2 \) is the permeability. As well as depending on both the fraction of pore space (\( \phi \)) and the typical pore size (\( \delta_p \)), the permeability typically depends on properties of the complex pore network, like the tortuosity and the ‘connectedness’ of the pores.

Darcy’s law (1.2) rests on a number of assumptions. The medium is assumed to be fully saturated by the fluid, so there are no effects of partial saturation. On the pore scale, inertia is assumed to be negligible compared to viscous drag, such that the pore-scale Reynolds number \( Re_p \) is small\(^1\). The lengthscales of the flow are also assumed to remain larger than the typical scale of the REV. The latter two assumptions are discussed in more detail in §1.2.4 below.

Throughout this thesis, we also make the assumption that density variations are small relative to the magnitude of the density itself; this is the (porous equivalent of the) Boussinesq approximation. Mathematically, the assumption is contained within the condition of incompressibility (1.1): variations in the density affect the buoyancy term in (1.2), but have a negligible effect on the velocity via conservation of mass.

1.2.2 Transport of solute or heat

The equation of state describes the dependence of the density \( \rho \) either on the concentration \( C \) of a solute, \( \rho(C) \) (as in the case of \( \text{CO}_2 \) and brine), or on the temperature \( T \), \( \rho(T) \). In the former case, the concentration field in the liquid

\(^1\)There have been numerous attempts to extend Darcy’s law or to re-derive the momentum equation for \( Re_p > O(1) \). These include simply appending inertial terms to Darcy’s law (e.g. Wooding 1957), or adding a quadratic drag term (the ‘Forchheimer equation’; see e.g. Joseph et al. 1982). In general, it is difficult to find a robust physical basis for these alternative momentum equations, and they are not considered in this thesis.
phase of the medium evolves by advection and diffusion, as described by
\[ \phi \frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla C = \phi \nabla \cdot (D \nabla C), \]  
(1.3)
where \( D \) is the solutal diffusivity, which we assume is constant.

In the case of thermal convection, one needs to consider the conservation of heat in both the solid and the liquid phases of the medium, which are coupled by the transfer of heat between the phases. In general, the transport equations for the temperature \( T_s \) of the solid phase and \( T_l \) of the liquid phase are given by
\[ (1 - \phi) \rho_s c_s \frac{\partial T_s}{\partial t} = (1 - \phi) \nabla \cdot (\alpha_s \nabla T_s) + K (T_s - T_l), \]  
(1.4a)
\[ \phi \rho_l c_l \frac{\partial T_l}{\partial t} + \rho_l c_l \mathbf{u} \cdot \nabla T_l = \phi \nabla \cdot (\alpha_l \nabla T_l) - K (T_s - T_l), \]  
(1.4b)
where \( \rho_{s,l}, c_{s,l}, \) and \( \alpha_{s,l} \) are the density, the specific heat capacity, and the thermal conductivity of the solid and liquid phases, respectively, and \( K \) is the volumetric heat-transfer coefficient between the phases. Throughout this thesis, we will make the simplifying assumption that there is no heat transfer to the solid phase \((K = 0)\); as such, the temperature of the liquid and solid are decoupled. The validity of this assumption is discussed in §1.2.4 below. We therefore need only model the evolution of the temperature field in the liquid region \((1.4b)\), which, on setting \( T_l = T \), reduces to
\[ \phi \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \phi \nabla \cdot (\kappa \nabla T). \]  
(1.5)
Here, \( \kappa = \alpha_l / (\rho_l c_l) \) is the thermal diffusivity of the liquid, which we assume is constant. Equations (1.3) and (1.5) therefore have an identical form, and so, under the assumption of negligible heat transfer to the solid phase, any analysis of thermal convection (for which \( \rho \) is a function of \( T \) alone) will be directly applicable to solutal convection (for which \( \rho \) is a function of \( C \) alone). For simplicity, both for solutal and thermal convection, we have neglected the effects of dispersion in the medium.
1.2.3 Dimensionless parameters

The ratio of the driving strength of buoyancy to the dissipative effects of diffusion and viscosity is given by the Rayleigh number $Ra$, defined in the case of thermal convection by

$$Ra = \frac{UH}{\phi\kappa} = \frac{\Delta \rho g \kappa H}{\phi\kappa\mu}, \quad (1.6)$$

where $U = \Delta \rho g K / \mu$ is the buoyancy velocity, $\Delta \rho$ is the driving density difference and $H$ is a typical length scale. For solutal convection, $\kappa$ is replaced by $D$ in (1.6).

The Rayleigh number can alternatively be thought of as the ratio of diffusive and convective time scales; in this sense, it is also a Peclét number. In this thesis, we focus on convective systems in which $Ra$ is large, and thus advection, rather than diffusion, provides the dominant transport mechanism.

The dimensionless measure of the convective transport, or flux, of buoyancy is given by the Nusselt number $Nu$. The Nusselt number is the ratio of the total flux $F^*$ of buoyancy to the diffusive flux that would occur if there were no convection. In the case of thermal convection driven by a temperature contrast $\Delta T$ across a depth $H$, the Nusselt number is given by

$$Nu = \frac{F^*}{\phi\kappa(\Delta T/H)}. \quad (1.7)$$

If there is no convection, $Nu = 1$. Based on dimensional analysis, $Nu = Nu(Ra)$, and the form of this relationship has been widely studied. One of the main results presented in chapter 2 is the characterization of this relationship for $Ra \gg 1$.

For solutal convection, the Nusselt number is sometimes known as the Sherwood number; for simplicity, throughout the thesis it will be referred to as the Nusselt number.

1.2.4 Discussion of assumptions at high $Ra$

We recall that a number of assumptions lie behind Darcy’s law (1.2). Two assumptions need particular consideration when the Rayleigh number is large. First, viscous terms are assumed to dominate inertial terms on the pore-scale; i.e., the pore-scale Reynolds number $Re_p$ is assumed to be small. Although this condition
cannot hold for arbitrarily large values of $Ra$, because $Ra$ is proportional to the buoyancy velocity, it can hold for $Ra \gg 1$ provided the pore scale remains small. More formally, we note that the typical pore size $\delta_p$ scales with $K^{1/2}$, and define both the Darcy number $Da = K/H^2 \sim (\delta_p/H)^2$ to be a dimensionless measure of the pore size, and the Prandtl number $Pr = \nu/\kappa$, where $\nu = \mu/\rho$, to be the ratio of viscous and thermal (or solutal) diffusivity. An estimate for the pore-scale Reynolds number gives $Re_p \sim U\delta_p/\nu \sim \phi Ra Da^{1/2}/Pr$, where $U$ is the buoyancy velocity. Darcy’s law is expected to remain valid if

$$Re_p \sim \frac{\phi Ra Da^{1/2}}{Pr} < O(1).$$

(1.8)

Note that, unlike for convection in a pure fluid (see, e.g. Linden 2000), $Pr$ does not enter the governing dimensionless equations for porous convection, and so the only role it plays is in setting the range over which Darcy’s law applies via (1.8).

Second, Darcy’s law is based on an assumption that the lengthscales of the flow are larger than the scale of the REV, and therefore much larger than the pore scale. At high $Ra$, the smallest lengthscales are diffusive, and are anticipated to scale like $H/Ra$ (see chapter 2). A comparison of the diffusive lengthscale with the pore scale $\delta_p \sim K^{1/2}$ suggests that Darcy’s law should remain valid if

$$Ra Da^{1/2} \ll O(1).$$

(1.9)

Throughout this thesis, we assume that (1.8) and (1.9) apply. For a CO$_2$ sequestration site, typical values of $Da$ lie in the range $10^{-19} \lesssim Da \lesssim 10^{-15}$, while $Pr > 1$, which suggests that Darcy’s law remains valid for at least $Ra \lesssim 10^6$. The majority of geophysical values of $Ra$ in a porous medium, and all the values considered in this thesis, lie below this bound.

The work in this thesis is, therefore, directly relevant to solutal convection at high $Ra$. To aid intuition, and in common with many previous studies of convection, however, we will use the terminology of thermally driven convection, except in chapters 5 and 6. As mentioned above, analysis of thermal convection is equally applicable to solutal convection under the assumption that there is no heat transfer to the solid phase of the medium. It should be noted that, in a physical
system, this assumption is likely to break down at large values of $Ra$, particularly when the temperature contrasts are large. However, while the specific physics of a particular system may vary, the results detailed in this thesis provide the tools to systematically understand the dynamics of high-Rayleigh-number porous convection in a variety of physical settings.

1.3 Rayleigh–Bénard convection at high Rayleigh number

The Rayleigh–Bénard cell provides a canonical system for the study of convection. The cell has lower and upper boundaries held at fixed hot and cold temperatures, respectively, and thus attains a statistically steady state, which allows for accurate characterization of both the convective flux through the system and the associated nonlinear dynamics. Of particular physical importance is the relationship between the convective flux of buoyancy, as described by the Nusselt number $Nu$, and the relative ‘strength’ of convection, as described by the Rayleigh number $Ra$. Below, we briefly discuss convection in a pure fluid Rayleigh–Bénard cell at high $Ra$, before providing an overview of convection in a porous medium, which will form the basis of this thesis.

1.3.1 Convection in a pure fluid Rayleigh-Bénard cell

The study of turbulent convection in a pure-fluid Rayleigh–Bénard cell has a long and rich history, and remains an enduring and active subject of fundamental interest in fluid dynamics (Siggia, 1994; Ahlers et al., 2009; Chillà & Schumacher, 2012). Characterization of the dependence of the convective flux $Nu$ on the Rayleigh number $Ra$ and the Prandtl number $Pr = \nu/\kappa$ is of particular interest. A very brief overview of the subject is given below.

The famous ‘classical’ scaling argument (Malkus, 1954; Howard, 1964) for the heat flux suggests that, for sufficiently large $Ra$, the dimensional heat flux becomes independent of the height $H$ of the domain, because the structure of the flow is dominated by plume shedding from thin boundary layers into a turbulent interior.
Equivalently, this argument can be thought of as a ‘marginally stable’ boundary-layer theory: diffusive boundary layers grow until they are unstable (based on a local boundary-layer Rayleigh number reaching a critical value), at which point heat is rapidly stripped from the layer into the interior, and the boundary layers grow again (see e.g. Graham & Steen 1994). This argument predicts a scaling of $Nu \sim Ra^{1/3}$ in a pure fluid.

However, the turbulent nonlinear dynamics of pure-fluid convection give rise to a system of more complexity than this simple argument suggests, and recent reviews by Ahlers et al. (2009) and Chillà & Schumacher (2012) provide a comprehensive overview of the different regimes of convection. For example, the widely cited theory of Castaing et al. (1989) suggested that shear in the boundary layers due to large-scale circulation could re-introduce a dependence on the height $H$ at larger $Ra$, to give a reduced scaling $Nu \sim Ra^{2/7}$. For very large values of $Ra$, a transition from the classical scaling described above to an ‘ultimate’ asymptotic scaling regime of $Nu \sim Ra^{1/2}$,\(^1\) in which shear-driven turbulence in the boundary layers gives an enhancement of the flux, has been theorised (Kraichnan, 1962; Spiegel, 1971) and predicted by rigorous upper bounds (Doering & Constantin, 1996; Plasting & Kerswell, 2003). According to this theory, for sufficiently large values of $Ra$ the flow is dominated by turbulence in the bulk; neither viscous or thermal boundary layers play an explicit role in the heat flux, which becomes independent of both the viscosity $\nu$ and the diffusivity $\kappa$.

There have been numerous experimental investigations of high-$Ra$ pure-fluid Rayleigh-Bénard convection. In particular, there have been a number of experiments using cryogenic helium gas (e.g. Heslot et al. 1987; Chavanne et al. 1997; Niemela et al. 2000; Roche et al. 2001; He et al. 2012), which has an extremely small kinematic viscosity giving rise to very large values of $Ra$. The evidence from these studies is not conclusive: for example, Niemela et al. (2000) found no transition to the ultimate state of convection up to $Ra = 10^{17}$, while Chavanne et al. (1997) appeared to find a transition near $Ra = 2 \times 10^{11}$. More recently, He et al. (2012) observed an apparent transition to the ultimate regime at $Ra \approx 5 \times 10^{14}$.

\(^1\)Non-trivial corrections to the theory, allowing for a viscous sub-layer, give a dependence on the Reynolds number, which corresponds to a reduced scaling exponent in $Nu(Ra)$ of $\sim 0.4$ (Grossmann & Lohse, 2011).
In addition, open questions remain as to the role of the Prandtl number $Pr$ on the convective dynamics (e.g. Roche et al. 2002; Xia et al. 2002; Calzavarini et al. 2005). In particular, the relationship $Nu(Pr)$ is not well understood in the ‘ultimate’ high-$Ra$ regime of convection. Experiments with cryogenic helium are complicated by the vanishing thermal diffusivity of the gas near to the critical point, which makes it difficult to vary $Ra$ and $Pr$ independently for very large values of $Ra$ (see, e.g. Niemela et al. 2000), while different theoretical arguments predict quite different dependences in this regime (Ahlers et al., 2009).

1.3.2 Convection in a porous Rayleigh–Bénard (‘Rayleigh–Darcy’) cell

Convection in a porous Rayleigh–Bénard cell has received rather less attention than its pure-fluid counterpart, particularly at high values of $Ra$. In order to avoid confusion with the pure-fluid Rayleigh–Bénard cell, throughout this thesis we refer to this porous cell as a Rayleigh–Darcy cell. Porous convection is mathematically rather simpler than pure fluid convection, primarily owing to the linearity of Darcy’s law, which also results in a system that is independent of the Prandtl number $Pr$.

The Rayleigh–Darcy cell is a ‘two-sided’ convective system, because there is convective transport away from both the upper and the lower boundaries. Natural convective systems in porous media are often driven by a source of buoyancy on only one boundary; we refer to such systems as ‘one-sided’. Convection in one-sided systems is discussed in detail in chapters 5 and 6.

Convection in a two-dimensional Rayleigh–Darcy cell for low and moderate values of $Ra$ ($Ra \lesssim 1300$) has been the subject of various studies (see Nield & Bejan 2006). For $Ra < Ra_{\text{crit}} = 4\pi^2$, a vertically linear and horizontally uniform temperature field is stable; there is no flow (Lapwood, 1948), and all the buoyancy transfer is diffusive ($Nu = 1$). For $4\pi^2 < Ra \lesssim 382$, the convective flow takes the form of large-scale convective rolls, which are steady and stable. The Nusselt number increases with $Ra$, and the relationship $Nu(Ra)$ can be well predicted by a weakly non-linear analysis (Nield & Bejan, 2006). For $382 \lesssim Ra \lesssim 1300$, convective instabilities in the boundary layers result in a series of bifurcations that
perturb, but do not completely break down, the background cellular structure of the flow (Robinson & O'Sullivan, 1976; Kimura et al., 1986; Graham & Steen, 1994). The perturbations take the form of ‘dripping’ plumes which grow from the boundary layers but are washed around with the background circulation. The growth and migration of these plumes gives rise to periodic, doubly periodic, or chaotic oscillations in the time-dependent Nusselt number. The dynamics exhibit significant hysteresis in this regime, and so the values of $Ra$ at which bifurcations occur are approximate.

Above $Ra \approx 1300$, the quasisteady background rolls are completely broken down by the growth of destabilizing plumes from the upper and lower boundaries (Otero et al., 2004). The change in the dynamical structure marks the transition to the ‘turbulent’ high-$Ra$ regime\(^1\).

In a porous medium, the classical scaling argument for $Nu$ discussed above predicts a linear scaling $Nu \sim Ra$ for large values of $Ra$. In fact, the ‘ultimate’ scaling argument, which suggests that the flux is independent of $\kappa$, also gives a linear scaling. In chapter 2, we examine the high-$Ra$ regime in a two-dimensional Rayleigh–Darcy cell in detail, and compare the measurements of the flux with this prediction. In chapter 7, we study the three-dimensional Rayleigh–Darcy cell at high $Ra$.

### 1.4 Layout

This thesis is laid out as follows. In chapter 2, we present direct numerical simulations of convection in a two-dimensional Rayleigh–Darcy cell for $Ra \leq 4 \times 10^4$, and examine in detail the convective dynamics at high $Ra$. Measurements\(^2\) of the Nusselt number $Nu$ are extremely well fitted in the high-$Ra$ regime ($Ra \gtrsim 1300$) by an expression of the form $Nu = \alpha Ra + \beta$, where $\alpha = 6.9 \times 10^{-3}$ and $\beta = 2.75$. This fit strongly suggests that the linear classical scaling $Nu \sim Ra$ (discussed above) is attained asymptotically. We show that the interior of the vigorously

\(^1\)The flow is turbulent in the sense that the dynamics are spatially and temporally chaotic on a range of scales, rather than in the sense of a turbulent energy cascade.

\(^2\)Note that, throughout this thesis, the term ‘measurements’ is used to describe data from numerical calculations, as well as to describe measurements from laboratory experiments.
1. INTRODUCTION

The convecting system is dominated by persistent vertical columnar flow. Remarkably, the columnar flow is increasingly well described as \( Ra \to \infty \) by a steady columnar ‘heat-exchanger’ solution with a single horizontal wavenumber \( k \). The wavenumber increases with \( Ra \), and measurements of \( k \) are approximately fitted by \( k \sim Ra^{0.4} \).

In chapter 3, we examine the stability of columnar convection in a porous medium. This work is motivated by the persistent quasisteady columnar flow observed in the previous chapter, and by the unexplained physical mechanism that controls the horizontal wavenumber \( k \) of this flow. We investigate the hypothesis that the stability of the columnar flow provides the mechanism for wavelength selection, by studying the linear stability of a steady unbounded ‘heat-exchanger’ flow. The dimensionless flow comprises interleaving vertical columns of horizontal wavenumber \( k \) and amplitude \( \hat{A} \) that are driven by a steady balance between vertical advection of a background linear density stratification and horizontal diffusion between the columns. We use a Floquet linear-stability analysis to show that the unbounded flow is always unstable, and determine the largest growth rate in the limit \( Ra \gg k/\hat{A} \) using a matched asymptotic expansion. The most unstable perturbation in this limit takes the form of vertically propagating pulses on the background columns. Direct numerical simulations show that the non-linear evolution of the instability results in a coarsening of the columnar flow. We apply the results of the stability analysis to the columnar flow in a two-dimensional Rayleigh–Darcy cell, by balancing time scales of propagation and growth. This scaling argument suggests that the columnar flow would be unstable if the wavenumber \( k \) were greater than \( k \sim Ra^{5/14} \), as \( Ra \to \infty \). A correction to this scaling for finite \( Ra \) gives a slightly stronger dependence on \( Ra \), in good agreement with the numerical measurements from chapter 2. The agreement demonstrated suggests that stability of the columnar flow may provide the hitherto unexplained mechanism that controls the horizontal structure of high-\( Ra \) porous convection.

In chapter 4, we present a numerical investigation of the flow in a porous cell containing a thin horizontal layer of much lower permeability than the rest of the cell. This work is motivated by the widespread presence of thin, roughly horizontal, low-permeability layering in geophysical aquifers. We show that, if both the height \( h \) and permeability \( \Pi \) of the interior layer are small compared with the height and permeability of the rest of the cell, the flow is a function of their ratio,
Ω = h/Π, only. We characterize the dependence of the convective flux and the associated dynamical structure of the flow on Ω, which can be thought of as the impedance due to the presence of the low-permeability layer. Two observations are particularly striking: first, the horizontal lengthscale of the plumes in the interior of the cell increases dramatically as Ω is increased; and second, the presence of an interior low-permeability layer can cause the Nusselt number Nu to increase from the value in a homogeneous cell with no interior layer. We explore the dependence of Nu(Ω) and the structure of the flow on Ra, and develop simple reduced models of the system to describe some of the observed features.

In chapter 5 and chapter 6, we extend our previous work on ‘two-sided’ statistically steady Rayleigh–Darcy convection to consider the evolution of convection in a ‘one-sided’ system. A one-sided system has a source of buoyancy on one boundary alone, and there is no steady state. In a closed domain, driven by a dense source on an upper boundary, convection gradually ‘shuts down’ owing to the increase in the average interior density. In chapter 5, we show that the evolution of the convective flux in this one-sided shutdown system can be directly calculated from the relationship Nu(Ra) in a two-sided statistically steady Rayleigh–Darcy cell (studied in chapter 2). We develop simple ‘box’ models that give excellent agreement with high-resolution numerical calculations. We also find a remarkable similarity in the dynamical structure of convection between the one-sided evolving system and the two-sided statistically steady system; vertical columnar plumes reach across the height of the domain, and their lateral scale evolves in very good qualitative agreement with measurements of k(Ra) from chapter 2. We extend this work to model the shutdown of convection with a general power-law equation of state.

In chapter 6, we build on the work of the previous chapter to consider different, more complex, physical systems, which comprise two fluid layers with an equation of state such that the solution that forms at the interface is more dense than either layer (as in the case of supercritical CO₂ overlying brine). We consider both immiscible and miscible fluids; in each case, the predictions of theoretical box models agree well with the results of high-resolution numerical simulations. We undertake both laboratory experiments and numerical simulations which show that interfacial deformation can dramatically enhance the convective flux.
1. INTRODUCTION

In chapter 7, we present the first numerical study of high-$Ra$ Rayleigh–Darcy convection in three dimensions. We give a brief overview and discussion of the features of the flow below the transition to the high-$Ra$ regime, as the system has been very little studied previously except for the range $Ra \lesssim 300$ in which the convection is steady. Measurements of $Nu(Ra)$ over the range $1750 \lesssim 2 \times 10^4$ are very well fitted by $Nu = \alpha_3 Ra + \beta_3$, for $\alpha_3 = 9.6 \times 10^{-3}$ and $\beta_3 = 4.6$. The flux in the high-$Ra$ regime is thus roughly $40\%$ larger than in two dimensions, and again appears to give the classical linear scaling $Nu \sim Ra$ as $Ra \to \infty$. We measure the dynamical structure of the flow, and show that a steady heat-exchanger model provides an increasingly good description of the interior exchange flow as $Ra \to \infty$. The dominant horizontal wavenumber of the interior flow is fitted by $k \sim Ra^{0.52\pm0.05}$ over this range of $Ra$.

Finally, in chapter 8, we summarize all of this work and discuss some of the implications of our results for the geological storage of CO$_2$. In appendix A, there is a detailed description of the numerical schemes that were developed and used throughout the thesis.
Chapter 2

Two-dimensional Rayleigh–Darcy convection at high Rayleigh number

The material contained in this chapter has been published in Physical Review Letters, under the title ‘Ultimate regime of high Rayleigh number convection in a porous medium’ (Hewitt et al., 2012).

2.1 Introduction

The Rayleigh–Darcy cell (porous Rayleigh–Bénard cell) provides an archetypal configuration in which to study convection in a porous medium. The cell has imposed temperatures on its upper and lower boundaries and thus attains a statistically steady state, which allows both for a detailed investigation of the convective dynamics and for an accurate measurement of the convective flux, as described by the Nusselt number $Nu$.

As discussed in chapter 1, various authors have studied and characterized the convective dynamics of the two-dimensional Rayleigh–Darcy cell for low and moderate values of the Rayleigh number $Ra$ (see Nield & Bejan 2006). We recall that, for $Ra < 4\pi^2$, there is no convection (Lapwood, 1948), while for $4\pi^2 < Ra < 1300$, the flow exhibits convective rolls, which undergo a series of bifurcations that per-
turb the background flow as $Ra$ is increased (Kimura et al., 1986; Graham & Steen, 1994). For $Ra \gtrsim 1300$, this quasisteady background flow breaks down completely, marking a transition to the high-$Ra$ regime of interest here (Otero et al., 2004).

The Nusselt number, which describes the transport of buoyancy in a system, provides perhaps the most physically important measure of convection. Characterization of the relationship $Nu(Ra)$ has been (and remains) the subject of extensive research, as discussed in §1.3.1. In particular, we recall the ‘classical’ scaling argument (Malkus, 1954; Howard, 1964) for convection in a pure-fluid Rayleigh–Bénard cell, which suggests that, for sufficiently large $Ra$, the heat transfer into the domain is independent of the height $H$ of the domain. The argument predicts a scaling of $Nu \sim Ra^{1/3}$ in a pure fluid.

For porous convection in a Rayleigh–Darcy cell at high $Ra$, the classical argument instead predicts a linear scaling $Nu \sim Ra$. In agreement with this prediction, a linear scaling has been shown to be a rigorous upper bound for the flux (Busse & Joseph, 1972; Doering & Constantin, 1998; Vitanov, 2000; Otero et al., 2004; Wen et al., 2012). However, in their direct numerical study of the high-$Ra$ regime, Otero et al. (2004) found a slightly reduced exponent $Nu \sim Ra^{0.9}$ for $1300 \lesssim Ra \leq 10^4$. Experimental results from a one-sided system with a convecting upper boundary and a deep or no-flux bottom boundary have given scalings closer to $Nu \sim Ra^{0.8}$ (Neufeld et al., 2010; Backhaus et al., 2011).

In this chapter, we use well-resolved direct numerical simulations of a two-dimensional Rayleigh–Darcy cell over the range $1300 < Ra \leq 4 \times 10^4$ to examine the dynamics and behaviour of the flux in the high-$Ra$ regime. In §2.2, we present the governing equations and non-dimensionalization, and briefly outline the numerical scheme that we employed (the numerical scheme is discussed in detail in appendix A). In §2.3, we present the numerical results, which reveal that, contrary to the previous indications of a sub-linear scaling, the linear classical scaling $Nu \sim Ra$ is attained asymptotically. In §2.4, we explore the dynamics of the flow in the high-$Ra$ regime. The dynamical structure of the flow is dominated by vertical columnar ‘megaplumes’ that extend across the interior of the domain. Near the upper and lower boundaries, the flow is instead dominated by the vigorous growth of small protoplumes, which are entrained into the interior megaplume flow. The flow in the interior is increasingly well described as $Ra \rightarrow \infty$ by a simple steady
2. 2D Rayleigh–Darcy convection

‘heat-exchanger’ solution with a single horizontal wavenumber $k$. Measurements of $k$ give an approximate scaling of $k \sim Ra^{0.4}$.

In §2.5, we summarize and discuss our results.

2.2 Governing equations and numerical method

2.2.1 Dimensional equations

We consider the flow of a Boussinesq fluid in a two-dimensional homogeneous and isotropic porous medium, with horizontal and vertical coordinates $x^*$ and $z^*$, respectively (dimensional variables are denoted with a *). We assume that the flow $u^*$ obeys Darcy’s law and is incompressible,

$$u^* = -\frac{K}{\mu} \left( \nabla p^* + \rho^* g \hat{z} \right), \quad (2.1)$$

$$\nabla \cdot u^* = 0, \quad (2.2)$$

where $K$ is the permeability of the porous medium and $\mu$ is the fluid viscosity, both of which are assumed to be constant, $p^*$ is the pressure field, $g$ is the acceleration due to gravity, and $\hat{z}$ is a unit vector in the positive $z^*$ direction. The density $\rho^*$ satisfies a linear equation of state with respect to the temperature field $T^*$,

$$\rho^* = \rho_0 \left[ 1 - a (T^* - T_0) \right], \quad (2.3)$$

with constant coefficient of thermal expansion $a$ and constant reference density and temperature $\rho_0$ and $T_0$ respectively. The temperature field evolves in time $t^*$ by advection and diffusion,

$$\phi \frac{\partial T^*}{\partial t^*} + u^* \cdot \nabla T^* = \phi \kappa \nabla^2 T^*, \quad (2.4)$$

where $\phi$ is the porosity of the porous medium and $\kappa$ is the thermal diffusivity, both again assumed to be constant. Note that we have neglected heat transfer to the solid phase of the medium in (2.4) (see §1.2).
2. 2D RAYLEIGH–DARCY CONVECTION

Figure 2.1: A schematic of the setup for the (a) dimensional and (b) dimensionless Rayleigh Darcy cell.

We consider a domain of depth $H$ and width $L^*$, with periodic boundary conditions on the sides $x^* = 0, L^*$ (figure 2.1a). We impose zero mass flux and fixed temperature on the top and bottom of the domain:

\[ T^* = T_0 + \Delta T, \quad w^* = 0 \quad \text{at} \quad z^* = 0, \]  
(2.5a)

\[ T^* = T_0, \quad w^* = 0 \quad \text{at} \quad z^* = H. \]  
(2.5b)

2.2.2 Dimensionless equations

We define the density scale $\Delta \rho = \rho_0 a \Delta T$ and the convective velocity scale $U = Kg\Delta \rho/\mu$. Lengths are scaled with $H$, velocity with $U$, pressure with $gH\Delta \rho$, and time with $\phi H/U$; we also introduce a rescaled dimensionless temperature $T$ given by

\[ T = \frac{T^* - T_0}{\Delta T}. \]  
(2.6)

This rescaling gives dimensionless equations

\[ \mathbf{u} = - (\nabla P - T\mathbf{\hat{z}}), \]  
(2.7)
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\[ \nabla \cdot \mathbf{u} = 0, \quad (2.8) \]

\[ \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \frac{1}{Ra} \nabla^2 T, \quad (2.9) \]

where \( P = p + z \rho_0 / \Delta \rho \) is a reduced pressure, and the Rayleigh number is given by

\[ Ra = \frac{UH}{\phi K} = \frac{\rho_0 a \Delta T g K H}{\phi K \mu}. \quad (2.10) \]

The thermal boundary conditions in (2.5) become

\[ T = 1 \text{ at } z = 0, \quad \text{and} \quad T = 0 \text{ at } z = 1. \quad (2.11) \]

The dimensionless system is shown schematically in figure 2.1(b).

Non-dimensionalizing in this way gives rise to \( O(1) \) dimensionless temperature and convective velocity and time scales, while diffusive time and length scales are \( O(Ra^{-1}) \). The Rayleigh number takes the role of an inverse diffusivity in (2.9). This choice of dimensionless variables aids numerical calculations by leaving the timescales for convergence to a statistically-steady state independent of \( Ra \).

The Nusselt number \( Nu \) is the dimensionless average heat flux though the system, scaled by the flux due to steady conduction alone. The heat flux can be determined by the diffusive flux through the lower boundary of the domain, which gives

\[ Nu = \langle nu(t) \rangle = \left\langle \frac{1}{L} \int_0^L \frac{\partial T}{\partial z} \bigg|_{z=0} \, dx \right\rangle, \quad (2.12) \]

where angle brackets \( \langle \rangle \) denote a long-time average and \( L = L^*/H \) is the dimensionless width of the domain. We define the expression inside the angle brackets of (2.12) to be the time-dependent horizontally averaged Nusselt number \( nu(t) \).

2.2.3 Numerical method

The requirement of incompressibility (2.8) can be satisfied by introducing a stream-function \( \psi \), with \((u, w) = (\psi_z, -\psi_x)\). We eliminate the pressure field \( P \) by taking
the curl of (2.7), which gives

\[ \nabla^2 \psi = -\frac{\partial T}{\partial x}. \]  

(2.13)

Equations (2.9) and (2.13) were solved numerically. The numerical method is outlined very briefly below, and is discussed in detail in appendix A.

Equation (2.13) was solved using a spectral method, and (2.9) with an alternating-direction implicit method. The diffusion and advection operators in (2.9) were discretised using standard second-order finite differences and flux-conservative techniques respectively. We used a vertical co-ordinate transformation in order to resolve the diffusive boundary layers at \( z = 0, 1 \) which have an anticipated depth \( \delta \sim Ra^{-1} \). The numerical simulations are second order in space and time, and have been extensively benchmarked against previous numerical results at lower values of \( Ra \) (Graham & Steen, 1994; Otero et al., 2004), as discussed in appendix A.

The numerical simulations were initialized in one of two ways: either with a small (random) perturbation to the steady conduction solution \( T = 1 - z, u = 0 \), or with the statistically-steady output from a simulation at a lower or similar \( Ra \). After some initial transient dynamics, which depend on the initialisation method, the system settles into a statistically steady state. Unlike at lower values of \( Ra \) (see, e.g., Otero et al. 2004), we have seen no evidence that the initial conditions play a role in the long-term behaviour of the system in the high-\( Ra \) regime.

2.3 Numerical results

2.3.1 Structure of the flow

For \( Ra \gtrsim 1300 \), the system cannot sustain the large-scale quasi-periodic roll structure found at lower \( Ra \), which is broken down as unsteady plumes from the boundaries drive a vigorous columnar exchange flow across the height of the domain. This transition in the dynamics marks the start of the ‘high-\( Ra \)’ regime, which is studied here.

The flow can be divided into three regions of differing dynamics, as illustrated
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![Figure 2.2: Snapshots of the temperature field for $L = 2$ at: (a) $Ra = 5000$; and (b) $Ra = 2 \times 10^4$, which highlights the three regions of differing dynamics, as discussed in the main text.](image)

in figure 2.2, which shows snapshots of the temperature field for $Ra = 5000$ and $Ra = 2 \times 10^4$. The interior region is dominated by predominantly vertical exchange flow, carried in columns or ‘megaplumes’ of a fairly regular and $Ra$-dependent wavelength. At the very top and bottom of the domain are thin diffusive boundary layers, where intermittent short-wavelength instabilities drive the growth of small ‘protoplumes’. Between the boundary layers and the interior columnar flow is a region where the dynamics are characterised by the rapid growth and vigorous mixing of protoplumes. Lateral flushing by the large-scale flow drives entrainment of the protoplumes into the interior megaplumes. As can be observed by a comparison of figure 2.2(a) and (b), the horizontal scale of both the protoplumes and the interior megaplumes decreases as $Ra$ increases.
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Figure 2.3: The instantaneous Nusselt number \( n_u(t) = \int \left. \partial T/\partial z \right|_{z=0} \, dx \) for: (a) \( Ra = 5000 \); and (b) \( Ra = 2 \times 10^4 \), with the vertical axis showing the range \([Nu/2, 3Nu/2]\). Panel (c) shows the same data as (b) on an expanded scale; the individual data points shown are separated by ten time steps \( \Delta t \), illustrating that the measurements are well resolved in time.

2.3.2 The Nusselt number

For \( Ra \gtrsim 1300 \), the time-dependent Nusselt number, \( n_u(t) \), of the statistically steady state exhibits chaotic fluctuations about the time-averaged Nusselt number \( Nu \). The typical frequency scales of these fluctuations increase with \( Ra \), while their relative amplitude decreases, as shown for \( Ra = 5000 \) and \( Ra = 2 \times 10^4 \) in figure 2.3. A numerical estimate of \( Nu \) is obtained by time-averaging until statistical uncertainty in the mean of \( n_u(t) \) is reduced to within 0.25%. The details of this averaging technique are given in appendix 2.A.

Figure 2.4 shows \( Nu(Ra) \) for \( Ra \leq 4 \times 10^4 \). The transition to the high-\( Ra \) regime is marked by a sharp discontinuity in \( Nu \) at \( Ra \approx 1300 \). A least-squares fit of the data beyond this point gives a scaling of \( Ra \sim Nu^{0.95 \pm 0.01} \), in approximate agreement with previous results (Otero et al., 2004). However, the numerical measurements for \( 1300 \leq Ra \leq 4 \times 10^4 \) are much more accurately fitted by an equation of the form

\[
Nu = \alpha Ra + \beta, \tag{2.14}
\]

where \( \alpha \approx 6.9 \times 10^{-3} \) and \( \beta \approx 2.75 \) are constants. Figure 2.4(b) shows a plot of \( Nu/Ra \) against \( Ra \), together with (2.14) and the best-fit power-law curve \( Nu \sim Ra^{0.95} \). We find that the linear fit (2.14) deviates from the data by less than 0.6%, while the power-law fit deviates by more than 2%, over the range shown.
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Figure 2.4: (a) The time-averaged Nusselt number $Nu(Ra)$, showing the onset of convection at $Ra = 4\pi^2$ and the transition to the high-$Ra$ regime at $Ra \approx 1300$. (b) The scaled Nusselt number $Nu/Ra$ in the high-$Ra$ regime, for different aspect ratios $L$, together with the data from Otero et al. (2004) for $Ra \leq 10^4$ for comparison. The best-fit power law $Nu \sim Ra^{0.95}$ (dotted line) does not capture the trend as $Ra$ increases; instead, the measurements are very well described by $Nu = \alpha Ra + \beta$, for $\alpha = 6.88 \times 10^{-3}$ and $\beta = 2.75$ (solid line).

The excellent fit provided by (2.14) strongly suggests that the classical linear scaling is attained asymptotically, and so the flux is asymptotically independent of the height of the domain. This result is perhaps surprising, given that the system is dominated by columnar exchange flow across the whole domain (fig. 2.2) which, we might imagine, could provide a mechanism by which information could be propagated between the upper and lower boundaries. We find that $Nu$ exhibits no systematic dependence on the aspect ratio $L$; the slight scatter in the measurements of fig. 2.4(b) is the result of extremely long-timescale fluctuations in the number of megaplumes in the domain, as discussed in §2.4.1 below.

2.4 Dynamics of the flow

2.4.1 The interior region

We observed in figure 2.2 that the interior of the flow in the high-$Ra$ regime is dominated by vertical columnar megaplumes. Space-time plots of the sign of the vertical velocity at $z = 0.5$ (figure 2.5) reveal the remarkable persistence of this columnar structure, particularly at higher $Ra$. The location of the columnar megaplumes
appears to be almost steady in time, despite significant short-timescale fluctuations in the position of the edges of the columns. There is some slight variability in the number of columns over extremely long timescales, which could be due to weak mode restriction imposed by the horizontal periodicity, although similar long-timescale variability is observed in calculations with larger aspect ratios $L$.

2.4.1.1 Heat-exchanger solution

Based on the observed persistence of the megaplumes in figure 2.5, we can develop a simple, steady model of the columnar flow in the interior. There is an exact ‘heat-exchanger’ solution to (2.9) and (2.13) in an unbounded domain, in which vertical advection of a background linear temperature gradient is exactly balanced by horizontal diffusion between neighbouring megaplumes, giving a steady solution,

$$T = \hat{A} \cos (kx) - \frac{k^2}{Ra} z, \quad (2.15a)$$

$$u = 0, \quad (2.15b)$$

$$w = \hat{A} \cos (kx). \quad (2.15c)$$
Figure 2.6: The temporally and horizontally averaged temperature profile $\langle T \rangle$ for $Ra = 1, 2, 4 \times 10^4$, as marked. The profiles are approximately linear through the interior of the domain, with a gradient that decreases with $Ra$.

The solution comprises interlocking columnar flow with amplitude $\hat{A}$ and a regular horizontal wavenumber $k$.

Equation (2.15a) shows that the horizontally averaged temperature profile is vertically linear. Numerical measurements of the temporally and horizontally averaged temperature $\langle T \rangle$ (figure 2.6) agree with this linear behaviour in the interior region. The gradient of $\langle T \rangle$ decreases as $Ra$ increases. We compare the amplitude of the columnar flow in the heat-exchanger model with the numerical calculations by measuring the root-mean-square (rms) temperature perturbations and velocity components, $T_{rms}$, $w_{rms}$ and $u_{rms}$. In the heat-exchanger model, $T_{rms} = w_{rms} = \hat{A}/\sqrt{2}$ and $u_{rms} = 0$, independent of $z$. Numerical measurements of $T_{rms}$, $w_{rms}$ and $u_{rms}$ at different values of $Ra$ (figure 2.7a) show very good agreement with this behaviour asymptotically: $u_{rms}$ decreases as $Ra$ increases, and $T_{rms}$ appears to tend towards $w_{rms}$, which is itself roughly independent of $Ra$, as $Ra \to \infty$.

These measurements indicate that the vigorously convecting system is dominated by a remarkably persistent columnar flow that becomes increasingly ordered and increasingly well-described by the steady heat-exchanger solution as $Ra$ increases. Moreover, the measurements presented in figure 2.7(a) suggest that $\hat{A}$ is asymptotically independent of $Ra$ and given by $\hat{A} = \sqrt{2}T_{rms} \approx \sqrt{2}(0.083) \approx 0.117$.
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Figure 2.7: The temporally averaged root-mean-square temperature $T_{\text{rms}}$ (red), vertical velocity $w_{\text{rms}}$ (blue) and horizontal velocity $u_{\text{rms}}$ (green): (a) measured at $z = 0.5$; and (b) plotted against $z$, for $Ra = 10^4$ (solid), $Ra = 2 \times 10^4$ (dashed), and $Ra = 4 \times 10^4$ (dotted).

as $Ra \to \infty$. This observation agrees with the indications from figure 2.4 that the classical linear scaling for $Nu(Ra)$ is attained asymptotically, and corroborates the validity of the heat-exchanger model for the interior flow: since the heat flux is dominated by advection in the interior at high $Ra$, the heat-exchanger model (2.15) gives $Nu \approx Ra \hat{A}^2/2 \approx 0.0069Ra$ as $Ra \to \infty$, in very good agreement with the measured value of the coefficient $\alpha$ in (2.14).

Figure 2.7(b) shows the variation in the rms temperature and velocity fields with $z$ for a selection of values of $Ra$. The heat-exchanger solution requires the rms values to be independent of $z$, and so we expect it to be valid across the interior, where the measured quantities vary slowly and $T_{\text{rms}} \approx w_{\text{rms}}$. Near to the upper and lower boundaries of the domain, however, the rms quantities vary significantly: $T_{\text{rms}}$ and $w_{\text{rms}}$ differ appreciably, and $u_{\text{rms}}$ grows. These observations signify that the heat-exchanger solution breaks down near to the upper and lower boundaries of the domain, where protoplumes dominate the dynamics of the flow.

We have also adapted the unbounded heat-exchanger solution (2.15) to model the effect of circulation in a finite domain, by including vertical variation with a wavenumber $m \ll k$. The adapted model is discussed in appendix 2.B. The model, which includes a non-zero horizontal velocity, gives good quantitative agreement.

\[1\] Interestingly, the average advective heat flux in the heat-exchanger model depends only on the amplitude $A$, and is independent of the wavenumber $k$. 

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with the behaviour of the rms temperature and velocity perturbations in figure 2.7(a), and reduces to the simple heat-exchanger solution (2.15) as \( Ra \to \infty \).

2.4.1.2 Measurements of the average wavenumber \( k \)

The heat-exchanger model *per se* leaves the wavenumber \( k \) of the columnar flow undetermined. We measured \( k \) by calculating the power spectra \( P(j) \) as a function of wavenumber \( j \) from the Fourier transform of the temperature field at \( z = 0.5 \). The average wavenumber \( k \) was given by the temporally averaged expected value from the power spectra,

\[
k = \left\langle \int jP(j) \, dj \right\rangle / \left( \int P(j) \, dj \right).
\]

We obtained very similar results by applying the same method to the vertical velocity field at \( z = 0.5 \). Measurements of \( k \) from (2.16) are shown in figure 2.8(a), and can be fitted by an approximate scaling

\[
k \approx 0.48Ra^{0.4},
\]

(figure 2.8b), although the data also hints at a possible decrease in the exponent for \( Ra \gtrsim 2 \times 10^4 \). There is some variation between different calculations, even for the same aspect ratio \( L \), which is likely due to fluctuations in the dominant wavenumber over extremely long timescales (as observed in figure 2.5).

Measurements of the time-averaged power spectra \( P(j) \) at \( z = 0.5 \) (figure 2.8c) give a clear peak, corresponding to the average wavenumber \( k \), and an exponential decay for larger wavenumbers. The measurements at different values of \( Ra \) collapse to give the same slope as a function of \( j/Ra^{0.4} \).

2.4.2 The protoplume region

In a bounded domain, the interior columnar-exchange flow feeds into and is fed by protoplumes near to the upper and lower boundaries. A plausible hypothesis

\footnote{A larger range of \( Ra \) would be required to verify any change in exponent. However, results from a stability analysis of the heat-exchanger solution (presented in chapter 3) are consistent with the measurements presented here and suggest an asymptotic scaling of \( k \sim Ra^{5/14} \) (5/14 \( \approx \) 0.357).}
is that the horizontal wavenumber $k$ and the amplitude $\hat{A}$ of the interior flow are determined by the interaction between the megaplumes and the protoplume regions. To examine the dynamics in these regions, we constructed space-time diagrams of the temperature in a slice at a fixed height just above the bottom boundary layer (which exhibits behaviour that is mirrored at the top). Figure 2.9 reveals a characteristic repeating ‘fish-bone’ pattern, which corresponds to persistent megaplume roots (the ‘backbones’) together with transient formation and entrainment of protoplumes on either side (the ‘ribs’).

The pattern of ribs shows bursts of protoplumes that typically commence near a larger established plume, while later protoplumes in the burst originate successively further away. We interpret this as propagation of instability along the boundary layer which drains the buoyancy accumulated since the previous burst. Concomitantly each new protoplume is entrained back towards the larger established plume. This coupled mechanism of instability and entrainment leads to episodic and highly time-dependent patterns of plume growth and flushing.
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Figure 2.9: Space-time plots of the temperature in a slice just above the lower boundary layer at $z = 100/Ra$, for: (a) $Ra = 5000$; and (b) $Ra = 2 \times 10^4$. These plots show both the directly measured temperature ($t < 120$) and the results of a plume-tracking algorithm ($t > 120$), which gives a way to analyse the dynamics of plumes in more detail. Megaplume roots are highlighted, and the ‘ribs’ of the fishbone structures (see the text) mark the formation and entrainment of protoplumes.

Counts from a plume-tracking algorithm of the number of plumes in the boundary layer (figure 2.10) indicate that the average number of protoplumes scales roughly with $Ra$, while the average number of megaplumes has a much weaker scaling of roughly $k \sim Ra^{0.4}$. This means that there are more protoplumes being entrained into each megaplume at higher values of $Ra$. In addition, visual
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Figure 2.10: The temporally averaged number of plumes in the boundary layer \((z = 10/Ra)\) for \(L = 2\), counted by a plume-tracking algorithm: the total number of plumes (red) is best fit by a scaling of \(Ra^{0.97 \pm 0.05}\), while the number of megaplumes alone is best fit by a scaling of \(Ra^{0.39 \pm 0.06}\), in rough agreement with the measurements of \(k\) in the interior (figure 2.8).

Comparison and rescaling of plots like figure 2.9\((a)\) and \((b)\) suggests that the typical timescales and lateral lengthscales of the protoplume ‘ribs’ in the fish-bone structures scale approximately like \(Ra^{-1}\). The lengthscales certainly decrease significantly more rapidly with \(Ra\) than the megaplume spacing, as can be seen by comparing the number of ribs and backbones between figure 2.9\((a)\) and \((b)\). We also observe that the patterns of ribs are increasingly initiated by protoplumes, as well as by megaplumes, as \(Ra\) is increased. This behaviour leads to increasingly ramified fish-bone patterns at higher \(Ra\), and is suggestive of a hierarchy of coarsening as \(Ra\) is increased. These observations strongly suggest that the average horizontal wavenumber \(k\) of the interior flow is not directly governed by the dynamics of protoplumes near the upper and lower boundaries.

2.5 Conclusions

We have found that numerical measurements of the Nusselt number in a Rayleigh–Darcy cell over the range \(1300 < Ra \leq 4 \times 10^4\) are extremely well fitted by \(Nu = \alpha Ra + \beta\), with \(\alpha = 6.9 \times 10^3\) and \(\beta = 2.75\). This fit strongly suggests that the classical linear scaling \(Nu \sim Ra\) is attained asymptotically. By implication,
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the dimensional flux is asymptotically independent of the height of the domain.

Given the increasingly vigorous nature of the dynamics at the boundaries, it is striking that the interior columnar flow displays such persistent regular structure as $Ra$ increases. Indeed, despite vigorous and time-dependent forcing from the protoplume regions, we have found that the steady heat-exchanger solution, which comprises purely vertical flow, provides a remarkably good description of the dynamics of the interior region asymptotically. This increasingly ordered behaviour as $Ra$ is increased is quite unlike the disordered turbulent dynamics in the interior of a pure-fluid Rayleigh–Bénard cell at high $Ra$ (e.g. Ahlers et al. 2009). The average horizontal wavenumber $k$ of the interior flow increases with $Ra$, and can be approximately fitted by a scaling of $k \sim Ra^{0.4}$ for $1300 < Ra \leq 4 \times 10^4$.

The episodic bursting and propagation of boundary-layer instabilities near the upper and lower boundaries of the domain give rise to the fish-bone structures shown in figure 2.9. The typical horizontal lengthscale of the resultant protoplumes approximately scales with $Ra^{-1}$, which is a much stronger than the dominant interior lengthscale $k^{-1} \sim Ra^{-0.4}$. The difference in scalings these suggests that the protoplumes do not govern the interior wavenumber $k$ directly. Motivated by this intriguing observation, in chapter 3 we will examine in detail whether the interior wavenumber is determined instead by the stability of the columnar flow itself. The results of the stability analysis are consistent with the numerical measurements of $k(Ra)$ presented in figure 2.8, and suggest an asymptotic scaling for the wavenumber of $k \sim Ra^{5/14}$.

Appendices

2.A Averaging the Nusselt number

The local time-dependent Nusselt number, $nu(t)$, is given by

$$\begin{align*}
    nu(t) &= -\frac{1}{L} \int_0^L \frac{\partial T}{\partial z} \bigg|_{z=0} \, dx = -\frac{1}{L} \frac{\partial \zeta}{\partial z} \int_0^L \frac{\partial T}{\partial \zeta} \bigg|_{\zeta=0} \, dx, \\
    &\quad \text{(2.18)}
\end{align*}$$
where \( \zeta(z) \) is the rescaled vertical coordinate (see appendix A). In the statistically steady high-\( Ra \) regime, \( nu(t) \) exhibits chaotic fluctuations about a mean (see figure 2.3). We measured and averaged \( nu(t) \) until the average had converged to a suitably defined tolerance. To reduce computation time, we used a ‘quadratic-box’ running average to reduce the convergence time.

We define the ‘quadratic-box’ (QB) average of length \( 2L \), \( Q_L(t) \), to be the weighted average,

\[
Q_L(t) = \frac{15}{16L^5} \int_{t-L}^{t+L} \left( L^2 - [\tau - t]^2 \right)^2 nu(\tau) \, d\tau.
\] (2.19)

We generate a running QB average \( Q_L(t) \) by averaging (2.19) over all previous time (for the sake of this discussion, \( t = 0 \) is taken to correspond to a time after all initial transients have decayed and the system is in a statistically steady state), to give

\[
\overline{Q}_L(t) = \frac{1}{t-2L} \int_{L}^{t-L} Q_L(\tau) \, d\tau.
\] (2.20)

Figure 2.11 shows an example of measurements of \( nu(t) \) at \( Ra = 2 \times 10^4 \), together with the standard running average (which simply averages all previous data points equally) and the QB running average. The QB average gives a much smoother signal than a standard running average. A QB will also give smoother
convergence than a simple unweighted box average would, because the averaging
function in (2.19) is only discontinuous in the second derivative rather than the
zeroth at $t \pm L$, which gives much more rapidly decaying Fourier modes.

The convergence of $\overline{Q}_L(t)$ is determined by specifying a convergence timescale
$t_{\text{conv}}$ and tolerance $\varepsilon$. We consider $\overline{Q}_L(t)$ to have converged to $Nu$ if

$$|\overline{Q}_L(t_1) - \overline{Q}_L(t_2)| < \varepsilon \left( \frac{\overline{Q}_L(t_1) + \overline{Q}_L(t_2)}{2} \right)$$

for all $t_1, t_2 \in [t - t_{\text{conv}}, t]$. (2.21)

We typically used values of $\varepsilon = 2.5 \times 10^{-3}$ (i.e. convergence to 0.25%), $t_{\text{conv}} = 100,$
and $L = 50.$

2.B The adapted heat-exchanger solution

In §2.4.1.1, we found that the flow in the interior of the Rayleigh–Darcy cell is
increasingly well described by a simple heat-exchanger solution as $Ra \rightarrow \infty$. The
heat-exchanger solution (2.15) comprises purely vertical columnar flow in an un-
bounded domain. In this appendix, we adapt the unbounded heat-exchanger so-
lution to model the effect of circulation in a finite domain, by including vertical
variation with a wavenumber $m \ll k$. The adapted heat-exchanger model takes
the form

$$T = \hat{T} \cos (kx) \sin (mz) - \frac{k^2}{Ra} \left( 1 + \frac{m^2}{k^2} \right) z,$$  (2.22a)

$$u = \hat{u} \sin (kx) \cos (mz),$$  (2.22b)

$$w = \hat{w} \cos (kx) \sin (mz),$$  (2.22c)

where

$$\hat{u} = \frac{km}{k^2 + m^2} \hat{T}, \quad \text{and} \quad \hat{w} = \frac{k^2}{k^2 + m^2} \hat{T}. \quad (2.23a, b)$$

Horizontal advection of temperature is neglected in this model, which is a valid ap-
proximation as long as $\hat{T} m \ll k^2$. We expect that $m$ is related to the height of the
domain, which implies that the more rapid horizontal variations with wavenumber
$k$ dominate as $Ra$ increases; hence the simple heat-exchanger solution (2.15) is
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Figure 2.12: Measurements of: (a) the average rms horizontal velocity $u_{\text{rms}}$ at $z = 0.5$, from direct numerical measurements (blue squares) and calculated from the adapted heat-exchanger model using (2.24) (red circles); and (b) the magnitude of the temporally and horizontally averaged vertical temperature gradient, from direct numerical measurements (blue squares), and calculated from the adapted heat-exchanger model using (2.25) (red circles).

recovered asymptotically.

Equations (2.22)–(2.23) provide three relationships which link five measurable unknowns, $\hat{T}$, $\hat{w}$, $\hat{u}$, $k$, and $\partial \langle T \rangle / \partial z$, together with one less easily measured, $m$. These relationships allow us to test the accuracy of the model. Two comparisons, for $\hat{u}$ and for $\partial \langle T \rangle / \partial z$, are presented below.

First, we consider the horizontal velocity $\hat{u}$. Elimination of $m$ from (2.23) gives an alternative expression for $\hat{u}$,

$$\hat{u} = \hat{w} \left( \frac{\hat{T}}{\hat{w}} - 1 \right)^{1/2}. \quad (2.24)$$

We also recall the relationships $T_{\text{rms}} = \hat{T}/\sqrt{2}$, $w_{\text{rms}} = \hat{w}/\sqrt{2}$, and $u_{\text{rms}} = \hat{u}/\sqrt{2}$. Figure 2.12(a) shows measurements of $u_{\text{rms}}$ together with the theoretical values obtained from (2.24) and the measurements of $T_{\text{rms}}$ and $w_{\text{rms}}$. The measurements give a very reasonable agreement with the predictions of the adapted heat-exchanger model, although there is roughly a 10% difference in magnitude.

Second, we consider the magnitude of the linear gradient of the temporally and horizontally averaged temperature profile, $\partial \langle T \rangle / \partial z$, that was shown in figure 2.6.
Elimination of $m$ from the theoretical expression for the gradient in (2.22a) using (2.23a), gives

\[ \left| \frac{\partial \langle T \rangle}{\partial z} \right| = \frac{k^2 \hat{T}^2}{Ra \hat{w}^2}. \] (2.25)

Figure 2.12(b) shows a comparison of direct measurements of the interior gradient with the calculated value obtained from (2.25) (together with measurements of $T_{rms}$ and $w_{rms}$). Again, we see a good qualitative fit, although with a difference in magnitude of $\sim 15\%$. A power-law fit of the measured data gives a $Ra$ exponent of $-0.27 \pm 0.05$, while the predicted asymptotic scaling from (2.25), using the rough fit $k \sim Ra^{0.4}$ and the asymptotic behaviour $\hat{T} \rightarrow \hat{w}$, gives $Ra^{-0.2}$. The variation in the data shown in figure 2.12 is related to the variation in the measurements of $k$ (figure 2.8), and is likely due to long-timescale changes in the number of plumes in the domain as discussed in §2.4.1.2.

There are at least two plausible reasons for the slight difference between theory and measurements in figure 2.12. First, the measurements of $k^2$ that we have used in (2.25) are calculated from measurements of $k$; however, since the interior flow contains more than one Fourier mode, this calculation will yield an underestimate of $k^2$ if it were measured and averaged directly. Second, there will be more horizontal heat transfer than the purely diffusive transfer that the model predicts, because of mixing due to transient dynamics in the interior of the Rayleigh–Darcy cell. So we might expect that vertical advection of heat, and therefore the background gradient of the flow, would be slightly larger than the model predicts in order to balance this increased horizontal transfer.
Chapter 3

Stability of columnar convection in a porous medium

The material contained in this chapter has been published in the Journal of Fluid Mechanics, under the title ‘Stability of columnar convection in a porous medium’ (Hewitt et al., 2013b).

3.1 Introduction

In chapter 2, we found that vertical columnar flow dominates the flow in a two-dimensional Rayleigh–Darcy cell at high Rayleigh number $Ra$. Curiously, the columnar flow not only persists, but becomes increasingly well organized as $Ra$ is increased. We found that, as $Ra$ increases, the interior columnar flow becomes increasingly well described by a steady ‘heat-exchanger’ solution, in which vertical advection of a background temperature gradient exactly balances horizontal diffusion (figure 3.1). The numerical measurements presented in chapter 2 gave an approximate scaling for the wavenumber $k$ of the columnar flow of $k \sim Ra^{0.4}$ over the range $1300 < Ra \leq 4 \times 10^4$ (see figure 2.8), although it was noted that there was some suggestion of a slightly smaller exponent asymptotically. While $k$ clearly increases with $Ra$, the amplitude $\hat{A}$ of the columnar flow tends towards a constant (see figure 2.7), consistent with an asymptotic Nusselt-number scaling $Nu \sim Ra$.

Columnar structures are also very widely observed in convective flow driven by
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a source of buoyancy on one boundary only. Following the onset of convection, flow below a dense source (or, equivalently, above a buoyant source) is marked by vigorous mixing at the boundary which feeds into persistent downwelling plumes, as observed in several experimental (Neufeld et al., 2010; Backhaus et al., 2011; Slim et al., 2013) and numerical (Pau et al., 2010; Hidalgo et al., 2012; Fu et al., 2013; Slim, 2014) studies. If the boundaries of the domain are impermeable then, over longer times, the convective flow weakens as the density in the interior increases towards that of the upper boundary. This ‘shutdown’ regime is studied in chapters 5 and 6: we will show in these chapters that the columnar flow across the interior of the domain persists throughout, with an average wavenumber $k$ that decreases slowly as the average interior density increased and the effective Rayleigh number decreased. The relationship between $k(t)$ and $Ra(t)$ gives excellent quantitative agreement with results from the Rayleigh–Darcy cell presented in chapter 2.

The physical mechanism that governs the wavenumber $k(Ra)$ has so far remained elusive. In chapter 2 we argued that $k$ is not controlled directly by the small-scale dynamics of protoplumes near the boundary, since these have a lateral scale of $Ra^{-1}$, which is a much stronger dependence on $Ra$ than the observed wavenumber exponent of about 0.4. It has been suggested by Wen et al. (2012, 2013) that the wavenumber is determined by the size of a ‘minimal flow unit’, which is set by the largest wavenumber $k$ for which the buoyancy flux remains independent of $k$. Solutions for steady convective flow in a narrow Rayleigh–Darcy cell (Corson, 2011) give a scaling of $k \sim Ra^{1/2}$ for the minimal flow unit, while recent numerical measurements of the minimal flow unit for unsteady flow suggest a slightly weaker dependence on $Ra$ (Wen et al., 2013), in rough agreement with the observed wavenumber scaling of $Ra \sim k^{0.4}$. This observation does not, however, provide a mechanism for the physical control of wavenumber. The aim of this chapter is to explore whether the wavenumber might be determined by the stability of the columnar flow.

Columnar ‘heat-exchanger’ flows are not only observed in porous media; similar flow is found in double-diffusive systems, in the form of ‘salt fingers’. These fingers can occur when the density is a function of two components with different molecular diffusivities, such as heat and salt, provided that the unstably distributed component (salt) has a lower diffusivity than the stably distributed component
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Figure 3.1: (a) A snapshot of the temperature field in a Rayleigh–Darcy cell at $Ra = 2 \times 10^4$ (see chapter 2), which is dominated by vertical columnar exchange flow across the domain; (b) the corresponding temporally and horizontally averaged temperature $\langle T \rangle (z)$, which shows the relatively weak linear temperature gradient across the interior of the domain; and (c) the temperature field of steady heat-exchanger flow with the same wavelength and background temperature gradient as (a).

(heat) (Huppert & Turner, 1981). Stability of the salt fingers has long been suggested as the controlling mechanism for their dynamical structure (Stern, 1969); it was explored in detail by Holyer (1981, 1984), and remains an active area of study (Schmitt, 2012; Radko & Smith, 2012). The Floquet analysis employed by Holyer (1984) to solve the linear-stability problem provides a starting point for our approach here.

In this chapter, we examine the stability of two-dimensional columnar heat-exchanger flow in a porous medium. The flow is driven by temperature differences between the columns, but the analysis is equally applicable to compositional convection (see §1.2). In §3.2, we set out the governing equations for heat-exchanger flow in an unbounded medium, and find that the flow is controlled by a single parameter, the rescaled amplitude $A$. In §3.3, we use Floquet theory to perform a linear-stability analysis of this flow. We show that the dominant instability for $A \gtrsim 17.2$ has double the horizontal wavelength of the background columns and a relatively small vertical wavenumber, and we determine the dependence on $A$ of the vertical wavenumber and growth rate of this mode. In §3.4, we present an asymptotic analysis of the most unstable perturbation for $A \gg 1$, and discuss the physical mechanism of instability. In §3.5, we explore the non-linear evolution of the instability for large $A$ using direct numerical simulations.
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In §3.6, we discuss the relevance of all these results for the scaling of the columnar wavenumber $k$ in a Rayleigh–Darcy cell at high $Ra$. A balance of the time scale for instability and the time scale for advection of perturbations across the domain suggests that the columnar flow should be unstable for wavenumbers $k \sim Ra^{5/14}$ as $Ra \to \infty$, while a correction to this asymptotic estimate gives a slightly stronger dependence on $Ra$ for $Ra < O(10^3)$. These scalings give good agreement with numerical measurements of the dominant wavenumber $k$ from the interior of a Rayleigh–Darcy cell.

We conclude with a summary of the main results and their implications in §3.7.

3.2 Governing equations

3.2.1 Dimensionless equations

We consider flow in a homogeneous, isotropic and unbounded two-dimensional porous medium, with horizontal and vertical coordinates $x$ and $z$, respectively. As in chapter 2, the flow $u = (u, w)$ is incompressible and satisfies Darcy’s law, and the density $\rho$ of the fluid is linearly related to the temperature $T$, which satisfies a transport equation. These equations are given in dimensionless variables by

$$\nabla \cdot \mathbf{u} = 0, \quad \mathbf{u} = - (\nabla P + \rho \hat{z}),$$  \hspace{1cm} (3.1a, b)

$$\rho = 1 - T, \quad \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \frac{1}{Ra} \nabla^2 T,$$  \hspace{1cm} (3.2a, b)

where $P$ is the reduced pressure (see §2.2.2). The Rayleigh number $Ra$ is given by

$$Ra = \frac{\rho_0 a \Delta T g \Pi H}{\phi \kappa \mu},$$  \hspace{1cm} (3.3)

where $\Pi$ is the permeability, $\phi$ is the porosity, $g$ is the gravitational acceleration, $\rho_0$ is a reference density, $a$ is the coefficient of thermal expansion, $\kappa$ is the thermal diffusivity and $\mu$ is the viscosity of the fluid, all of which are assumed to be constant. In common with the rest of this thesis, we have assumed that there is negligible heat transfer to the solid phase of the medium, and, as such, these equations are
equally applicable to compositional convection. We have non-dimensionalized with respect to a temperature scale $\Delta T$, which determines the buoyancy-velocity scale $U = \rho_0 \beta \Delta T g \Pi / \mu$, and with respect to a length scale $H$, which determines the convective time scale $\phi H / U$. In the case of a Rayleigh–Darcy cell, these scales would correspond to the driving temperature difference across the domain and the height of the domain, respectively, as in chapter 2.

We satisfy (3.1a) by introducing a streamfunction $\psi$, where $(u, w) = (\partial \psi / \partial z, -\partial \psi / \partial x)$. We take the curl of (3.1b) to eliminate the pressure, and combine with the equation of state (3.2a) to obtain

$$\nabla^2 \psi = -\frac{\partial T}{\partial x}. \quad (3.4)$$

Equations (3.2b) and (3.4) govern the flow.

Steady ‘heat-exchanger’ flow provides an exact solution of (3.2b) and (3.4) (see chapter 2; §2.4.1.1) in which vertical advection of a background linear temperature gradient by interleaving columns of exchange flow balances horizontal diffusion between the columns; the horizontal velocity is zero, and the vertical velocity is directly proportional to the sinusoidal variation of temperature across the columns. The heat-exchanger solution $[\psi_0, T_0]$ is characterized by a wavenumber $k$ and amplitude $\hat{A}$, and is given by

$$T_0 = \hat{A} \cos kx - \frac{k^2}{Ra} z, \quad \psi_0 = -\frac{\hat{A}}{k} \sin kx, \quad u_0 = 0, \quad w_0 = \hat{A} \cos kx, \quad (3.5a, b, c, d)$$

(cf. (2.15)), where $u_0 = \partial \psi_0 / \partial z$ and $w_0 = -\partial \psi_0 / \partial x$ are the corresponding horizontal and vertical velocity of the flow. The average vertical advective heat flux for heat-exchanger flow scales with $\hat{A}^2$, and is independent of the wavenumber $k$.

### 3.2.2 Re-scaled equations

The heat-exchanger flow (3.5) is governed by three parameters, $k$, $\hat{A}$, and $Ra$, which describe the wavenumber, the amplitude, and the relative strength of advection and diffusion, respectively. We can scale out two of these apparent degrees of
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freedom by setting

\[ X = kx; \quad \Theta = \frac{Ra}{k} \frac{T}{T_0}; \quad \Psi = Ra \psi; \quad \tau = \frac{k^2}{Ra} t. \]  \hfill (3.6)

The governing equations (3.4) and (3.2b) become

\[ \nabla^2 \Psi = -\frac{\partial \Theta}{\partial X}, \quad \frac{\partial \Theta}{\partial \tau} + \frac{\partial \Psi}{\partial Z} \frac{\partial \Theta}{\partial X} - \frac{\partial \Psi}{\partial X} \frac{\partial \Theta}{\partial Z} = \nabla^2 \Theta, \]  \hfill (3.7a, b)

and the heat-exchanger solution (3.5) becomes

\[ \Theta_0 = A \cos X - Z, \quad \Psi_0 = -A \sin X, \quad U_0 = 0, \quad W_0 = A \cos X. \]  \hfill (3.8a, b, c, d)

The rescaled strength of the flow

\[ A = \frac{\hat{A}Ra}{k}, \]  \hfill (3.9)

is now the only free parameter. Equation (3.8) gives the background flow for the stability analysis of the subsequent sections of this chapter.

3.3 Linear-stability analysis

3.3.1 Theory

We consider small perturbations \[ \tilde{\Psi}, \tilde{\Theta} \] to the background heat-exchanger flow (3.8) of the form

\[ \tilde{\Psi} = \text{Re} \left\{ F(X) \exp (\sigma t + i\alpha Z) \right\}, \quad \tilde{\Theta} = \text{Re} \left\{ G(X) \exp (\sigma t + i\alpha Z) \right\}, \]  \hfill (3.10a, b)

where \(|F|, |G| \ll 1\). By retaining only terms that are linear in \(F\) and \(G\), the governing equations (3.7) become

\[ F'' - \alpha^2 F = -G', \quad (\sigma + i\alpha A \cos X) G + F' - i\alpha A \sin X F = G'' - \alpha^2 G. \]  \hfill (3.11a, b)

Owing to the spatial dependence of the coefficients in (3.11b), we cannot as-
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sume a simple-harmonic normal-mode form for $F$ and $G$. Instead, we utilise the periodicity of the equations: the coefficients are periodic in $X$ with period $2\pi$, and, therefore, (3.11) forms a Floquet system. Floquet theory (see Jordan & Smith 1999, for example) implies that the eigenmodes $y_j(X)$ of any homogeneous system of linear ordinary differential equations that has periodic coefficients with period $\lambda$ can be written in the form $y_j(X) = p_j(X) \exp(i\beta_j X)$, where $p_j$ is periodic with period $\lambda$, and $\beta_j$ is a (possibly complex) constant. If the eigenmodes are also required to be spatially periodic, then $\beta_j$ must be real. In (3.11), $\lambda = 2\pi$, and so the function $p_j(X)$ can be written as a sum of complex exponentials of the form $\exp(i n X)$ for integer $n$ (Beaumont, 1981). We therefore look for spatially periodic eigenmodes of the form

$$\begin{bmatrix} F \\ G \end{bmatrix} = \text{Re} \left\{ \exp(i\beta X) \sum_{n=-\infty}^{\infty} \begin{bmatrix} F_n \\ G_n \end{bmatrix} \exp(inX) \right\},$$

(3.12)

where $\beta$ is real. Due to the invariance of (3.12) under integer shifts in $\beta$ and under reflection $\beta \rightarrow -\beta$, we can pick $0 \leq \beta \leq 1/2$ without loss of generality. We refer to $\beta$ as the horizontal wavenumber of the perturbation; strictly, $\beta$ is the wavenumber of the largest horizontal scale, and the infinite sum allows for perturbations on smaller scales.

The eigenvalue $\sigma$ is given as a function of $\alpha$ and $\beta$ by substituting the Fourier sum (3.12) into (3.11) and rewriting $\sin X$ and $\cos X$ in terms of complex exponentials. Equation (3.11) becomes

$$i\gamma_n^2 F_n = - (\beta + n) G_n,$$

(3.13a)

$$i(\beta + n) F_n - \frac{\alpha A}{2} (F_{n-1} - F_{n+1}) = - (\gamma_n^2 + \sigma) G_n - \frac{i\alpha A}{2} (G_{n-1} + G_{n+1}),$$

(3.13b)

where $\gamma_n^2 = (\beta + n)^2 + \alpha^2$. Eliminating $F$ between (3.13a) and (3.13b) gives

$$\left[ \frac{(\beta + n)^2}{\gamma_n^2} - \gamma_n^2 - \sigma \right] G_n = \frac{i\alpha A}{2} \left[ \left( 1 + \frac{\beta + n + 1}{\gamma_{n+1}^2} \right) G_{n+1} + \left( 1 - \frac{\beta + n - 1}{\gamma_{n-1}^2} \right) G_{n-1} \right].$$

(3.14)
Equation (3.14) can be written as an infinite matrix equation of the form

\[ MG = \sigma G, \quad (3.15) \]

where the vector \( G = ( \cdots, G_{n-1}, G_n, G_{n+1}, \cdots ) \), and \( M \) is an infinite (tridiagonal) matrix. Solutions to (3.15) are found by looking for eigenvectors \( G \) of \( M \) with eigenvalues \( \sigma \). The real part of \( \sigma \) gives the growth rate of perturbations.

3.3.2 Solutions

3.3.2.1 The limit of large horizontal scales

The equations simplify dramatically if we only consider perturbations on the largest horizontal scales, which is achieved by severely truncating the infinite sum in (3.12) such that \( G_n = 0 \) for all \( n \neq 0 \). In this long-wavelength limit, the columnar flow is completely decoupled from the perturbation, which is equivalent to setting \( A = 0 \) and losing the effect of flow on stability. Equation (3.14) reduces to the standard linear-stability analysis of a linear background temperature field about rest (Nield & Bejan, 2006), and the growth rate is given by the usual Rayleigh modes,

\[ \sigma = \frac{\beta^2}{\beta^2 + \alpha^2} - \left( \frac{\beta^2 + \alpha^2}{\beta^2 + \alpha^2} \right). \quad (3.16) \]

The flow is unstable if \( \beta > \beta^2 + \alpha^2 \). If there is no constraint on the size of the domain, then the growth rate is maximized by \( \alpha \ll \beta \ll 1 \), which gives a limiting growth rate \( \text{Re}\{\sigma\} = 1 \). If the perturbation is constrained in a finite domain, then the instability takes the form of one or more large convective rolls.

3.3.2.2 Numerical solutions that incorporate smaller scales

We incorporated the effects of smaller horizontal modes on the stability of the flow by retaining more terms in the Fourier sum in (3.12) and solving (3.15) numerically. We found eigenvalues \( \sigma \) by truncating the infinite sum in (3.15) to \(-N \leq n \leq N\), for some integer \( N(\alpha, \beta, A) \), which was increased until the relative error in the eigenvalue with the largest real part (growth rate) was less than \( 10^{-5} \). We denote the eigenvalue with the largest real part \( \hat{\sigma}(\alpha, \beta, A) \).
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Figure 3.2: Contours of the growth rate $\text{Re}\{\hat{\sigma}\}$ (as marked) against the horizontal wavenumber $\beta$ and the vertical wavenumber $\alpha$ at amplitudes: (a) $A = 0$; (b) $A = 2^3$; (c) $A = 2^5$; and (d) $A = 2^{12}$. The marginal-stability curve is independent of $A$ (§3.3.2.3). The maximum growth rate is initially $\text{Re}\{\hat{\sigma}\} = 1$, which is attained at $\alpha = \beta = 0$. As $A$ increases, a mode with horizontal wavenumber $\beta = 0.5$ and $\alpha > 0$ becomes increasingly unstable. For $A \gtrsim 17.2$ (c,d), this mode has a growth rate that is greater than 1.

Figure 3.2 shows contour plots of the growth rate $\text{Re}\{\hat{\sigma}\}$ against the vertical and horizontal wavenumbers $\alpha$ and $\beta$, for different values of $A$. For all $A$, we find that the growth rate is negative for $\alpha > 1/2$, and this range is therefore not shown. We also recall that we only need to consider values of $\beta$ in the range $0 \leq \beta \leq 1/2$ due to the symmetries of the system.

Figure 3.2 reveals three interesting features. First, the marginal-stability curve $\text{Re}\{\hat{\sigma}\} = 0$ appears to be independent of the amplitude $A$. This observation is confirmed analytically in §3.3.2.3. Second, for $A \lesssim 17.2$, the most unstable mode
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Figure 3.3: (a) The maximum growth rate $\text{Re}\{\sigma_M\}$, which asymptotically scales like $A^{4/9}$ as shown in the inset, and (b) the magnitude of the corresponding phase speed $c_M = -\text{Im}\{\sigma_M\}/\alpha_M$, which tends to the maximum background velocity $A$ asymptotically, as shown in the inset. The cross signifies the first data point after the change of most unstable mode at $A \approx 17.2$.

occurs at $\alpha = \beta = 0$ and has constant growth rate $\text{Re}\{\hat{\sigma}\} = 1$, which is the same as the case $A = 0$ discussed above in §3.3.2.1. Third, a new mode with $\beta = 1/2$ and $\alpha > 0$ becomes increasingly unstable as $A$ is increased, and, for $A \gtrsim 17.2$ (figure 3.2c,d), the new mode has a growth rate that exceeds that of the zero-wavenumber mode. For all higher values of $A$, this mode is the most unstable.

The most unstable mode is defined by the wavenumbers $(\alpha_M(A), \beta_M(A))$ that maximize the growth rate $\text{Re}\{\hat{\sigma}(\alpha, \beta, A)\}$ over $\alpha$ and $\beta$. We label the most unstable mode as $\sigma_M(A) = \hat{\sigma}(\alpha_M, \beta_M, A)$, and the corresponding cut-off value for convergence of the Fourier sum in (3.12) as $N_M(A) = N(\alpha_M, \beta_M, A)$.

The maximum growth rate $\text{Re}\{\sigma_M\}$ and the phase speed $c_M = -\text{Im}\{\sigma_M\}/\alpha_M$ are shown in figure 3.3. The change in the most unstable mode at $A \approx 17.2$ can be observed as the point where the maximum growth rate begins to increase and the phase speed becomes non-zero. Both $\text{Re}\{\sigma_M\}$ and $|c_M|$ show an asymptotic power-law dependence on $A$, which is very well fitted by

$$\text{Re}\{\sigma_M\} = 0.231A^{4/9}, \quad c_M = \pm A \quad \text{as} \quad A \to \infty. \quad (3.17a, b)$$

The most unstable mode, therefore, propagates at the maximum speed of the background flow, either up or down depending on the alignment of the perturbation.
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(see §3.3.2.4 below). (In fact, we find that the magnitude of the phase speed for all unstable modes with $\alpha > 0$ is asymptotically given by $A$, while that of the stable modes is zero.)

The wavenumbers of the most unstable mode are both zero for $A \lesssim 17.2$. At $A \approx 17.2$, the vertical wavenumber $\alpha_M$ becomes non-zero, and gradually decreases as $A$ increases further (figure 3.4a). Asymptotically, $\alpha_M$ is very well fitted by

$$\alpha_M = 0.332A^{-1/9} \quad \text{as} \quad A \to \infty.$$  

(3.18)

The corresponding horizontal wavenumber $\beta_M$ is 1/2 for all $A \gtrsim 17.2$, as suggested by the results of figure 3.2, which means that the most unstable perturbation has twice the wavelength of the background flow.

The cut-off value $N_M = N(\alpha_M, \beta_M, A)$ increases like $A^{2/9}$ for large $A$ (figure 3.4b). Since larger wavenumbers in the Fourier sum in (3.12) describe shorter horizontal scales, the need to increase $N_M$ for convergence suggests that the smallest horizontal scales of the most unstable perturbation decrease like

$$N_M^{-1} \sim A^{-2/9} \quad \text{as} \quad A \to \infty.$$  

(3.19)

In §3.4, we confirm that the truncated Fourier sum remains an accurate representation of the solution by comparison with an asymptotic expansion of the differential equations (3.11).

3.3.2.3 Marginal stability

The results of figure 3.2 suggest that the marginal-stability curve is independent of the amplitude $A$. Here we verify this suggestion analytically.

Marginal stability occurs when $\text{Re}\{\hat{\sigma}\} = 0$. Numerical results for general $A > 0$ suggest that the eigenvector $G$ corresponding to the marginally stable modes takes the simple form $G_{-1} = \pm G_0$, and $G_n = 0$ for $n \neq 0, -1$. Motivated by this observation, and the corresponding form of $F_n$ from (3.13a), we consider eigenvectors $[F, G]$ of the form

$$F = \pm [\sin \beta X + \sin (1 - \beta)X], \quad G = \mp [\cos \beta X + \cos (1 - \beta)X]. \quad (3.20a, b)$$
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Figure 3.4: (a) The vertical wavenumber $\alpha_M$ of the most unstable mode, which asymptotically scales like $A^{-1/9}$ as shown in the inset, and (b) the cut-off $N_M = N(\alpha_M, \beta_M, A)$ for the Fourier sum in (3.12), which asymptotically scales like $A^{2/9}$ as shown in the inset. The origin of the discontinuity at $A \approx 10^7$ is unclear. The cross signifies the first data point after the change of most unstable mode at $A \approx 17.2$.

On substituting (3.20) into the advection-diffusion equation (3.11b), we obtain

$$\left[ \sigma + (\beta^2 + \alpha^2 - \beta) \right] G = i\alpha A \left[ \sin XF - \cos XG \right],$$

(3.21)

which, by using double-angle formulae and (3.20), reduces to

$$\left[ \sigma + (\beta^2 + \alpha^2 - \beta) \right] = \pm i\alpha A.$$  
(3.22)

The eigenfunctions (3.20) must also satisfy Poisson’s equation (3.11a); this gives the requirement that

$$\beta = \beta^2 + \alpha^2,$$

(3.23)

which is precisely the marginal-stability relationship for $A = 0$ given in (3.16). Combining (3.22) and (3.23) gives

$$\sigma = \pm i\alpha A,$$

(3.24)

which corresponds to a phase speed of $|c| = A$ and a growth rate of zero.

The marginal-stability curve (3.23) is, therefore, independent of $A$, as are the corresponding eigenfunctions $[F, G]$ (3.20), provided $A > 0$. Interestingly, the
eigenfunctions do differ from those for $A = 0$, which are pure Fourier modes with
wavenumber $\beta$; the presence of background flow with unit wavenumber introduces
an additional component to the marginally stable perturbation with wavenumber
$1 - \beta$.

### 3.3.2.4 Structure of the most unstable perturbation

For $A \lesssim 17.2$, the most unstable mode has $\alpha_M = \beta_M = 0$, growth rate $\text{Re}\{\sigma_M\} = 1$
and phase speed $c_M = 0$. The instability takes the form of a roll-like perturbation
of the background temperature gradient, with a wavelength that is independent
of the background columnar flow. At $A \approx 17.2$, a different mode becomes the
most unstable, which has half the horizontal wavenumber of the background flow
$\beta_M = 1/2$. The vertical wavenumber and phase speed of this mode are also both
non-zero.

Figure 3.5 shows the structure of the most unstable mode for $A = 2.5 = 32$
(figure 3.5a,c) and $A = 2^{20} \approx 10^6$ (figure 3.5b,d). The perturbation takes the form
of tall, thin, counter-rotating rolls (figure 3.5a,b; right-hand plots). Each roll has
width $2\pi$, and is centred on a downwelling of the background columnar flow. The
whole perturbation has horizontal period $4\pi$. The temperature perturbation $\tilde{\Theta}$
takes the form of claw-shaped pulses centred on the upwellings of the background
flow (figure 3.5a; left-hand plot), which, for larger amplitudes (figure 3.5b; left-
hand plot), split into two neighbouring pulses of the same sign.

The vertical velocity $\tilde{W}$ and temperature $\tilde{\Theta}$ of the dominant perturbation (fig-
ure 3.5c,d) are symmetric about $X = 2n\pi$ for integer $n$, and are almost indistin-
guishable from each other. As $A$ increases, the profiles of $\tilde{\Theta}$ and $\tilde{W}$ become
increasingly sinusoidal in the intervals $(2n\pi, 2(n+1)\pi)$, but their gradients change
by an $O(1)$ amount through increasingly narrow regions centred on $X = 2n\pi$. The
horizontal velocity $\tilde{U}$ either diverges away from or converges into these regions.

The perturbations shown in figure 3.5 have a phase speed $c_M = A$ to leading
order, and thus move upwards at the maximum speed of the background flow. If
the perturbation were shifted horizontally by $\pi$, the pulses would be centred on
the downwellings of the background flow and the phase speed would be $c_M = -A$;
the growth rate and vertical wavenumber would be unchanged.
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Figure 3.5: The structure of the most unstable perturbation (a,c) for \( A = 2^5 \) and (b,d) for \( A = 2^{20} \). Panels (a) and (b) show contours of the perturbation temperature \( \tilde{\Theta} \) (left) (scaled to unit amplitude), at intervals of 0.4, and streamlines (right) with arrows showing the direction of the flow, together with schematic profiles of the background flow \( \Theta_0 = W_0 \) (top). The perturbation is doubly periodic, with horizontal period \( 4\pi \) and vertical period \( 2\pi/\alpha_M \). Panels (c) and (d) show horizontal profiles of the perturbation quantities (scaled to unit amplitude): upper plots show the temperature \( \tilde{\Theta} \) (solid) and vertical velocity \( \tilde{W} = -\partial \tilde{\Psi}/\partial X \) (dashed) at \( Z = \pi/2\alpha_M \); lower plots show the horizontal velocity \( \tilde{U} = \partial \tilde{\Psi}/\partial Z \) (solid) at \( Z = \pi/\alpha_M \), together with the background columnar flow \( \Theta_0 \) (dotted) scaled by \( A \). The vertical velocity and temperature perturbations are almost indistinguishable. The perturbations shown here propagate upwards; the same perturbations shifted horizontally by \( \pi \) would propagate downwards and have the same growth rate.
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3.4 Asymptotic analysis of linear stability for $A \gg 1$

Motivated by the structure of the most unstable perturbation as just described, and in order to understand the physical balances behind the instability, we examine the linear stability of heat-exchanger flow in the asymptotic limit $A \gg 1$. In this limit, the dominant balance in the advection–diffusion equation (3.11b) is most obviously between horizontal advection of the background temperature by the perturbation $\sim \alpha A \sin XF$ and vertical advection of the perturbation flow by the background velocity $\sim \alpha A \cos XG$. However, the perturbation plotted in figure 3.5(d) shows that advection cannot dominate everywhere; the temperature gradient changes by an $O(1)$ amount through regions centred on $X = 2n\pi$ for integer $n$, which suggests the presence of boundary layers in which horizontal diffusion enters the leading-order balance.

We first observe that the linearized governing equations (3.11) exhibit a number of symmetries. Suppose that, for a given eigenvalue $\sigma(A,\alpha)$, we have solutions $[F(X),G(X)]$. It is clear from the form of (3.11) that $[-F(-X),G(-X)]$, $[F(2\pi + X),G(2\pi + X)]$, and $[-F(2\pi - X),G(2\pi - X)]$ are all also solutions, as are any linear combinations of these. Thus we are free to construct solutions with any given reflectional symmetry around $X = 0$ and $X = \pm \pi$. Motivated by the symmetries of the most unstable mode shown in figure 3.5, we consider a solution $[F,G]$ in which $G$ is even under reflection about $X = 0$ and odd under reflection about $X = \pm \pi$, and $F$ is odd under reflection about $X = 0$ and even under reflection about $X = \pm \pi$. Such a solution is periodic with period $4\pi$.

As discussed above, we anticipate boundary-layer regions located near $X = 2n\pi$, for integer $n$, in which horizontal diffusion ($G''$) enters the leading-order balance in (3.11b). We therefore look for an asymptotic solution over the range $0 \leq X \leq 2\pi$, which has the symmetries of $[F,G]$ discussed above, with an inner region near $X = 0$ where diffusion is important, and an outer region away from $X = 0$ where the advection terms dominate.

In order to motivate the asymptotic scalings, we also recall the measured scalings from the full Floquet analysis of §3.3 for the growth rate $\text{Re}\{\sigma\} \sim A^{4/9}$, the phase speed $c_M = -\text{Im}\{\sigma\}/\alpha_M = A$, and the vertical wavenumber $\alpha_M \sim A^{-1/9}$.
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(see 3.17 and 3.18).

3.4.1 Asymptotic expansion

We consider the limit of large amplitude $A$ and of small vertical wavenumber $\alpha$, such that $\alpha A \gg 1$ and $\alpha \ll 1$, and we try

$$\sigma = -i\sigma_0 \alpha A + \sigma^*, \tag{3.25}$$

where $|\sigma^*| \ll \alpha A$, and $\sigma_0$ is an $O(1)$ constant to be determined. The perturbation equations (3.11) can be rewritten as

$$F'' + G' = \alpha^2 F, \quad \alpha A (\cos X - \sigma_0) G - \alpha A \sin XF + \sigma^* G + F' = G'' - \alpha^2 G. \tag{3.26a, b}$$

The boundary conditions come from the symmetries of the solution as discussed above, and are given by

$$F(0) = G'(0) = G(\pi) = F'(\pi) = 0. \tag{3.27}$$

Based on the limits $\alpha A \gg 1$, $\alpha \ll 1$, the leading-order behaviour of (3.26) away from $X = 0$ is given by

$$F' + G = c_0, \quad (\cos X - \sigma_0) G - \sin XF = 0, \tag{3.28a, b}$$

where $c_0$ is a constant of integration that comes from the first integral of (3.26a). Equation (3.28) has solutions

$$F = (\cos X - \sigma_0) \left(1 + c_0 \int \frac{dX}{\cos X - \sigma_0}\right), \quad G = \sin X \left(1 + c_0 \int \frac{dX}{\cos X - \sigma_0}\right), \tag{3.29a, b}$$

where, without loss of generality, the arbitrary amplitude of the perturbations has been scaled to unity. Based on the form of the numerical solutions in figure 3.5, we assume that there are no leading-order discontinuities in $F$ at $X = 0$ or in $G$ at $X = \pi$. The boundary conditions (3.27) thus imply that $\sigma_0 = 1$ and that $c_0 = 0,$
such that the leading-order outer solutions are given by

\[ F = \cos X - 1, \quad G = \sin X. \]  \hfill (3.30a, b)

The leading-order phase speed \( c = -\text{Im}\{\sigma\}/\alpha = \sigma_0 A \) is given by \( c = A \), as we found numerically in (3.17b)

Since \( \sigma_0 = 1 \), the coefficients \( \cos X - \sigma_0 \) and \( \sin X \) of the \( O(\alpha A) \) terms in (3.26b) both vanish as \( X \to 0 \), which suggests an inner boundary-layer region there, as indicated by the numerical solutions. We look for a balance in (3.26b) between the advection terms, horizontal diffusion \( G'' \) and growth \( \sigma^* G \). This balance gives \( \alpha A X^2 G \sim \alpha A X F \sim \sigma^* G \sim G/X^2 \). From (3.30b), we also have that \( G \sim X \) as \( X \to 0 \). Based on these balances, we define the following inner variables:

\[ \xi = (\alpha A)^{1/4} X; \quad s = (\alpha A)^{-1/2} \sigma^*; \quad g(\xi) = (\alpha A)^{1/4} G(X); \quad f(\xi) = (\alpha A)^{1/2} F(X). \]  \hfill (3.31a, b, c, d)

Rewritten in terms of the inner variables, the governing equations (3.26) become

\[ f'' + g' = \alpha^2 (\alpha A)^{-1/2} f, \quad g'' - \left(s - \frac{i \xi^2}{2}\right) g + i \xi f = (\alpha A)^{-1/2} \left(f' + \alpha^2 g\right). \]  \hfill (3.32a, b)

At leading-order,

\[ f' + g = \gamma_0, \quad g'' - \left(s - \frac{i \xi^2}{2}\right) g + i \xi f = 0. \]  \hfill (3.33a, b)

The constant of integration \( \gamma_0 \) in (3.33a) is determined by matching with the outer region: by integrating (3.26a) and substituting from (3.30a), we obtain to leading order

\[ F' + G = \alpha^2 \int_\pi^X (\cos X - 1) \, dX = \alpha^2 (\sin X - X + \pi), \]  \hfill (3.34)

where the lower limit of the integral has been determined from the boundary conditions (3.27c, d). The right-hand side of (3.34) is given by \( \alpha^2 \pi \) to leading order as \( X \to 0 \), which, together with the inner scalings (3.31c, d), determines the
constant of integration in (3.33a) as
\[
\gamma_0 = \alpha^2 (\alpha A)^{1/4} \pi = (\alpha A^{1/9})^{9/4} \pi.
\]  
(3.35)

The boundary conditions for (3.33) are given by the two symmetry conditions (3.27a, b) \( f(0) = g'(0) = 0 \) and a matching condition that \( g \to \xi \) as \( \xi \to \infty \). In appendix 3.A, we consider the generic behaviour of the solutions of (3.33), and find that the matching condition constitutes two constraints on the differential equation; we therefore have four conditions on a third-order system, which is sufficient to determine the unknown eigenvalue \( s \). We solve (3.33) numerically, and determine \( s \) as a function of the rescaled vertical wavenumber

\[
\alpha^* \equiv \alpha A^{1/9},
\]  
(3.36)

(cf. 3.35). The leading-order growth rate is then given by \( \Re\{\sigma^*\} = (\alpha A)^{1/2} \Re\{s(\alpha^*)\} \) from (3.31b), or alternatively

\[
\Re\{\sigma^*\} = A^{4/9} \Re\{S(\alpha^*)\}, \quad \text{where} \quad S(\alpha^*) = \alpha^{1/2} s(\alpha^*).
\]  
(3.37)

Numerical solutions for the leading-order scaled growth rate \( \Re\{S(\alpha^*)\} \) are shown in figure 3.6(a). The eigenvalue with the maximum growth rate is given by \( S = 0.2308 - 0.182i \) and occurs at \( \alpha^* = 0.332 \), such that \( \Re\{\sigma^*\} = 0.2308 A^{4/9} \) at \( \alpha = 0.332 A^{-1/9} \). These values agree extremely well with the measurements presented in figures 3.3(a) and 3.4(a) for the maximum growth rate \( \Re\{\sigma_m\} \) and the corresponding vertical wavenumber \( \alpha_m \), respectively. Since the imaginary part of \( S \) is negative, the second-order correction to the phase speed is positive, and is given by \( -\Im\{\sigma^*\}/\alpha = 0.55 A^{5/9} \). The dependence of \( \Re\{S\} \) on the wavenumber \( \alpha^* \) (figure 3.6a) shows very good agreement between the asymptotic analysis and the full solutions of the Floquet analysis for large \( A \), as do the eigenfunctions \([f, g]\) of (3.33), which give the leading-order behaviour of \([F, G]\) near \( X = 0 \) (figure 3.6b).

The leading-order growth rate \( \Re\{S(\alpha^*)\} \) increases for small \( \alpha^* \) and decreases for large \( \alpha^* \) (figure 3.6a). In appendix 3.B, in order to understand this behaviour, we analyse the leading-order equations for the inner region (3.33) in the asymptotic
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\[ \xi = (\alpha A)^{1/4}X \]

Figure 3.6: Asymptotic solutions \( (A \gg 1) \) and full numerical solutions of the eigenvalue problem (3.15). (a) The leading-order scaled growth rate \( \text{Re}\{S\} = \alpha^{1/2}\text{Re}\{s\} = A^{-4/9}\text{Re}\{\sigma^*\} \) against the scaled vertical wavenumber \( \alpha^* = \alpha A^{1/9} \): the asymptotic solution (line), and the full numerical solutions for \( A = 2^{10} \) (crosses), \( A = 2^{20} \) (squares), and \( A = 2^{30} \) (dots). (b) The solution \([f, g] = [(\alpha A)^{1/2}F, (\alpha A)^{1/4}G]\) (solid and dashed lines, respectively) of (3.33), together with full solutions of (3.15) for \( A = 2^{30} \) (solid and hollow circles, respectively).

limits \( \alpha^* \ll 1 \) and \( \alpha^* \gg 1 \). The physical basis for the decay in the growth rate at small and large \( \alpha^* \) is discussed below.

3.4.2 Physical mechanism of instability for \( A \gg 1 \)

It has proved difficult to unravel the precise details of the physical mechanism of instability, largely owing to the fact that the growth rate depends on a subtle second-order interaction between boundary-layer regions and the main flow. However, based on the form of the asymptotic equations, we can make various observations about the relevant physical components that control the propagation and growth of perturbations.

The leading-order evolution of the most unstable perturbation for \( A \gg 1 \) is neutral propagation at speed \( c = \pm A \), which is the maximum speed of the background flow. The neutral propagation is the result of a leading-order advective balance between two processes: horizontal advection of the background temperature field \( \Theta_0 \) by the perturbation velocity \( \tilde{U} \), and vertical advection of the perturbation temperature field \( \tilde{\Theta} \) by the background velocity \( W_0 \). We illustrate this balance by working in a frame of reference moving with the perturbation, as sketched in figure...
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3.7. We consider an upwards propagating perturbation \( c = +A \), but the discussion equally applies to downwards propagating perturbations. Since the vertical wavenumber \( \alpha_M \) is small, Darcy’s law implies that the perturbation temperature \( \tilde{\Theta} \) and vertical velocity \( \tilde{W} \) are proportional. By mass conservation, the horizontal velocity \( \tilde{U} \) is strongest where the vertical variation of \( \tilde{W} \) is largest, which occurs where \( \tilde{W} \) vanishes. The perturbation flow therefore takes the form of tall thin circulating cells. Horizontal advection of \( \Theta_0 \) by \( \tilde{U} \) leads to an induced temperature perturbation (shown dashed on the right-hand side of figure 3.7) that is vertically out of phase with the original temperature perturbation. Downwards vertical advection of the induced temperature perturbation by the background flow \( W_0 \) (in this propagating frame) balances the horizontal advection in such a way that the original perturbation is sustained.

The leading-order advective balance gives a neutrally propagating mode. Growth occurs because of horizontal diffusion in the thin boundary-layer regions centred on the lines \( X = 2n\pi \), across which the temperature gradient changes significantly. The importance of diffusion can be seen by an examination of (3.33\text{b}), which shows that the two advective processes described above are balanced by diffusion \( (g'') \) and growth \( (sg) \) in these boundary-layer regions. Indeed, (3.33\text{b}) also shows that the advective processes, which have imaginary coefficients, and diffusion, which has a real coefficient, are vertically out of phase, so that we might expect the rescaled eigenvalue \( s \) to have both a non-zero imaginary part, which gives a correction to the phase speed, and a non-zero real part, which gives growth.

The strength of diffusion, which must determine the growth rate, depends on the rescaled vertical wavenumber \( \alpha^* \). We found in §3.4.1 that the growth rate decreases at both large and small \( \alpha^* \) (figure 3.6a). For \( \alpha^* \ll 1 \), the perturbation cells are very long, and, by continuity, the horizontal velocity is weak. The boundary-layer regions, which have a width that is set by the strength of the horizontal advection, are therefore wider (as in (3.31\text{a})), so the diffusive flux is weaker, and the growth rate decreases. Conversely, for \( \alpha^* \gg 1 \), the horizontal velocity is strong. In this limit, the perturbation in the boundary-layer regions takes a different form: the temperature is smoothed out by strong horizontal advection, and the leading-order advective balance no longer gives discontinuities in the temperature gradient (see appendix 3.B). Owing to this smoothed temperature profile, diffu-
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Figure 3.7: A schematic of the instability for $A \gg 1$, in a frame of reference moving with the perturbation. The background vertical velocity $W_0 = A \cos X - A$ in this frame is shown at the top. The left-hand side shows streamlines of the perturbation flow; the perturbation temperature $\tilde{\Theta}$ is proportional to the vertical velocity $\tilde{W}$, and locations at which pulses form on the background columns as a result of the instability are marked with a $\oplus$. The right-hand side shows horizontal profiles (all scaled to unit amplitude) along the lines of constant $z$ as marked. Each plot shows the background temperature field $\Theta_0$ (dotted), together with one of the perturbation velocities (solid) as labelled on the right; in each plot, the velocity not shown is zero. The plots at $Z = \pi/\alpha_M$ and $Z = 2\pi/\alpha_M$ also show the induced temperature perturbations (dashed) that result from horizontal advection of the background field $\Theta_0$ by $\tilde{U}$. The neutral propagation of the perturbation is sustained by downwards advection of the induced temperature perturbation by the background velocity $W_0$. 
sion only enters the balance at higher order, and so both the diffusive flux and the growth rate decrease. We therefore find that there is a balance between diffusion being too weak for $\alpha^* \ll 1$ and horizontal velocity being too strong for $\alpha^* \gg 1$, which gives rise to an optimal wavenumber $\alpha^* = 0.332$ at which the growth rate is maximum.

Interestingly, the instability process discussed above is independent of the background linear temperature gradient. Indeed, the analysis of §3.4.1 shows that the term describing advection of the background temperature gradient ($F'$) does not enter the asymptotic equations. This contrasts with the control of the instability for small $A$ by the background temperature gradient.

Another interesting implication of the above discussion is that thermal diffusion provides a destabilizing mechanism for the flow. In appendix 3.C, we examine a related system of columnar-exchange flow of two fluids of different densities in the absence of diffusion, and we find that the flow is always neutrally stable. This observation supports the idea that diffusion is required for the growth of perturbations. There is some parallel between the role of thermal diffusion here and the role of viscosity in the stability of plane Poiseuille flow (e.g. Drazin 2002), where the flow is linearly unstable for sufficiently large Reynolds numbers, but is linearly stable in the inviscid limit.

### 3.5 Evolution of the instability in the non-linear regime

In order to explore the development of the instability beyond the linear regime, we examined heat-exchanger flow using high-resolution direct numerical simulations. We set the temperature $\Theta = \Theta_0 + \tilde{\Theta}$ to be the steady heat-exchanger solution $\Theta_0 = A \cos X - Z$, as in (3.8a), plus an initially small perturbation $\tilde{\Theta}(X, Z, \tau)$, and then solved the non-linear governing equations (3.7) for the evolution of $\tilde{\Theta}$ numerically. In order to clearly observe the non-linear evolution of the instability, we used doubly periodic boundary conditions for $\tilde{\Theta}$ and for the corresponding streamfunction $\tilde{\Psi}$ (given by 3.7a). We used a vertical period of $2\pi/\alpha_M \approx 18.9 A^{1/9}$, which is the height of the most unstable mode calculated in §3.3. The initial value
of $\tilde{\Theta}$ was proportional to the most unstable mode.

Snapshots of the temperature field $\Theta$ at different times for $A = 2^8 = 256$ and horizontal period $L = 8\pi$ are shown in figure 3.8(a–d), together with the corresponding magnitude of the perturbation over time (figure 3.8(e)) and dominant wavenumber of the flow (figure 3.8(f)). The linear growth of the instability leads to the formation of pulses (figure 3.8(a)) which move with the background flow. Once the pulses have reached a certain size, the amplitude stops growing, and the flow becomes unstable to a secondary instability, which breaks the symmetry of the solution and results in less regular motion (figure 3.8(b,c)). The system gradually re-organizes into columnar flow with a quarter of the wavenumber of the original flow (figure 3.8(d)), but the same background temperature gradient, which remains imposed by the representation $\Theta = \Theta_0 + \tilde{\Theta}$.

However, the wavenumber and background gradient of a steady heat-exchanger flow are linked by (3.5a); hence if the wavenumber decreases and the gradient is fixed, the flow can no longer be a steady solution of the governing equations. Instead, we find that the amplitude of the flow grows exponentially (figure 3.8(e)). It is straightforward to show that the governing equations permit unsteady columnar flow with a fixed background temperature gradient for any wavenumber $\kappa$; this generalized time-dependent columnar flow is given by

$$\Theta = Ae^{(1-\kappa^2)\tau} \cos \kappa X - Z, \quad W = Ae^{(1-\kappa^2)\tau} \cos \kappa X, \quad (3.38a, b)$$

for any amplitude $A$. The steady solution $\kappa = 1$ (3.8) can be thought of as the marginally stable solution: if $\kappa > 1$, horizontal diffusion dominates and the amplitude decays; if $\kappa < 1$, advection dominates and the amplitude grows. In the results of figure 3.8, the system ultimately adopts a wavenumber $\kappa = 1/4$, and the magnitude of the flow grows like $e^{15\tau/16}$ (figure 3.8(e)). We note that the continued exponential growth at late times only arises because it can feed off the fixed background temperature gradient that is imposed in an effectively infinite domain.

The main conclusion from this calculation is that the non-linear evolution of the instability leads to a reduction of the wavenumber of the flow. We have also carried out simulations in domains with different horizontal periods $L$; in each case
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Figure 3.8: Nonlinear dependence of the instability for $A = 2^8$ and horizontal period $L = 8\pi$. Snapshots of the temperature field $\Theta(X, Z, \tau)$ at times: (a) $\tau = 4$, the growth of pulses on the background flow that result from linear instability; (b) $\tau = 7$ and (c) $\tau = 11$, the secondary instability; and (d) $\tau = 14$, the growing heat-exchanger flow with a quarter of the original wavenumber (3.38). Panel (e) shows the magnitude of the perturbation over time, as measured by the L2 norm and scaled by the initial magnitude; dots correspond to the pictures in the previous panels. The asymptotic growth of the most unstable mode (from (3.17a)) and the growth of the unsteady exchange flow (3.38) are also shown, for comparison. Panel (f) shows the dominant wavenumber $k$ of the flow (measured by a Fourier transform of the temperature field at $Z = 0.5$), for simulations with different horizontal periods $L$ as marked; in each case, the wavenumber decreases towards the fundamental mode $2\pi/L$.

the flow coarsened due to a secondary instability, leaving one upwelling and one downwelling column in the domain (figure 3.8f).
3.6 Implications for two-dimensional convection in a porous medium

In this section, we return to the linear-stability analysis of §3.3 and consider the implications of this analysis for columnar flow in a vertically confined domain. Specifically, we investigate whether stability might provide the mechanism that controls the horizontal scale of the columnar flow in the interior of a two-dimensional Rayleigh–Darcy cell at high $Ra$.

3.6.1 The wavenumber of columnar flow in a Rayleigh–Darcy cell at high $Ra$

Flow in a Rayleigh–Darcy cell for $Ra \gtrsim 1300$ is dominated in the interior by columnar flow. This nearly steady interior flow is fed from the upper and lower boundaries of the cell by vigorous mixing and merging of short-wavelength protoplumes (see figure 3.1a). The numerical measurements presented in chapter 2, which are taken from a cell of height $H = 1$ for the range $1300 \leq Ra \leq 4 \times 10^4$, suggest that the columnar flow in the interior of the cell is increasingly well described by the steady heat-exchanger solution in (3.5) as $Ra \to \infty$. Measurements of the dominant wavenumber $k$ over the same range were approximated by $k \approx 0.48Ra^{0.4}$, although there are significant fluctuations in the data, and there is some suggestion of a slightly weaker exponent at very large $Ra$ (see §2.4.1.2).

It is important to note that there are some significant differences between the columnar flow in a Rayleigh–Darcy cell at high $Ra$ and the steady unconfined heat-exchanger flow that has been the subject of this chapter so far. Most notably, the cell has a finite height, and the flow in the interior is fed by time-dependent protoplumes at the upper and lower boundaries as discussed above, whereas the heat-exchanger flow (3.5) has an infinite height, and any disturbances propagate indefinitely. It is, nonetheless, interesting to try applying some of the results from the stability of unconfined heat-exchanger flow to the flow in a vertically confined domain, and to compare the resultant scalings of this simple analysis with numerical measurements of the dominant wavenumber $k$.

In ideal heat-exchanger flow, the amplitude of the temperature and vertical ve-
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Figure 3.9: Measurements of the amplitude of the temperature $\hat{T}$ (dots) and vertical velocity $\hat{w}$ (circles) of the columnar flow in the interior of a Rayleigh–Darcy cell (adapted from figure 2.7). The amplitudes appear to tend to approximately the same constant value, $\hat{T}, \hat{w} \to 0.117$, as $Ra \to \infty$. (This result is directly equivalent to the asymptotic ‘classical’ linear scaling of the Nusselt number with $Ra$, as observed in chapter 2.) For comparison with the linear-stability analysis, we choose $\hat{A} = \hat{w}$.

In a vertically confined domain, we hypothesize that a perturbation to the steady columnar flow will destabilize the flow if the time scale for growth of the perturbation is shorter than the time scale for the perturbation to advect from one boundary to the other. We assume that the regions of protoplumes at the upper and lower boundaries provide perturbations to the columnar flow on a range of scales. Since the height of the Rayleigh–Darcy cell in rescaled co-ordinates ($\S 3.2.2$) is $H = k$, the time scale for advection of the most unstable perturbation across the domain for $A \gg 1$ is $H/c_M = k/A$ (from 3.17$b$), and the time scale for growth of the most unstable perturbation is $1/\text{Re}\{\sigma_M\} = 1/(0.231A^{4/9})$ (from 3.17$a$). A comparison of these time scales, which is the hypothesized condition for instability, gives

$$\frac{k}{A} \gtrsim \frac{1}{0.231A^{4/9}} \quad \text{for} \quad A \gg 1,$$

(3.39)
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Figure 3.10: Measurements of the wavenumber $k$ from a Rayleigh–Darcy cell of height $H = 1$ and aspect ratio either $L = 1$ or $L = 2$, taken from figure 2.8: (a) the wavenumber $k(Ra)$ (dots) together with the asymptotic stability estimate (3.40) (dashed line) and the approximate correction to the asymptotic scaling for finite $Ra$ and $A$ from (3.41) (solid line); and (b) the scaled wavenumber $k/Ra^\lambda$ for trial exponents $\lambda = 5/14$ (dots), $\lambda = 0.4$ (crosses), and $\lambda = 0.5$ (circles), together with the asymptotic stability estimate (3.40) (dashed line) and the correction from (3.41) (solid line), both scaled by $0.7Ra^{5/14}$. The measured data follows the trend of the correction (solid line) over this range of $Ra$.

which reduces to

$$k \gtrsim 2.6 (\hat{w}Ra)^{5/14} \gtrsim 1.2 Ra^{5/14} \quad \text{for} \quad Ra \gg 1,$$

(3.40)
on using $A = \hat{A}Ra/k = \hat{w}Ra/k$ and the observation that $\hat{w} \to 0.117$ as $Ra \to \infty$. We note that, since (3.40) is simply obtained by a comparison of time scales, we would not expect the numerical pre-factor in (3.40) to be accurate, beyond giving a rough estimate of the order of magnitude.

For $A \lesssim O(10^4)$, both the growth rate and the phase speed of the most unstable mode are found numerically to be slightly larger than the asymptotic scalings (3.17) (see inset to figure 3.3). In addition, for $Ra \lesssim O(10^4)$, the amplitude $\hat{w}$ is slightly larger than its asymptotic value (see figure 3.9). We found simple empirical fits $\Re\{\sigma_M\} \approx 0.231A^{4/9} + 0.34A^{-0.2}$ and $c_M \approx A + 0.55A^{0.55}$ to the numerical data for $A \gtrsim 17.2$, and $\hat{w} \approx 0.117 + 2900Ra^{-1.8}$ to the amplitude for $Ra \geq 1300$. By using these fits in the balance of time scales $k/c_M \sim 1/\Re\{\sigma_M\}$, as above, with $A = \hat{w}Ra/k$, we obtain a correction for finite $Ra$ and $A$ to the asymptotic
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stability estimate (3.40). This approximate correction \( k(Ra) \) is given implicitly by the equations

\[
k = \frac{A + 0.55A^{0.55}}{0.231A^{4/9} + 0.34A^{-0.2}}; \quad kA = Ra \left(0.117 + 2900Ra^{-1.8}\right).
\]

(3.41)

Figure 3.10(a) shows measurements of the time-averaged dominant wavenumber \( k(Ra) \) from a Rayleigh–Darcy cell for \( 1300 < Ra \leq 4 \times 10^4 \), together with the asymptotic stability estimate (3.40) (dashed line), and the approximate correction to the asymptotic scaling, given by the solution of (3.41) (solid line). The measured data lies inside the stable region, and appears to give good agreement with the trend of the stability estimates.

In order to examine this agreement more closely, we can rescale the wavenumber and the stability estimates by different trial powers of \( Ra \) (figure 3.10(b)). As a preliminary observation, we can see from this rescaling that the measured data exhibits a distinctly weaker scaling than \( k \sim Ra^{1/2} \), which was identified as the ‘minimal flow unit’ for steady convection (Corson, 2011). Instead, as found in chapter 2, the data is fairly well described by the scaling \( k \sim Ra^{0.4} \) over this range of \( Ra \), which is slightly stronger than the asymptotic stability estimate \( k \sim Ra^{5/14} \). However, it is also evident that the estimate corrected for finite \( Ra \) and \( A \) (solid line) differs appreciably from the asymptotic estimate (dashed line) over this range of \( Ra \), and that the measured data follows the trend of the correction. (The parameter \( A \) for the data shown lies in the range \( 25 \lesssim A \lesssim 150 \).) In particular, although there is significant scatter, the data appears to show a slight trend towards a lower exponent at the highest values of \( Ra \), in agreement with the prediction of the stability estimate.

The measured data does, therefore, appear to be consistent with the theoretical stability estimate. Given the very different boundary conditions between the Rayleigh–Darcy cell and the unconfined heat-exchanger flow, this qualitative agreement is notable. Figure 3.10(b) suggests that the Rayleigh number for the measured data is still too low to observe the hypothesized asymptotic scaling \( k \sim Ra^{5/14} \); numerical measurements of \( k \) at higher values of \( Ra \) would be needed to confirm this suggestion.
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3.6.2 The onset of the high-$Ra$ regime in a Rayleigh–Darcy cell

Working on the hypothesis that stability controls the horizontal scale of the interior flow in a Rayleigh–Darcy cell, it is natural to consider what happens as $Ra$ decreases, or, equivalently, as the re-scaled amplitude of the flow $A$ decreases. In §3.3.2, we found that the nature of the dominant instability in an unbounded domain changes completely when $A \lesssim 17.2$. A similar dramatic change is observed in the dynamics of the Rayleigh–Darcy cell as $Ra$ decreases below $Ra \approx 1300$ (Graham & Steen, 1994; Otero et al., 2004), from columnar-exchange flow in the interior for $Ra \gtrsim 1300$ to large-scale convective rolls for $Ra \lesssim 1300$.

Numerical measurements of $k$ and $\hat{A} = \hat{w}$ at $Ra = 1380$, which is just above the onset of high-$Ra$ convection, give a value of $A \approx 14.5$ (alternatively, using $\hat{A} = \hat{T}$ gives $A \approx 15.6$), which is remarkably close to the bifurcation value $A \approx 17.2$ in the linear-stability problem. In fact, since the most unstable mode of the unbounded flow for $A < 17.2$ has zero wavenumber in both directions, which is not physically achievable in a finite domain, we would expect the Rayleigh–Darcy cell to have a slightly lower bifurcation value of $A$. The rough agreement demonstrated here provides an intriguing direction for further investigation, and again suggests that stability criteria may play an important role in the dynamical structure of the Rayleigh–Darcy cell.

3.7 Conclusions

We have examined the stability of columnar convection in a two-dimensional porous medium. The flow is characterized by dimensionless horizontal wavenumber $k$, amplitude $\hat{A}$, and background temperature gradient $-k^2/Ra$. The stability of the flow in an unbounded domain is a function of the parameter $A = \hat{A}Ra/k$ alone.

We used a Floquet analysis to determine the eigenvalues $\sigma$ of the linear-stability problem (3.11) numerically. Somewhat surprisingly, the marginal-stability curve $\text{Re}\{\sigma\} = 0$ is independent of $A$ and thus given by the usual criterion $\beta = \beta^2 + \alpha^2$ for stability of a linear temperature field, where $\beta$ and $\alpha$ are the horizontal and
vertical wavenumbers, respectively. For small $A$, the most unstable mode is given by $\alpha = \beta = 0$, and has growth rate $\text{Re}\{\sigma\} = 1$; this mode is an instability of the background linear temperature gradient, and is independent of the columnar flow. However, at $A \approx 17.2$, a different mode becomes the most unstable. This mode has double the horizontal period of the background flow ($\beta = 1/2$), takes the form of vertically propagating pulses on the background columns, and has a growth rate that increases with $A$. Asymptotically, the vertical wavenumber of the most unstable mode is given by $\alpha = 0.332A^{-1/9}$, the growth rate by $\text{Re}\{\sigma\} = 0.2308A^{4/9}$, and the vertical phase speed by $|c| = A$. The sign of $c$ changes if the perturbation is shifted horizontally by $\pi$ (a quarter period).

For $A \gg 1$, advective processes dominate the flow across almost all of the domain: horizontal advection of the background temperature by the perturbation flow balances vertical advection of the perturbation temperature by the background flow. In the absence of any diffusion, this advective balance would simply give a neutrally stable propagating mode. However, the temperature gradient changes significantly across thin boundary-layer regions that are centred on the maxima (for upwelling perturbations) or minima (for downwelling perturbations) of the background flow. Horizontal diffusion in these boundary-layer regions provides a mechanism for growth, as discussed in §3.4.2. Interestingly, the instability is independent of the background vertical temperature gradient in the limit $A \gg 1$, and is driven entirely by the columnar flow.

Numerical simulations of the non-linear evolution of the instability for $A \gtrsim 17.2$ in a periodic domain show that perturbations initially grows in accordance with linear theory, before the flow undergoes a secondary instability. After a period of reorganization, the system evolves into a new columnar flow with a smaller wavenumber than the original flow.

Persistent vertical columnar structures have also been observed in three-dimensional porous convection (e.g. Pau et al. 2010; Fu et al. 2013, and chapter 7 below), and it seems likely that many of the ideas discussed in this chapter could be extended to three dimensions. However, while it is straightforward to write down three-dimensional heat-exchanger base flows, the linear-stability analysis of such flows is much more complicated than in two dimensions (primarily owing to the double expansion in the Floquet analysis). In fact, even the leading-order
advection–propagation balance for $A \gg 1$ does not yield analytic solutions in three-dimensions, unlike in two dimensions (see (3.30)). A three-dimensional stability analysis is left for future work. A detailed investigation of the interior flow of statistically steady three-dimensional porous convection is presented in chapter 7.

This work was motivated by the hitherto unexplained mechanism that controls the horizontal wavenumber of the columnar flow in the interior of a two-dimensional Rayleigh–Darcy cell at high $Ra$. Numerical measurements of this flow suggest that it is increasingly well described by the steady heat-exchanger solution as $Ra \to \infty$ (chapter 2). By a comparison of the time scales for growth and propagation of the most unstable mode, we derived an asymptotic stability estimate $k \sim (\hat{A}Ra)^{5/14}$ for the wavenumber $k$ of vertically confined heat-exchanger flow. In a Rayleigh-Darcy cell, the amplitude $\hat{A}$ is given by the amplitude of the temperature $\hat{T}$ or the vertical velocity $\hat{w}$, which numerical measurements suggest are asymptotically equal and independent of $Ra$. The estimated stability boundary thus reduces to $k \sim Ra^{5/14}$ as $Ra \to \infty$. For $Ra < O(10^5)$, the stability boundary has a slightly stronger dependence on $Ra$ than this asymptotic scaling. Although numerical measurements in a Rayleigh–Darcy cell at higher $Ra$ would be required to verify the asymptotic scaling $k \sim Ra^{5/14}$, the stability boundary gives good agreement with the previously unexplained trend of numerical measurements of $k(Ra)$ over the range $1300 < Ra \leq 4 \times 10^4$.

The results of this chapter, therefore, support the hypothesis that the stability of the interior columnar flow provides the mechanism that controls the wavenumber $k$ in Rayleigh–Darcy convection. The vigorous large-wavenumber dynamics of protoplume formation at the upper and lower boundaries force the system over a range of small scales, and the columnar flow adopts the smallest scale for which it can remain stable over the height of the domain, which is given by $k \sim Ra^{5/14}$ as $Ra \to \infty$. Any smaller scale of columnar flow would be unstable, and the resulting instability would lead to a coarsening of the flow.
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Appendices

3.A Generic behaviour of solutions of (3.33)

Equation (3.33) can be re-written as a single differential equation for \( f \) by substituting \( g = \gamma_0 - f' \) into (3.33b) to obtain

\[
f''' + \left( \frac{i\xi^2}{2} - s \right) f' - i\xi f = \gamma_0 \left( \frac{i\xi^2}{2} - s \right)
\]  

(3.42)

We seek solutions that satisfy \( f(0) = f''(0) = 0 \) and the matching condition \( f \rightarrow -\xi^2/2 \) (equivalently \( g \rightarrow \xi \)) as \( \xi \rightarrow \infty \). In order to determine the unknown eigenvalue \( s \), we require four boundary conditions for the third-order system (3.42). It is not clear, per se, whether the matching condition constitutes one or two constraints; this depends on the generic behaviour of the solutions as \( \xi \rightarrow \infty \).

A WKB approximation to (3.42) in the limit \( \xi \rightarrow \infty \) gives leading-order solutions of the form

\[
f \sim c\xi^2 - \gamma_0\xi + d_\pm \xi^b \exp \left[ \pm \frac{(1-i)}{4} \xi^2 \right] + O(1) \quad \text{as} \quad \xi \rightarrow \infty,
\]  

(3.43)

where \( b \) would be determined at the next order, and \( c \) and \( d_\pm \) are constants. The matching condition \( f \rightarrow -\xi^2/2 \) requires both that \( c = -1/2 \) and that \( d_+ = 0 \). It therefore constitutes two constraints, and we have sufficient conditions to determine the eigenvalue \( s \) in (3.33).

3.B Variation of the growth rate Re\{S\} for \( \alpha^* \ll 1 \) and \( \alpha^* \gg 1 \)

In §3.4.1, we determined the leading-order growth rate \( \text{Re}\{\sigma^*\} = A^{4/9}\text{Re}\{S\} \) as a function of the rescaled vertical wavenumber \( \alpha^* \), and found that \( \text{Re}\{S(\alpha^*)\} \) increased for small \( \alpha^* \) and decreased for large \( \alpha^* \) (figure 3.6a). In this appendix, in order to understand this behaviour, we examine the limits \( \alpha^* \ll 1 \) and \( \alpha^* \gg 1 \).
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Figure 3.11: The leading-order growth rate $\text{Re}\{S\}$ (solid) as a function of the scaled vertical wavenumber $\alpha^*$, together with the predictions from the asymptotic analysis for $\alpha^* \ll 1$ (3.45) and $\alpha^* \gg 1$ (3.47) (dashed).

For clarity, we re-write (3.33) and (3.37) here as

\[
\begin{align*}
    f' + g &= \alpha^{9/4} \pi, \\
    g'' - \left( s - i\xi^2 \right) g + i\xi f &= 0, \\
    S &= \alpha^{s/2}. \quad (3.44a, b, c)
\end{align*}
\]

The boundary conditions are $f(0) = g'(0) = 0$ and $g \to \xi$ as $\xi \to \infty$.

In the limit $\alpha^* \ll 1$, (3.44a) becomes $f' = -g$ to leading order, while (3.44b) remains unchanged; the solution to these equations gives an eigenvalue $s = (1-i)/2$ that is independent of $\alpha^*$ to leading order. (The corresponding expression for the eigenfunction $f$ can be found analytically in integral form, but the expression is not elucidating.) Hence

\[
\text{Re}\{S\} = \frac{1}{2} \alpha^{s/2} \quad \text{for} \quad \alpha^* \ll 1. \quad (3.45)
\]

In the limit $\alpha^* \gg 1$, the balance in (3.44a) requires that the eigenfunctions $[f, g]$ are $O(\alpha^{9/4})$ to leading-order. We write $g = \alpha^{9/4} g_0 + g_1 + O(\alpha^{-9/4})$ and $f = \alpha^{9/4} f_0 + f_1 + O(\alpha^{-9/4})$, and expand $s = s_0 + \alpha^{-9/4} s_1 + O(\alpha^{-9/2})$. The matching condition as $\xi \to \infty$ only applies at second order and is given by $g_1 \to \xi$; the first-order condition is instead given by $g_0 \to 2\pi$ (or, equivalently, $f_0 \to -\pi\xi$), which comes from the form of the solution as $\xi \to \infty$ given by (3.43) in appendix 3.A.
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The solution of (3.44a,b) at leading order is given by \([f_0, g_0] = [-\pi \xi, 2\pi]\) and \(s_0 = 0\); neither diffusion \(g''\) or growth \(sg\) enter the leading-order balance, which is instead simply between the advective terms. At second order, (3.44a,b) become

\[
f'_1 = -g_1, \quad g''_1 + \frac{i\xi^2}{2}g_1 - 2\pi s_1 + i\xi f_1 = 0,
\]

which can be solved numerically, together with boundary conditions \(f_1(0) = g'_1(0) = 0\) and \(g_1 \to \xi\) as \(\xi \to \infty\), to give an eigenvalue \(s_1 = 0.1164 - 0.048i\). Thus

\[
\text{Re}\{S\} = 0.1164 \alpha^*^{-7/4} \quad \text{for} \quad \alpha^* \gg 1.
\]

Figure 3.11 shows that the leading-order asymptotic predictions of \(\text{Re}\{S(\alpha^*)\}\) for small and large wavenumber from (3.45) and (3.47) give very good agreement with the full solution of figure 3.6(a). The physical basis for the decay in the growth rate at small and large \(\alpha^*\) was discussed in §3.4.2.

3.C Stability of piecewise uniform exchange flow in the absence of diffusion

In the main text of this chapter, we examined the stability of density-driven heat-exchanger flow, in which vertical advection balanced horizontal diffusion between the interleaving columns. Motivated by the interesting observation in §3.4.2 that diffusion acts as a destabilizing mechanism for the columnar flow, in this appendix we examine the related system of exchange flow of two distinct fluids of different densities in the limit of negligible diffusion. The fluids again flow in interleaving columns, as shown in figure 3.12.

The governing equations for the flow are incompressibility and Darcy’s law (3.1). The system is horizontally periodic, and each period contains an upwelling column of unit width and uniform velocity \(w\) and a downwelling column of width \(\lambda^{-1}\) and velocity \(-\lambda w\) by continuity (figure 3.12). The interface between the \(j^\text{th}\) and \((j+1)^\text{th}\) columns is labelled by \(X_j\). The density is piecewise uniform, and so
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the governing equations combine to give

\[ \nabla^2 p = 0, \quad (3.48) \]

in each column.

We look for a pressure perturbation \( \tilde{p}_j \) in the \( j \)th column and a corresponding interfacial perturbation \( \tilde{X}_j \) of the form

\[ \tilde{p}_j = \pi_j(x) \exp(\sigma t + i\alpha z), \quad \tilde{X}_j = \xi_j \exp(\sigma t + i\alpha z). \tag{3.49a,b} \]

The horizontal variation \( \pi_j \) of the perturbed pressure is found by solving \( (3.48) \), which gives

\[ \pi_j(x) = A_j \cosh(\alpha (x - X_j)) + B_j \sinh(\alpha (x - X_j)). \tag{3.50} \]

The constants \( A_j, B_j \) and \( \xi_j \) are determined by continuity of pressure and a kinematic condition for each column at \( X_j + \tilde{X}_j \), which are linearized to give

\[ \pi_j(X_j) = \pi_{j-1}(X_j), \tag{3.51a} \]

\[ \left( \frac{\partial}{\partial t} + w_j \frac{\partial}{\partial z} \right) \tilde{X}_j = - \left. \frac{\partial \tilde{p}_j}{\partial z} \right|_{x=X_j}, \tag{3.51b} \]

\[ \left( \frac{\partial}{\partial t} + w_{j-1} \frac{\partial}{\partial z} \right) \tilde{X}_j = - \left. \frac{\partial \tilde{p}_{j-1}}{\partial z} \right|_{x=X_j}. \tag{3.51c} \]

By substituting \( (3.49) \) and \( (3.50) \) into \( (3.51) \) and eliminating \( \xi_j \), we obtain

\[ A_{j+1} = A_j \cosh \alpha d_j + B_j \sinh \alpha d_j, \tag{3.52a} \]

\[ B_{j+1} = \frac{\sigma + i\alpha w_{j+1}}{\sigma + i\alpha w_j} \left( A_j \sinh \alpha d_j + B_j \cosh \alpha d_j \right), \tag{3.52b} \]

where \([d_j, w_j]\) are the width and velocity of the \( j \)th column, given by \([1, w]\) for even \( j \) and \([\lambda^{-1}, -\lambda w]\) for odd \( j \).
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Figure 3.12: A schematic showing the interleaving flow of two distinct fluids of different densities, in columns with width ratio $\lambda$.

We consider perturbations that are periodic over $2N$ columns, for some integer $N$. Therefore, we equate the perturbations to the interface at $X_{2N}$ with those at $X_0$. The application of (3.52) $2N$ times gives a dispersion relation for $\sigma$ of the form

$$\det \left( M^N - I \right) = 0,$$

(3.53)

where $I$ is the identity matrix. The matrix $M$ is given by

$$M = \begin{pmatrix} C_\lambda & S_\lambda \\ \Gamma S_\lambda & \Gamma C_\lambda \end{pmatrix} \begin{pmatrix} C_1 & S_1 \\ \Gamma^{-1} S_1 & \Gamma^{-1} C_1 \end{pmatrix}; \quad \Gamma = \frac{\sigma + i\alpha w}{\sigma - i\alpha \lambda w},$$

(3.54a, b)

where $C_1 = \cosh \alpha$, $S_1 = \sinh \alpha$, $C_\lambda = \cosh (\alpha/\lambda)$, and $S_\lambda = \sinh (\alpha/\lambda)$.

Equation (3.53) has solutions if and only if $M^N$ has eigenvalue 1, or equivalently $M$ has an eigenvalue that is an $N^{th}$ root of unity. Moreover, it is easily shown that the determinant of $M$ is 1, and so the product of the eigenvalues of $M$ is 1. Thus, (3.53) has solutions if and only if the eigenvalues of $M$ are a conjugate pair of $N^{th}$ roots of unity. We label these eigenvalues $\mu_{\pm} = a \pm ib$, for some real $a$ and $b$ with $|a|, |b| \leq 1$. Then (3.53) is equivalent to

$$\det \left( M - \mu_{\pm} I \right) = 0,$$

(3.55)

which can be reduced to

$$(1 + \Gamma^2) S_1 S_\lambda + 2 (C_1 C_\lambda - a) \Gamma = 0,$$

(3.56)
Equation (3.56) is a quadratic for $\Gamma$, which has discriminant

$$
\Delta = 4 \left[ (C_1 - C_\lambda)^2 + 2(1 - a)C_\lambda C_1 + a^2 - 1 \right].
$$

(3.57)

Since $C_1 C_\lambda \geq 1$ and $|a| \leq 1$, (3.57) implies that $\Delta \geq (a - 1)^2 \geq 0$, and so solutions $\Gamma$ of (3.56) must be real. This constraint, together with (3.54b), requires that $\sigma$ is pure imaginary, which holds for any width ratio $\lambda$, velocity $w$, periodicity $N$, or wavenumber $\alpha$. Therefore, in the absence of diffusion, the columnar exchange flow of two distinct fluids of different densities is neutrally stable to all wavelengths; perturbations are advected by the flow without growth or decay. This result is similar to the observation in §3.4.2 that the leading-order advection balance for heat-exchanger flow gives neutral propagation, and growth is only possible because of diffusion.
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Chapter 4

High Rayleigh number convection in a porous medium containing a thin low-permeability layer

The material contained in this chapter has been submitted to the Journal of Fluid Mechanics, under the title ‘High Rayleigh number convection in a porous medium containing a thin low-permeability layer’ (Hewitt et al., 2014a).

4.1 Introduction

Porous media are often modelled as homogeneous (as in the rest of this thesis), and described by uniform averaged properties like the porosity and permeability. Natural porous media, however, are rarely homogeneous. In particular, geophysical aquifers commonly consist of a series of roughly horizontal layers of rock of distinctly different permeabilities (Monkhouse, 1970; Phillips, 2009). Layering of this sort can frequently be observed on exposed rock faces in quarries or coastal cliffs, such as the Jurassic sandstone cliffs at Bridport in Dorset, UK (Morris & Shepperd, 1982). Both the permeability and the depth of layers can be much smaller than those of the main formation: the exposed Aztec sandstone in Nevada, for example, at over a kilometre in depth, is characterized by multiple very thin (∼ 1 cm) horizontal layers that are several orders of magnitude less permeable than the
main formation (Sternlof et al., 2006). An important example for the geological storage of CO\textsubscript{2} is the Utsira sand formation at the Sleipner field in the North Sea, where roughly 1 million tonnes of CO\textsubscript{2} have been sequestered every year since 1996 (Bickle et al., 2007; Boait et al., 2012). Seismic images have revealed that the flow of injected CO\textsubscript{2} is significantly affected by the presence of nine low-permeability roughly horizontal mudstone layers which intersperse the formation, and are much thinner (roughly 1 − 5 m deep) than the formation itself (roughly 200 m deep) (Bickle et al., 2007).

The study of convection in inhomogeneous or anisotropic media has tended to focus on the onset of convection and the subsequent dynamics of the flow at low Rayleigh numbers (Simmons et al., 2001; Ennis-King et al., 2005; Nield & Bejan, 2006). In media comprising layers of high and low permeability, McKibbin & O’Sullivan (1980, 1981) found that, as the permeability contrast between the layers is increased, there is a transition in the flow dynamics from large-scale convective rolls to local convective structures confined to the higher-permeability layers. McKibbin & Tyvand (1983) examined the flow at low $Ra$ in a medium with thin low-permeability layers, and found that the presence of these layers can significantly increase the critical Rayleigh number for the onset of convection. They modelled the flow under the assumption that both the height and permeability of the low-permeability layers were small but their ratio was $O(1)$; we adopt a similar approach here for the case of vigorous high-$Ra$ convection.

In this chapter, we use high-resolution numerical simulations to examine the impact of a thin, horizontal, low-permeability layer on the strength and dynamical structure of high-$Ra$ convection in a porous medium. We consider a cell comprising an identical upper and lower layer, between which there is a thin interior layer of a lower permeability. The whole cell is heated from below and cooled from above. The flow thus attains a statistically steady state, which allows for a systematic examination of the effect of a thin low-permeability layer on the heat flux through the cell and on the associated flow structure. In the limit in which there is no interior layer, the cell is identical to the homogeneous Rayleigh–Darcy cell discussed in chapter 2. All physical properties of the fluid and the medium except the permeability are assumed to be constant throughout the cell; in particular, we assume for simplicity that the porosity $\phi$ of the medium is uniform, and
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is thus independent of the permeability (see appendix 4.A for a discussion of this assumption).

The chapter is laid out as follows. In §4.2, we present the governing equations and non-dimensionalization. In §4.3, we discuss our numerical results. We show that, in the limit that both the dimensionless thickness $h$ and permeability $\Pi$ of the low-permeability interior layer are small, the flow can be described solely by their ratio $\Omega = h/\Pi$. In §4.3.4, we examine in detail the dependence on $\Omega$ of the dynamical structure of the flow and the flux $Nu$, and in §4.3.5 we investigate the dependence of the flow on $Ra$, across the range $2500 \leq Ra \leq 2 \times 10^4$. In §4.4, we develop simple one-dimensional models of the system that capture some of the observed features of the relationship $Nu(\Omega)$, and we discuss the limitations of the models. Finally, in §4.5, we summarize and discuss our main results.

4.2 Governing equations

We consider the flow of a Boussinesq fluid in a two-dimensional porous medium, with horizontal and vertical coordinates $x^*$ and $z^*$ respectively. The medium comprises a thin interior layer between a relatively deep upper and lower layer (figure 4.1a). The combined depth of the three layers is $z^* = H$. The upper and lower layers have uniform permeability $K_1$, while the thin interior layer has uniform permeability $K_2 < K_1$ and depth $h^* \ll H$, and lies between $z_1^* = (H - h^*)/2$ and $z_2^* = (H + h^*)/2$. Within each layer, the medium is homogeneous and isotropic.

We assume that the flow $u^* = (u^*, w^*)$ in all three layers is incompressible and is governed by Darcy’s law. The equation of state $\rho^*(T^*)$ is linear, and the temperature field $T^*$ satisfies an advection–diffusion transport equation. These equations are given by

\[ \nabla \cdot u^* = 0, \]

\[ \mu u^* = \begin{cases} -K_1 (\nabla p^* + \rho^* g z^*) & 0 \leq z^* \leq z_1^*, \ z_2^* \leq z^* \leq H, \\ -K_2 (\nabla p^* + \rho^* g z^*) & z_1^* < z^* < z_2^*, \end{cases} \]

\[ \rho^* = \rho_0 [1 - a (T^*-T_0)], \]
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\[ \phi \frac{\partial T^*}{\partial t^*} + \mathbf{u}^* \cdot \nabla T^* = \phi \kappa \nabla^2 T^*, \]  

(4.1d)

where \( \mu \) is the viscosity, \( p^* \) is the pressure, \( g \) is the gravitational acceleration, \( \hat{z}^* \) is a unit vector in the \( z^* \) direction, \( \rho_0 \) and \( T_0 \) are a constant reference density and temperature, respectively, \( a \) is the coefficient of thermal expansion, \( \phi \) is the porosity of the medium, and \( \kappa \) is the constant thermal diffusivity in the liquid phase. As in the rest of this thesis (see §1.2), heat transfer to the solid phase of the medium is neglected; as such, these equations are equally applicable to compositionally driven convection.

On the upper and the lower boundaries of the domain, the vertical velocity vanishes and a fixed temperature is imposed, such that

\[ T^*|_{z^*=0} = T_0 + \Delta T, \quad T^*|_{z^*=H} = T_0, \quad w^*|_{z^*=0,H} = 0, \]  

(4.2)

where \( \Delta T \) is a fixed unstable (positive) temperature difference. The pressure, temperature and normal velocity are continuous at the internal boundaries \( z^* = z_{1,2}^* \).

We non-dimensionalize the system with respect to the depth \( H \) of the whole domain, the permeability \( K_1 \) of the upper and lower layers, the density difference across the domain \( \Delta \rho = \rho_0 a \Delta T \), and the convective time scale \( \phi H \mu / (g \Delta \rho K_1) \). The dimensionless rescaled temperature is given by \( T = (T^* - T_0) / \Delta T \). In dimensionless variables, the governing equations (4.1) reduce to

\[ \nabla \cdot \mathbf{u} = 0, \]  

(4.3a)

\[ \mathbf{u} = \begin{cases} 
- (\nabla p - T \hat{z}) & 0 \leq z \leq z_1, z_2 \leq z \leq 1, \\
- \Pi (\nabla p - T \hat{z}) & z_1 < z < z_2,
\end{cases} \]  

(4.3b)

\[ \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \frac{1}{Ra} \nabla^2 T, \]  

(4.3c)

where \( p = [p^* + \rho_0 g z^*] / (\Delta \rho g H) \) is a reduced pressure, \( \Pi = K_2 / K_1 < 1 \) is the ratio of the two permeabilities. The dimensionless edges of the interior layer are given
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\[ z^* = H \quad T^* = T_0 \]
\[ z^* = z_2^* \quad K_1 \]
\[ z^* = z_1^* \quad K_2 \]
\[ z^* = 0 \quad T^* = T_0 + \Delta T \]

\( (a) \)

\[ z = z_2 \quad z = z_1 \]
\[ z = z_1 \]
\[ z = 1 \]
\[ T = 0 \]

\( (b) \)

\[ T = 1 \]

Figure 4.1: A schematic showing the system under consideration, with the permeability of each layer and the thermal boundary conditions marked, for (a) dimensional and (b) dimensionless variables.

by \( z_{1,2} = (1 \mp h)/2 \). The parameter \( Ra \) is the Rayleigh number, given by

\[ Ra = \frac{g \Delta \rho K_1 H}{\phi \kappa \mu}. \tag{4.4} \]

The dimensionless boundary conditions on the upper and lower boundaries of the domain are given from (4.2) by

\[ T|_{z=0} = 1, \quad T|_{z=1} = 0, \quad w|_{z=0,1} = 0, \quad (4.5) \]

(figure 4.1b). The conditions at the internal interfaces between the different layers are given by continuity of temperature, pressure and normal velocity,

\[ [T] = [p] = [w] = 0 \quad \text{at} \quad z = z_1, z_2. \tag{4.6} \]

As in chapter 2, incompressibility (4.3a) is satisfied by the introduction of a streamfunction \( \psi \) which obeys \((u, w) = (\partial \psi / \partial z, -\partial \psi / \partial x)\). We eliminate the pressure field by taking the curl of (4.3b), which gives

\[ \nabla^2 \psi = \begin{cases} 
-\partial T / \partial x & 0 \leq z \leq z_1, \quad z_2 \leq z \leq 1, \\
-\Pi \partial T / \partial x & z_1 < z < z_2.
\end{cases} \tag{4.7} \]

We incorporate the boundary condition for the pressure at the interfaces with the interior layer by combining (4.6) with Darcy’s law (4.3b), to give the boundary
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conditions in terms of discontinuities of the horizontal velocity:

\[ u|_{z=z_1^+} = \Pi u|_{z=z_1^-}, \quad u|_{z=z_2^-} = \Pi u|_{z=z_2^+}. \]  (4.8)

The flow is described by three dimensionless parameters: the Rayleigh number \(Ra\); the permeability ratio \(\Pi\); and the relative thickness of the low-permeability layer \(h = h^*/H\). The statistically steady convective flux, or, in dimensionless variables, the Nusselt number \(Nu(Ra, \Pi, h)\), can be defined as the temporally and horizontally averaged heat flux at any height \(z\), and is here given by

\[ Nu = \langle nu(t) \rangle = \left\langle \frac{-1}{L} \int_0^L \frac{\partial T}{\partial z} \bigg|_{z=0} \, dx \right\rangle, \]  (4.9)

where \(nu(t)\) is the instantaneous horizontally averaged flux through the boundary at a given time \(t\), and \(L\) is the aspect ratio of the cell. The angle brackets \(\langle \rangle\) signify a long-time average.

We solved (4.3c) and (4.7) numerically. The numerical method is discussed very briefly here, and is described in more detail in appendix A, §A.2.1. We imposed periodic boundary conditions on the cell in the \(x\) direction at \(x = 0, L\). Unless otherwise stated, all the numerical results presented in this chapter have aspect ratio \(L = 4\). We employed a vertical coordinate transformation in order to fully resolve both the thin boundary layers at the upper and lower boundaries of the domain, and the interfaces between the different layers inside the cell. The initial condition for all calculations, unless explicitly noted in the text, was given by a linear vertical temperature gradient with a small random perturbation. After an initial period of reorganization, the flow attains a statistically steady state. At high \(Ra\), the local flux through the boundary \(nu(t)\) exhibits chaotic fluctuations about a mean in this state, and the computations are continued until the Nusselt number (4.9) has converged to within 0.25% of its mean.

4.3 Numerical results

In this section we present our numerical measurements and discuss the observations. We focus initially in §§4.3.1–4.3.4 on simulations at \(Ra = 5000\), which is an
appreciably higher value than the onset of the high-\(Ra\) regime for homogeneous Rayleigh–Darcy convection (see chapter 2). We then examine the dependence of the system on \(Ra\) in §4.3.5. The effects of the interior low-permeability layer on the convective dynamics are more complicated than might be anticipated, and thus we describe the observations in some detail. A summary of the main observations is given in §4.3.6.

### 4.3.1 Numerical results for \(Ra = 5000\)

Snapshots of the statistically steady temperature field for different values of the thickness \(h\) of the low-permeability layer and two different permeability ratios \(\Pi\) are shown in figures 4.2 and 4.3. The homogeneous case \(h = 0\) (equivalently \(\Pi = 1\)) is shown in figure 4.2(a).

The structure of the flow changes significantly as the thickness of the low-permeability layer increases. For homogenous convection (figure 4.2a), the flow is dominated away from the boundaries by columnar megaplumes with a roughly regular horizontal wavelength (see chapter 2). The horizontal scale of these plumes increases significantly as \(h\) is increased (figure 4.2b–f). The flow increasingly resembles an ordered array of cells, each of which is half the height of the domain and comprises a thin vertical plume flowing up/down and a much wider plume carrying the return flow. For the smaller value of \(\Pi\) (figure 4.3), the horizontal scale of the flow increases even more rapidly as \(h\) is increased. In fact, for sufficiently large values of \(h\), the horizontal scale of the plumes appears to have become so broad that protoplumes form near the low-permeability layer (figure 4.3c–e). There is significant variability in the structure of the flow between different simulations, as exemplified by figure 4.2(e,f) which, contrary to the general trend just discussed, show a flow with \(h = 0.08\) which has a smaller horizontal lengthscale than a flow with \(h = 0.04\).

Profiles of the horizontally and temporally averaged temperature \(\langle T \rangle\) (figures 4.2,4.3) show that the temperature difference across the low-permeability layer increases as \(h\) is increased. The background stratification also appears to depend on \(h\): for homogeneous convection (figure 4.2a), the profile has a very weak negative gradient throughout the interior of the domain, whereas, as \(h\) is
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Figure 4.2: Snapshots of the temperature field $T$ for $Ra = 5000$, $\Pi = 0.04$, and varying thickness $h$ of the low-permeability layer: (a) $h = 0$ (no low-permeability layer), (b) $h = 0.005$, (c) $h = 0.01$, (d) $h = 0.02$, (e) $h = 0.04$, and (f) $h = 0.08$. The white bars on the left mark the location and thickness of the low-permeability layer. The temporally and horizontally averaged temperature $\langle T \rangle (z)$ (solid) is shown on the right-hand side, together with the temperature averaged only over fluid with $w > 0$ (dashed) and only over fluid with $w < 0$ (dot-dashed).

increased, (figure 4.2b–f and figure 4.3), the gradient becomes positive, giving an
apparent stable background stratification in each layer. Measurements of the average temperature restricted to either the upwelling or the downwelling regions alone (figures 4.2, 4.3 dashed and dot-dashed lines) do not show as large a stratification as the full profiles of $\langle T \rangle$, although the fluid is still slightly stratified, particularly in the plumes that carry fluid towards the low-permeability layer.

Figure 4.4(a) shows measurements of the Nusselt number as a function of the thickness $h$ of the low-permeability layer for different values of $\Pi$ and for an
The Nusselt number $Nu$ for $Ra = 5000$: (a) as a function of the thickness $h$ of the low permeability layer, and (b) as a function of the impedance $\Omega = h/\Pi$, where $\Pi$ is the permeability ratio. The data points are for $\Pi = 0$ (squares), $\Pi = 0.005$ (circles), $\Pi = 0.01$ (stars), $\Pi = 0.02$ (crosses), $\Pi = 0.04$ (pluses), $\Pi = 0.08$ (dots). The solid line in (a) is the theoretical prediction for an impermeable interior layer (see §4.4.2). For homogeneous convection (i.e. the limit $h \to 0$), $Nu = 37.25$ (dashed line, taken from the results of chapter 2). Surprisingly, the Nusselt number initially increases with $\Omega$, before decreasing for $\Omega \gtrsim 0.25$.

Surprisingly, $Nu$ does not decrease monotonically as $h$ is increased, as might be expected from the increasing proportion of the domain that is occupied by low-permeability material. Instead, $Nu$ first increases for small $h$ ($\Pi \neq 0$), before decreasing for larger $h$. The measurements for $\Pi \neq 0$ roughly collapse onto a single curve when plotted as a function of the quantity $\Omega = h/\Pi$ (figure 4.4(b)), as discussed in the following section. The case $\Pi = 0$ is quite different since all the heat flux across an impermeable layer must be by diffusion.

### 4.3.2 Dependence on $\Omega = h/\Pi$

The measurements of $Nu$ collapse onto a single curve as a function of $\Omega = h/\Pi$ (figure 4.4b). This dependence can be simply understood by examination of the governing equations for $h, \Pi \ll 1$. In this limit, Darcy’s law (4.3b) implies that the horizontal velocity in the low-permeability layer is small ($O(\Pi)$), while the vertical
velocity is $O(\Pi/h)$ and given by

$$w = -\Pi \left( \frac{\partial p}{\partial z} - T \right) = -\frac{\Pi}{h} \left[ p(z_2) - p(z_1) + O(h) \right].$$

(4.10)

The flow through the low-permeability layer is therefore predominantly vertical if $h, \Pi \ll 1$ and $\Pi/h = O(1)$, and it is driven by pressure differences, rather than by buoyancy. In this limit, the flow is controlled by the parameter $\Omega = h/\Pi$, which is a form of impedance, being a ratio of pressure difference and Darcy velocity.

We can parameterize the effect of the low-permeability layer in the distinguished limit $h, \Pi \to 0$ with the impedance $\Omega = h/\Pi$ remaining finite. The derivative of (4.10) with respect to $x$ and the continuity conditions for $w$ and $p$ from (4.6) give

$$\Omega \frac{\partial w}{\partial x} \approx u(z_2) - u(z_1).$$

(4.11)

We note that there is no requirement of continuity for the horizontal velocity $u$ at $z = z_{1,2}$. In the limit $h, \Pi \to 0$, (4.11) reduces to a jump condition for $u$, given by

$$\Omega \frac{\partial w}{\partial x} \bigg|_{z=0.5} = [u]_{z=0.5}.$$

(4.12)

The temperature and vertical velocity are continuous at $z = 0.5$ in this limit.

### 4.3.3 Reduced numerical simulations

Motivated by the results of the previous section, we developed a simplified numerical scheme in which the thin low-permeability layer is parameterized by the jump condition (4.12), together with continuity of temperature and vertical velocity, at $z = 0.5$ (see Appendix A, §A.2.1 for details). This parameterization both simplifies the numerical computations and appreciably reduces the numerical cost, as there is no longer a low-permeability layer to be resolved. We refer to these simulations as ‘reduced’, to distinguish from ‘full simulations’ in which the low-permeability layer is fully represented and resolved.

Measurements of $Nu(\Omega)$ from reduced simulations give good agreement with results from full simulations for different values of $h$ and $\Pi$ (figure 4.5). The slight difference in some of the measurements at large values of $\Omega$ is because of
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Figure 4.5: The Nusselt number $\text{Nu}(\Omega) = \text{Nu}(h/\Pi)$ from full simulations for $10^{-3} \leq h \leq 0.2$ and $10^{-4} \leq \Pi \leq 0.1$ (dots; includes the data from figure 4.4) and from reduced simulations (crosses) for $Ra = 5000$. The results give good agreement, and tend to the homogeneous value $\text{Nu} = 37.25$ (dashed line) in the limit $\Omega \to 0$.

the relatively large values of $h$ in some of the full simulations. There is also some scatter in the measurements of $\text{Nu}$, which is related to variability in the horizontal structure of the flow, as discussed in §4.3.4.2 below.

Figure 4.5 shows that $\text{Nu}$ increases gradually with $\Omega$ to give a maximum of $\text{Nu} \approx 41.2$ at $\Omega \approx 0.25$. This is an increase of approximately 10% from the value of $\text{Nu}$ for homogeneous convection. For $\Omega \gtrsim 0.25$, $\text{Nu}$ decreases rapidly. For $\Omega \gtrsim 5$, measurements from reduced simulations level off at roughly a quarter of the value of $\text{Nu}$ for homogeneous convection, while measurements from full simulations appear to continue to decrease slowly.

4.3.4 The dynamical structure of the flow

We have observed that the dynamical structure of the flow changes significantly with $h$ and $\Pi$ (figure 4.2, 4.3), and we showed in the previous section that the flow is a function of $\Omega = h/\Pi$ only, for $h, \Pi \ll 1$. In this section, we describe in detail the change in the flow with $\Omega$, and the corresponding form of $\text{Nu}(\Omega)$.

4.3.4.1 Dependence on $\Omega$

For $\Omega \lesssim 0.05$ (figure 4.6a: i and ii), the flow resembles homogeneous flow. The dynamics are dominated by predominantly vertical columnar flow across the full
height of the domain with a fairly small wavelength. The average widths of upwelling and downwelling plumes are roughly equal throughout the domain, although there are substantial fluctuations in the location of the edges of the columnar megaplumes (figure 4.6b). The Nusselt number does not change appreciably for $\Omega \lesssim 0.05$.

For $0.05 \lesssim \Omega \lesssim 0.3$ (figure 4.6a: iii and iv), the flow increasingly resembles a series of cells of half the height of the domain. In the lower layer, the cells take the
form of a wide hot upwelling plume neighbouring a much thinner cold downwelling plume. As the upwelling plume impinges on the low-permeability layer, some fluid spreads laterally and is entrained into the downwelling return flow, while some ‘leaks’ through into the upper layer and feeds the base of a thin upwelling plume there. The cells have a complementary form in the upper layer. As Ω is increased in this range, the horizontal lengthscale of the flow increases significantly. The flow also appears to become increasingly ‘ordered’, in that there is much less temporal variability in the location and width of the plumes than at lower values of Ω (figure 4.6c). The Nusselt number increases over this range of Ω, which is surprising since, for fixed thickness h, this implies that the flux increases as the permeability of the low-permeability layer is decreased.

For $0.3 \lesssim \Omega \lesssim 5$ (figure 4.6a: v), the horizontal lengthscale of the flow continues to increase. In this range, the horizontal flow along the boundary of the low-permeability layer appears to be unstable to the growth of protoplumes, which perturb the cellular structure of the flow. The Nusselt number decreases markedly in this range of Ω.

At $\Omega \approx 5$, the structure of the flow changes completely. For $\Omega \gtrsim 5$ (figure 4.6a: vi), the flow resembles two layers of homogeneous columnar convection, each of half the original height and half the original temperature contrast, placed one on top of the other. Unlike at lower values of Ω, there are no plumes that reach across the full height of the domain. The Nusselt number appears to be roughly constant for $\Omega \gtrsim 5$.

Figure 4.7 shows four sets of temporally averaged measurements of the flow, with each set at a value of Ω selected to be in one of the ranges discussed above. For $\Omega = 0.04$ (figure 4.7a), $\langle T \rangle$ is roughly uniform in the interior of the domain, except for a small temperature difference across the interior boundary at $z = 0.5$. Similarly, the temperature fluctuations and velocities are fairly uniform, with some small deviations near $z = 0.5$.

For $\Omega = 0.25$ and $\Omega = 1.28$ (figure 4.7b,c), the temperature difference across the low-permeability layer is larger than in figure 4.7(a), and the rms quantities vary appreciably near $z = 0.5$. The average temperature field $\langle T \rangle$ has a weak stable stratification in the upper and lower layers of the domain. There is a notable asymmetry between upwelling and downwelling plumes which varies with
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Figure 4.7: Measurements from reduced simulations at $Ra = 5000$. Left panels show $\langle \overline{T} \rangle (z)$ (solid), together with the average temperature of upwelling fluid (dashed) and the average temperature of downwelling fluid (dot-dashed). Centre panels show the temporally averaged proportion $\phi_w$ of the fluid with $w > 0$, which reveals the asymmetry between the widths of upwelling and downwelling plumes. Right panels show the temporally averaged rms temperature perturbations $T_{\text{rms}}(z)$ (red, solid) and velocities $w_{\text{rms}}(z)$ (blue, dashed) and $u_{\text{rms}}(z)$ (green, dot-dashed). (a) $\Omega = 0.04$, (b) $\Omega = 0.25$, (c) $\Omega = 1.28$, and (d) $\Omega = 10$; corresponding to figure 4.6(a) parts (ii), (iv), (v), and (vi), respectively.

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Figure 4.8: Measurements from reduced simulations at $Ra = 5000$ of the temporally averaged rms temperature perturbations and velocities at $z = 0.5$. The Nusselt number $Nu(\Omega)$ from figure 4.5 is shown above for comparison. The vertical velocity at $z = 0.5$ is approximately zero for $\Omega \gtrsim 5$; this reflects the transition (dashed line) from dominantly advective to dominantly diffusive transport across the low-permeability layer.

There is a clear change in the trend of the rms measurements at $\Omega \approx 5$ (figure 4.8). In particular, $w_{\text{rms}} \approx 0$ for $\Omega \gtrsim 5$, which means that there is no appreciable advective flux through the low-permeability layer. We interpret the change in the dynamics as a transition from advection to diffusion as the dominant transport mechanism across the low-permeability layer. For convenience, we will refer to the regime for $\Omega \gtrsim 5$ as the ‘diffusion regime’, and to the regime for $\Omega \lesssim 5$ as the ‘advection regime’.

4.3.4.2 Hysteresis

We observed some variation in the measurements of $Nu(\Omega)$ between simulations at the same value of $\Omega$ started with different random perturbations to the same initial state (figure 4.6a, dots). We also observed systematic differences between
Figure 4.9: Instantaneous measurements from a reduced simulation at $Ra = 5000$ and $\Omega = 0.25$. 

(a) The temperature variation $T - \overline{T}$ (solid) and the vertical ‘leakage’ velocity $w$ (dashed) at $z = 0.5$. 

(b) The horizontal velocities $u_+$ (solid) immediately above the low-permeability layer, and $u_-$ (dashed) immediately below the low-permeability layer.

series of simulations with different initial states (figure 4.6a, dots and crosses). The differences in $Nu(\Omega)$ appear to be related to differences in the number of cells in the domain, as can be seen by a comparison of two flow structures at $\Omega = 0.25$ (figure 4.6a: iii and iv). The fact that there can be different numbers of cells for the same value of $\Omega$ is likely due to the restriction imposed by the horizontal periodicity of the domain. Once the flow develops a particular structure, we find that the structure can persist as an apparently statistically steady state for a long time.

4.3.4.3 Profiles at the low-permeability layer

Figure 4.9 shows profiles of the temperature variation and velocities at $z = 0.5$ at $\Omega = 0.25$. The vertical ‘leakage’ velocity $w$ through the low-permeability layer forms a clear piecewise-linear triangular profile (figure 4.9a). Simulations from across the range $0.05 \lesssim \Omega \lesssim 5$ show similar linear profiles for $w$. The temperature variation $T - \overline{T}$ is in phase with $w$, but has a more rounded profile.

The horizontal velocities $u_+$ and $u_-$ just above and just below the low-
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permeability layer (at \( z = 0.5^+ \) and \( z = 0.5^- \), respectively, form an offset repeating sawtooth profile (figure 4.9b). The profiles reveal something of the cellular structure of the flow. In the upper half of the domain, for example, hot fluid that has leaked up across the layer is swept laterally as a buoyant boundary layer and converges into thin regions where \( u_+ \) changes rapidly from positive to negative (figure 4.9b). These regions, which are also centred on the positive maxima of the leakage velocity \( w \) (figure 4.9a), correspond to thin upwelling plumes. In the regions between the thin upwelling plumes there are broad regions of downwelling relatively cold fluid, which impinge on the low-permeability layer and are deflected into the lateral flow discussed above, roughly like a stagnation-point flow. The flow in the lower half of the domain has a complementary form, offset laterally by half a period, such that the thin upwelling plumes in the upper half of the domain lie above the broad upwelling regions in the lower half of the domain, and the thin downwelling plumes in the lower half of the domain lie below the broad downwelling regions in the upper half of the domain.

4.3.5 Dependence on \( Ra \)

We have, thus far, focused on the flow at a fixed value of \( Ra = 5000 \). Figure 4.10(a) shows measurements of \( Nu(\Omega) \) for different values of \( Ra \) in the range \( 2500 \leq Ra \leq 2 \times 10^4 \), scaled by the Nusselt number \( Nu_0(Ra) \) for homogeneous Rayleigh–Darcy convection. There are two particularly interesting features of this plot. First, the initial trend in \( Nu(\Omega) \) as \( \Omega \) is increased changes with the value of \( Ra \): for \( Ra = 2500 \), \( Nu \) increases by over 30% before then decreasing, while for \( Ra = 2 \times 10^4 \), \( Nu \) decreases monotonically. Second, \( Nu \) is approximately independent of \( \Omega \) for \( \Omega \gtrsim 5 \). This observation can be explained by the fact that the flux across the low-permeability layer is diffusive in this regime, and so is independent of \( \Pi \). The transition to the diffusion regime appears to occur at a value of \( \Omega \) that is roughly independent of \( Ra \), which is perhaps surprising given that the Rayleigh number can be interpreted as a measure of the relative strength of advection and diffusion.

Measurements of the time-averaged modal horizontal wavenumber \( k(\Omega) \) at \( z = 0.5 \) (figure 4.10b) are somewhat noisy, which reflects the degree of hystere-
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Figure 4.10: Measurements from reduced simulations for $Ra = 2500$ (dots), $Ra = 5000$ (crosses), $Ra = 10^4$ (pluses) and $Ra = 2 \times 10^4$ (circles). (a) The Nusselt number $Nu(\Omega)$, scaled by the Nusselt number $Nu_0$ for homogeneous convection (from chapter 2). (b) The time-averaged modal wavenumber $k$ scaled by $2\pi$, as measured from a Fourier transform of the temperature field at $z = 0.5$ for $\Omega < 5$ (the advection regime) and at $z = 0.75$ for $\Omega > 5$ (the diffusion regime). The inset shows the data for $\Omega < 5$ on a log-log scale, together with the scaling $k \sim \Omega^{-1/2}$ (see §4.4.1 for a theoretical prediction of this scaling). Note that the simulations at $Ra = 2 \times 10^4$ have aspect ratio $L = 2$, rather than $L = 4$.

sis that can affect the flow. For small $\Omega$, the wavenumber tends to the value for homogeneous convection (measurements of which are approximately fitted by $k = 0.48Ra^{0.4}$; see (2.17) in chapter 2). The wavenumber decreases for $\Omega \gtrsim 0.1$, which roughly coincides with the value of $\Omega$ at which $Nu/Nu_0$ begins to differ appreciably from 1. The subsequent decrease in $k$ can be approximately fitted by a scaling of $k \sim \Omega^{-1/2}$ (figure 4.10b inset).

For $\Omega \gtrsim 5$ in the diffusion regime, the temperature is roughly uniform at
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Figure 4.11: Snapshots of the temperature field from reduced simulations for \( \Omega = 0.1 \) (left) and \( \Omega = 0.3 \) (right), together with profiles of \( \langle T \rangle (z) \) (solid lines) and the average temperature of fluid with \( w > 0 \) (dashed lines) and of fluid with \( w < 0 \) (dot-dashed lines). (a) \( Ra = 2500 \), (b) \( Ra = 5000 \), (c) \( Ra = 10^4 \), and (d) \( Ra = 2 \times 10^4 \). In (d), the simulations have an aspect ratio \( L = 2 \); the snapshot is shown twice for comparison with the other simulations which have \( L = 4 \).

\( z = 0.5 \); in this range we instead measure the average wavenumber \( k \) at \( z = 0.75 \), in the middle of the upper layer. The wavenumber is slightly larger than the wavenumber for homogeneous convection, as can be understood by a simple rescaling of the height and length scales. The flow in each half of the domain resembles homogeneous Rayleigh–Darcy convection in a layer with half the height and half the temperature difference, which gives an effective Rayleigh number four times smaller than \( Ra \) and an effective wavenumber that is half the measured value. This rescaling, together with the relationship \( k \sim Ra^{0.4} \), suggests that the measured wavenumber should be roughly a factor of \( 2/4^{0.4} \approx 1.15 \) larger than the homogeneous value, and this prediction is consistent with the measurements shown in figure 4.10(b).

Figure 4.11 shows a comparison of snapshots of the flow for different values of \( Ra \). For \( \Omega = 0.1 \), the flow has an ordered cellular structure at each value of \( Ra \), although the dominant horizontal lengthscale of the flow decreases as \( Ra \) is
increased, and the asymmetry in the widths of upwelling and downwelling plumes is clearer at larger $Ra$. For $\Omega = 0.3$, however, the qualitative structure of the flow varies with $Ra$. In particular, the flow for larger $Ra$ (figure 4.11c,d) is affected by the formation of protoplumes near the interior boundary, and, as a result, the flow appears more disordered than the cellular flow at smaller values of $Ra$ (figure 4.11a, b).

It is interesting to note (with reference to figure 4.10a), that $Nu$ increases between $\Omega = 0.1$ and $\Omega = 0.3$ for the lower values of $Ra$ (figure 4.11a,b), but decreases over this range for the higher values (figure 4.11c,d). Based on the observations above, the increase in $Nu$ with increasing $\Omega$ at moderate $Ra$ appears to coincide with an increasingly ordered cellular flow structure. Conversely, the absence of such an increase at higher $Ra$ coincides with the growth of protoplume instabilities near the low-permeability layer, which break down the cellular structure and lead to a more disordered flow.

### 4.3.6 Summary of main observations

We have shown that the dynamics of the statistically steady flow depend only on the ratio $\Omega = h/\Pi$ for $h, \Pi \ll 1$ and for a given value of $Ra$. The horizontal lengthscale of the flow increases as $\Omega$ is increased. For small values of $\Omega$, the structure of the flow resembles homogeneous columnar flow. For larger values of $\Omega$, the flow adopts an ordered cellular structure which, for sufficiently large $\Omega$, is unstable to the formation of protoplumes near the interior boundary. For even larger values of $\Omega$, there is a distinct transition when the advective flux across the inner boundary becomes weaker than the diffusive flux.

For $Ra = 5000$, we found that the Nusselt number initially increases with $\Omega$, to a maximum at $\Omega \approx 0.25$. For larger values of $\Omega$, $Nu$ then decreases. Beyond the transition to the diffusion regime at $\Omega \approx 5$, $Nu$ is independent of $\Omega$ in the reduced model. In full simulations with a finite thickness $h$ of the low-permeability layer, $Nu$ continues to decrease in the diffusion regime as $h$ is increased (figure 4.5).

There are two main differences in this behaviour at different values of $Ra$. First, the initial increase in $Nu$ with $\Omega$ weakens at larger values of $Ra$, and at $Ra = 2 \times 10^4 \ Nu(\Omega)$ decreases monotonically. Second, as $Ra$ is increased, the
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formation of protoplumes near the inner boundary appears to occur at a lower value of $\Omega$. The decrease in the horizontal wavenumber $k$ over the range of $\Omega$ for which $Nu$ decreases is roughly fitted by $k \sim \Omega^{-1/2}$ (figure 4.10b). The value of $\Omega \approx 5$ at which there is a transition in the flow to the diffusion regime appears to be roughly independent of $Ra$.

4.4 Simple theoretical models

In order to develop some understanding of the observed behaviour of $Nu(\Omega)$, in this section we describe simple one-dimensional models of the statistically steady convective system. These models provide a tentative basis for interpretation of the dynamical behaviour that we have observed, but further refinement will be required for a fuller understanding (see §4.4.3). We describe two simple models, one for each of the regimes identified in §4.3: first, in §4.4.1, for the advection regime ($\Omega \lesssim 5$); and second, in §4.4.2, for the diffusion regime ($\Omega \gtrsim 5$).

For simplicity, we make the assumption in both models that the horizontally averaged temperature $T$ is approximately uniform in each of the upper and lower layers of the domain, except in thin boundary regions near $z = 0$, $z = 0.5$ and $z = 1$. (This approximation neglects any background stratification.) We therefore set

$$T = \Theta(\Omega) \text{ in } z > 0.5, \quad \text{and} \quad T = 1 - \Theta(\Omega) \text{ in } z < 0.5. \quad (4.13)$$

In chapter 2, we found that, in a homogeneous layer of unit depth with average interior temperature $T = 0.5$, the convective heat flux $Nu$ is well described for $Ra \gtrsim 1300$ by the empirical parameterization $Nu = \alpha Ra + \beta$, where $\alpha = 6.9 \times 10^{-3}$ and $\beta = 2.75$. A simple rescaling of the depth and temperature scales in the definitions of $Nu$ and $Ra$ allows the heat flux through a layer of depth $\hat{H}$ with average interior temperature $\Theta$ to be described by

$$Nu = 4\alpha \Theta^2 Ra + 2\beta \frac{\Theta}{\hat{H}}, \quad (4.14)$$

where $\alpha$ and $\beta$ are given above. We use (4.14) to parameterize the convective flux
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Figure 4.12: Schematic diagrams of the model system. (a) A sketch of the flow (solid lines) through and near the low-permeability layer in the advection regime (see §4.4.1), and the isotherm along which $T = 0.5$ (dashed line). (b) A profile of the horizontally averaged temperature $\bar{T}$ for the advection regime. (c) A profile of $T$ for the diffusion regime.

through the upper and lower layers in the models outlined below.

4.4.1 Advevtive transport across the low-permeability layer

Figure 4.12(a) shows a schematic diagram of the flow in the advection regime. In the upper and lower layers, we model the flow as a series of circulating cells of depth $1/2$ and width $\lambda$. Broad downwelling (upwelling) flow in the upper (lower) layer with typical vertical velocity $w_B$ impinges on the low-permeability layer, and either ‘leaks’ through the layer with typical velocity $w_L$ or spreads laterally with typical velocity $u$ (figure 4.12a).

The leakage velocity $w_L$ is driven by the vertical pressure difference $[p]$ across the low-permeability layer, which, owing to the symmetry of the system, is also the horizontal pressure difference over the distance $\lambda$ between neighbouring plumes. From the vertical component of Darcy’s law inside the layer and the horizontal component outside of the layer, we therefore have

$$[p] \sim \Omega w_L \sim u \lambda,$$  \hspace{1cm} (4.15)

(cf. (4.12)). Measurements of $w_L$, $u$ and $\lambda$ from simulations give good agreement
The pressure difference \([p]\) must also be related to the density contrasts between the upper and lower layers. Just above the low-permeability layer, relatively hot fluid of temperature \(\sim 1 - \Theta\) that has leaked from below spreads laterally beneath relatively cold fluid of temperature \(\sim \Theta\). We model this lateral flow as a thin buoyant boundary layer of hot fluid which is driven by a hydrostatic pressure difference

\[
[p] \sim \Delta \Theta \eta,
\]

where \(\eta\) is the depth of the boundary layer (figure 4.12a) and \(\Delta \Theta = 1 - 2\Theta\) is the density difference between the hot and cold fluid (figure 4.12b). Under the assumption that advection dominates the flow near to the low-permeability layer, so that diffusion can be neglected, we deduce that \(\eta\) is an isotherm (figure 4.12a) with a slope \(\sim \eta/\lambda\) set by the relative strength of vertical and horizontal flow. Hence

\[
\frac{\eta}{\lambda} \sim \frac{w_L}{u}.
\]

The velocities \(w_L\) and \(u\) are also related to the typical vertical velocity \(w_B\) of the broad downwelling or upwelling regions by conservation of volume flux, which gives

\[
u \sim (w_B - w_L) \lambda.
\]

Equations (4.15)–(4.18) provide five scaling relationships which describe the unknown variables \(u, w_L, [p], \lambda\) and \(\eta\) in terms of \(\Delta \Theta, \Omega\), and \(w_B\). The equations combine to give \(w_B - w_L \sim \Delta \Theta/\Omega\) and a simple scaling of

\[
w_L \sim \Theta - \nu \frac{\Delta \Theta}{\Omega},
\]

for the leakage velocity \(w_L\), where \(\nu\) is an undetermined constant of proportionality and \(w_B \sim \Theta\) by Darcy’s law.

We close the system by balancing the leakage heat flux \(\sim Ra w_L \Delta \Theta\) through the low-permeability layer with the convective heat flux in the upper and lower layer given by (4.14). Such a balance gives a quadratic equation for \(\Theta\) of the form
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\[ 4\alpha \Theta^2 + \frac{2\beta \Theta}{Ra} = \gamma (1 - 2\Theta) \left[ \Theta - \nu \frac{(1 - 2\Theta)}{\Omega} \right], \quad (4.20) \]

where \( \gamma \) is another constant of proportionality. (Note that we have set the depth scale \( \hat{H} \) in (4.14) to unity in order that \( Nu \) reduces to the homogeneous value for small \( \Omega \).)

Equation (4.20) can be readily solved for \( \Theta \) (the resultant expression is convoluted and not given here) and has one real root in the range \( 0 \leq \Theta \leq 1/2 \) if \( \Omega > O(\nu \alpha / \gamma) \). In fact, since \( \alpha = O(10^{-3}) \) and \( Ra \geq O(10^3) \), (4.20) can be well approximated by setting the left-hand side equal to zero, provided that \( \gamma = O(1) \) or larger. The simple solution of the resultant equation is given by

\[ \Theta = (2 + \Omega / \nu)^{-1}, \quad (4.21) \]

which can be combined with (4.14) to give an expression for the flux of the form

\[ Nu = \frac{\alpha Ra}{(1 + \Omega/2\nu)^2} + \frac{\beta}{(1 + \Omega/2\nu)}. \quad (4.22) \]

The predictions of \( Nu(\Omega) \) from (4.22) for \( \nu = 3 \) are shown in figure 4.13, and give a reasonably good qualitative fit with the data. The parameter \( \nu \) was chosen to give a rough fit across the range of \( Ra \). The model does not describe the initial increase in \( Nu \) with \( \Omega \) at moderate values of \( Ra \) (e.g. in figure 4.13a).

The model also gives a prediction for the scaling of the width \( \lambda \) of the cells. Equations (4.15)–(4.17) combine to give \( w_L \sim \Delta \Theta \lambda^2 / \Omega^2 \), which can then be combined with (4.19) to give

\[ \lambda \sim \left( \frac{\Omega^2 \Theta}{\Delta \Theta} - \nu \Omega \right)^{1/2} \sim \Omega^{1/2}, \quad (4.23) \]

using (4.21). The model therefore predicts that the lengthscale between plumes increases like \( \Omega^{1/2} \), or, equivalently, the horizontal wavenumber decreases like \( \Omega^{-1/2} \), in agreement with the numerical measurements of the wavenumber \( k \) in figure 4.10(b).
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Figure 4.13: A comparison of measurements of $Nu(\Omega)$ from reduced simulations and the predictions of the model for the advection regime with $\nu = 3$ (solid lines, from (4.22)) and for the diffusion regime (dashed lines, from (4.26)). (a) $Ra = 5000$, (b) $Ra = 10^4$, and (c) $Ra = 2 \times 10^4$.

4.4.2 Diffusive transport across the low-permeability layer

For sufficiently large values of $\Omega$, the flux through the low-permeability layer is primarily diffusive. In the diffusion regime, the system resembles two layers of homogeneous columnar convection placed one on top of the other, with boundary-layer regions above and below the low-permeability layer as well as near the upper and lower boundaries of the domain (figure 4.12c).

The diffusive flux across the low-permeability layer of thickness $h$ is given by

$$Nu \approx \frac{\Delta \Theta}{h} = \frac{1 - 4\Theta}{h}, \quad (4.24)$$

(figure 4.12c). We eliminate $\Theta$ by equating (4.24) with the convective flux through the upper and lower layers, which is given by (4.14) with $\hat{H} = 1/2$. The resultant quadratic equation for $\Theta(h)$ has one real root in the range $0 \leq \Theta \leq 1/2$, which can be back-substituted into (4.24) to give

$$Nu = \frac{1}{\alpha Ra h^2} \left[ (\alpha Ra + 2\beta) h + 2 - 2\sqrt{\alpha Ra h + (1 + \beta h)^2} \right]. \quad (4.25)$$

The prediction of $Nu(h)$ from (4.25) was shown by the solid line in figure 4.4(a); it shows that $Nu$ decreases as $h$ is increased, and gives very good agreement with numerical measurements for $\Pi = 0$.

For $h, \Pi \ll 1$, the interior temperature and Nusselt number from (4.25) reduce
4. Convection in a layered medium

To

\[ \Theta = \frac{1}{4} - O(h) \quad \text{and} \quad Nu = \frac{1}{4} \alpha Ra + \beta - O(h). \]  

(4.26a, b)

Thus, in the limit \( h, \Pi \to 0 \), \( Nu \) is a constant. Predictions of (4.26b) give fairly good agreement with measurements from reduced simulations at large \( \Omega \) (figure 4.13, dashed lines), although they appear to slightly underestimate the measurements. It is likely that this underestimate is related to the implicit assumption in the model that the temperature at the edge of the low-permeability layer is uniform. In measurements from reduced simulations, we observed non-zero horizontal fluctuations in \( T \) at \( z = 0 \) (figure 4.7d), which will induce flow, potentially leading to thinner diffusive boundary layers above and below the low-permeability layer and a slightly larger flux than the model predicts.

4.4.3 Discussion

The results of figure 4.13 demonstrate that simple one-dimensional models can give a reasonable qualitative description of the relationship \( Nu(\Omega) \). The model for the advection regime also predicts that the dominant horizontal wavenumber decreases like \( \Omega^{-1/2} \), in agreement with the numerical measurements in figure 4.10(b). The model is based on a number of assumptions, and some of these are briefly discussed here.

The model takes the form of a balance between the heat flux through the upper and lower layers and the heat flux through the low-permeability layer, each of which is parameterized in terms of the average temperature in each half of the domain. The heat flux through the upper and lower layers is related to the convective flux for homogeneous Rayleigh–Darcy convection by a rescaling of temperatures and lengths. The model for the heat flux through the low-permeability layer has three key components: a relationship between the pressure-driven vertical flow across the layer and horizontal flow above and below the layer (4.15); a relationship between the pressure and the temperature difference across the layer (4.16), which incorporates an expression for the boundary-layer depth near to the layer (4.17); and conservation of volume flux (4.18).

The second relationship is the least straightforward to model. In order to generate a simple closed model, we assumed that heat is advected without diffusing...
near to the low-permeability layer, which gives rise to the scaling in (4.17). Inspection of isotherms and streamlines from the numerical simulations suggests that vertical diffusion may not be completely negligible in these regions; however, it is not clear how to incorporate a balance between diffusion and both horizontal and vertical advection into the simple model.

The boundary-layer scaling in (4.16) relies on the assumption that the lateral flow on either side of the layer is not weak relative to the vertical flow across the layer. This assumption breaks down in the limit \( \Omega \to 0 \), as the homogeneous flow is predominantly vertical throughout the interior of the domain. In fact, we find that there are no real solutions to (4.20) if \( \Omega \) is sufficiently small (\( \Omega < O(\nu \alpha / \gamma) \)), which likely reflects the breakdown of this assumption.

The observed increase in \( Nu \) with \( \Omega \) for small \( \Omega \) is not captured by the simple model in the advection regime. Our numerical results suggest that the increase in \( Nu \) is related to the flow becoming more ‘ordered’ (see e.g. figure 4.6), although this is a qualitative observation and it is not clear how an increased ‘order’ leads to an increased flux. An additional interesting feature of the increase in \( Nu \) is that the effect is smaller at larger values of \( Ra \), and so, by implication, it is not associated with asymptotically large values of \( Ra \). We have been unable to find a simple physical model for the increase in \( Nu \) with \( \Omega \), and the effect remains puzzling.

4.5 Conclusions

We have undertaken a detailed numerical investigation of statistically steady convection at high \( Ra \) in a domain containing an interior low-permeability layer of height \( h \) and relative permeability \( \Pi < 1 \). In the limit \( h, \Pi \ll 1 \), the flow depends only on the parameter \( \Omega = h/\Pi \), and the low-permeability layer can be parameterized by a jump condition for the horizontal velocity at \( z = 0.5 \). Reduced numerical simulations which solve the jump condition give good agreement with fully resolved numerical simulations for a range of values of \( h \) and \( \Pi \).

In §4.3.4, we examined the structure of the flow for \( Ra = 5000 \), in the reduced framework \( h, \Pi \ll 1 \). For \( \Omega \gtrsim 0.05 \), the flow develops an ordered cellular structure with a horizontal length scale that increases with \( \Omega \). Each cell is roughly half the
height of the domain, and comprises a thin vertical plume carrying fluid in one direction and a much wider plume carrying the return flow, together with some ‘leakage’ of buoyancy across the low-permeability layer. Remarkably, $Nu$ increases as $\Omega$ is increased (i.e. as the permeability of the interior layer is decreased) in this dynamical regime. For $0.3 \lesssim \Omega \lesssim 5$, the horizontal lengthscale of the flow continues to increase but $Nu$ decreases. The flow can be unstable to the formation of protoplumes near the low-permeability layer in this range of $\Omega$. For $\Omega \gtrsim 5$, advection through the low-permeability layer is weaker than diffusion, and the flow structure changes completely to resemble two layers of homogeneous columnar convection placed one on top of the other. The statistically steady flow structure and the associated flux appear to be sensitively affected by the initial conditions, which is likely owing to restriction imposed on the flow by the horizontal periodicity of the domain.

In §4.3.5, we explored the dependence of this behaviour on $Ra$. We found that the initial increase in $Nu$ with $\Omega$ is more pronounced at smaller $Ra$ and less pronounced at larger $Ra$. As $Ra$ is increased, the value of $\Omega$ above which the flow near the low-permeability layer is unstable to the growth of protoplumes appears to decrease. Measurements of the dominant horizontal wavenumber $k$ at $z = 0.5$ suggest that the increase in the horizontal lengthscale with $\Omega$ roughly fits a scaling of $k \sim \Omega^{-1/2}$.

In §4.4, we developed simple one-dimensional models that describe the behaviour of $Nu(\Omega)$, for both the advection and the diffusion regime. The model for the advection regime also predicts that the dominant horizontal wavenumber scales with $\Omega^{-1/2}$, in agreement with the numerical measurements. This model was discussed in §4.4.3. The model for the diffusion regime has no free parameters and gives fairly good agreement with both full and reduced numerical results.

Two observations from this work are particularly striking: the dramatic increase in the horizontal lengthscale of the flow with $\Omega$, and the unexpected increase in $Nu$ with $\Omega$ for moderate values of $Ra$. These observations could have interesting consequences in geophysical and industrial settings.
Appendix

4.A Discussion of the assumption of uniform porosity

For simplicity, in the main body of this paper we made the assumption that the porosity \( \phi \) is uniform throughout the domain, and is, by implication, independent of the permeability \( K \). In a physical system, it is likely that \( \phi \) would vary with \( K \). However, typical models of the relationship \( K(\phi) \) (such as the Kozeny–Carman model) suggest that the porosity scales with roughly the cube root of the permeability (Bear, 1988), and so changes in the porosity are likely to be much weaker than changes in the permeability.

Here we briefly consider the qualitative effect of a lower porosity in the low-permeability layer. Suppose that the porosity of the upper and lower layers is \( \phi_1 \), while that of the low-permeability layer is \( \phi_2 < \phi_1 \). The flow \( u \) is determined by the solution of the Poisson equation (4.3b), and is thus not directly dependent on the porosity. Under the assumption that the flow through the low-permeability layer is not dominated by time-dependent dynamics, the advective flux through the layer, which scales with \( wT \), is also not significantly affected by a decrease in the porosity. The diffusive flux, however, is scaled by a factor of \( \phi_2/\phi_1 \), because the diffusivity is multiplied by the porosity (see (4.1d)). Thus, we anticipate that a lower porosity in the low-permeability layer would not have an appreciable effect on the flux in the advection regime, but would lead to a lower flux in the diffusion regime. As a result, the transition between advection and diffusion regimes would likely occur at a larger value of \( \Omega \). A simple parameterization of the effect of a lower porosity in the low-permeability layer could be incorporated into our model of the flux in the diffusion regime (§4.4.2) by including a factor of \( \phi_2/\phi_1 \) in (4.24); this parameterization is equivalent to the rescaling \( h \rightarrow (\phi_1/\phi_2)h \).
Chapter 5

Shutdown of convection in a porous medium I: fixed interface

The material contained in both this and the following chapter has been published in the Journal of Fluid Mechanics, under the title ‘Convective shutdown in a porous medium’ (Hewitt et al., 2013a). This chapter contains the first half of the paper. The paper was also the subject of a ‘Focus on Fluids’ review article (Pritchard, 2013).

5.1 Introduction

In chapter 2, we explored in detail the flow in a Rayleigh–Darcy cell, which provides a canonical system for the study of convection. The Rayleigh–Darcy cell is a ‘two-sided’ system, in which there is convective transport away from both the upper and lower boundaries. The system therefore attains a statistically steady state, which allows both for examination of the dynamical structures and emergent patterns of the flow, and for accurate characterization of the convective flux.

Natural convective systems in porous media tend instead to be driven by a source of buoyancy on one boundary alone. We refer to such systems as ‘one-sided’. There are fundamental questions relating to the differences and similarities of the dynamics between one-sided and two-sided convective systems, some of which we address in this chapter and the next. For clarity, when we consider one-sided systems we will assume throughout that the convective flow is downwards,
5. CONVECTIVE SHUTDOWN I: FIXED INTERFACE

away from an active upper boundary. All the other boundaries of the domain are
assumed to be impermeable and perfectly insulating. Furthermore, in contrast
to the previous chapters of this thesis, we consider systems in which convection
is driven solely by compositional density differences, such that the density \( \rho^* \) of
the fluid is a function of the concentration of solute \( C^* \) only. It should be noted,
however, that the governing equations are equally applicable both to convection
from a buoyant source at the base of the domain, and to thermal convection,
provided that heat transfer in the solid phase of the medium can be neglected (as
discussed in §1.2).

This chapter and the next are closely linked, and, for clarity, are introduced
together. The principal objective of this chapter is to examine the relationship
between two-sided and one-sided convection with a fixed upper boundary. Then,
in chapter 6, we will extend these ideas to examine different physically motivated
one-sided systems, each of which comprises two fluid layers with a moving interface
(such as in the case of sequestered CO\(_2\) and brine).

Previous work on the two-dimensional Rayleigh–Darcy cell was discussed in
§1.3. This work has focused on examining the dimensionless heat (or solute) flux
through the cell, as described by the Nusselt number \( \text{Nu} \), and the corresponding
dynamical structures of the flow, as functions of the Rayleigh number \( Ra \). In
chapter 2, we examined the flow in a Rayleigh–Darcy cell in the ‘high-\( Ra \)’ regime
(\( Ra \gtrsim 1300 \)). We recall that the dynamical structure in this regime is dominated
by vertical columnar ‘megaplumes’ that extend across the interior of the domain,
and are driven by entrainment and mixing of small ‘protoplumes’ near the upper
and lower boundary. Numerical measurements of \( \text{Nu} \) were extremely well described
by a function of the form \( \text{Nu} = \alpha Ra + \beta \), for constant \( \alpha \) and \( \beta \) (see §2.3).

In contrast to the two-sided statistically steady Rayleigh–Darcy configuration,
the dynamics and the buoyancy flux in a one-sided convective system evolve over

time. Many previous studies of one-sided convective systems have focused on the
conditions required for the onset of convection, which presents significant theoret-
ical challenges as the diffusive base state is both time-dependent and nonlinear.
Various theoretical studies (Riaz et al., 2006; Xu et al., 2006; Hassanzadeh et al.,
2006; Slim & Ramakrishnan, 2010; Daniel et al., 2013) have been complemented
by direct numerical investigations (Riaz et al., 2006; Hassanzadeh et al., 2007) and
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laboratory experiments (Fernandez et al., 2002; Backhaus et al., 2011; Slim et al., 2013) that explore the onset of convection.

After onset, the convective flow is dominated by large dense plumes which merge and coarsen as they descend. These descending plumes are fed by the entrainment of smaller plumes near the upper boundary, which are themselves generated episodically by short-wavelength instabilities in the boundary layer. The system evolves independently of the depth of the domain until the largest plumes reach the lower boundary. There have been a number of numerical studies for \( Ra \lesssim O(10^3) \) which examine the evolution of the dynamics and the merging of descending plumes before they interact with the lower boundary (Pau et al., 2010; Hassanzadeh et al., 2007; Slim, 2014). Slim et al. (2013) performed experiments in a Hele-Shaw cell for \( 100 < Ra < 1700 \), and categorized the evolution of the system from the onset of convection in detail. Experimental studies at high \( Ra \) by Neufeld et al. (2010) for \( 5 \times 10^4 < Ra < 6 \times 10^5 \) in a quasi-2D porous medium, and by Backhaus et al. (2011) for \( 6 \times 10^3 < Ra < 9 \times 10^4 \) in a Hele-Shaw cell, provided measurements of the convective flux after the onset of convection.

When the descending plumes reach the lower boundary, the domain begins to fill up with dense fluid. Once this dense fluid reaches the upper boundary, the dynamics of the system change and the convective flux begins to decrease. The qualitative behaviour of the flux in this ‘shutdown’ regime has been observed in numerical simulations by Hassanzadeh et al. (2007) for \( Ra < 1000 \), although they provided no theoretical analysis of the system. Slim et al. (2013) presented experimental results in this regime for \( 100 < Ra < 1700 \), and derived a phenomenological model which describes the evolution of the flux based on an ad hoc parameterization of the typical boundary-layer depth. Slim (2014) studied the same system numerically. We are not aware of any studies that explore the shutdown regime, in which the convective flux steadily decreases, for \( Ra > 1700 \).

In this chapter and the next, we focus on the evolution of the dynamics and the convective flux during the shutdown regime for \( Ra > O(10^3) \). In this chapter, we show that the evolution of the flux in this one-sided problem can be directly calculated using measurements of the convective flux from a Rayleigh–Darcy cell. We develop a simple theoretical ‘box’ model for this system that uses these measurements to predict the timescales for shutdown, and compare the results to high-
resolution numerical simulations. Furthermore, we find that the dynamical structure of the flow in the shutdown regime exhibits a remarkable similarity to that in a Rayleigh–Darcy cell: the flow is dominated by vertical columnar ‘megaplumes’ that extend across the height of the domain, and the lateral spacing of these plumes increases as the average concentration increases and the system shuts down, in excellent quantitative agreement with measurements from a Rayleigh–Darcy cell. Motivated by previous experimental systems (Neufeld et al., 2010; Backhaus et al., 2011) with a nonlinear density curve, we also examine how the rate of shutdown depends on the form of the density $\rho^*(C^*)$ by considering a power-law equation of state.

In chapter 6, we will develop these ideas to model convective systems comprising two fluid layers, with an interface that that is free to move, as discussed in more detail in §6.1.

### 5.2 Overview of physical systems for chapters 5 and 6

In this chapter and the next, we explore three different model systems for one-sided convection in a porous medium, each with different physical applications (figure 5.1). The systems are distinguished primarily by different properties of the active interface at the top of the convecting region: the first system is a ‘fixed-interface’ system, in the sense that the interface is stationary and is located at a fixed upper boundary; the second and third systems are ‘free-interface’ systems, in the sense that the active interface is free to move and divides the convecting region below from a non-convecting region of fluid above. The second and third systems are distinguished by whether the fluids on either side of the interface are immiscible or miscible, as discussed below.

The first system, studied in this chapter, is the ‘fixed-interface’ system, in which the convective flux away from an interface does not significantly change its height. There are a broad range of geophysical systems for which this is an excellent approximation, including the convection of saline groundwater driven by evaporation at the upper surface (Duffy & Al-Hassan, 1988; Wooding et al.,
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Figure 5.1: A schematic diagram showing typical equations of state $\rho^*(C^*)$, vertical concentration profiles $C^*(z^*)$, and vertical density profiles $\rho^*(z^*)$, for each of the three physical systems outlined in the text (§5.2). In each case the maximum density $\rho^*_{m}$ is attained at concentration $C^*_{m}$, the interfacial height is given by $z^* = h^*$, and the domain has constant depth $H^*$: (a) the ‘fixed-interface’ system, with a stationary upper boundary $z^* = h^* = H^*$ held at concentration $C^*_{m}$; (b) the ‘immiscible’ (free-interface) system, in which fluid with concentration $C^*_+ \overlineslash C^*_-$ overlies fluid with initial concentration $C^*_-$, and the upper fluid is partially soluble in the lower; (c) the ‘miscible’ (free-interface) system, in which the two fluids are fully soluble, and the interfacial height $z^* = h^*$ is given by the isopycnal of maximum density.
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1997a,b), and the extraction of geothermal energy driven by underground heat sources (Cheng, 1978; Goldstein et al., 2011). We consider a fluid that initially contains a dissolved solute at some concentration $C^*_\text{\text{-}}$. The upper boundary of the domain is held at a fixed larger concentration $C^*_m$. We consider a density curve that increases monotonically from $\rho^*(C^*_\text{-})$ to $\rho^*_m = \rho^*(C^*_m)$. A typical density curve for such a system is shown schematically in figure 5.1(a), together with vertical profiles of the concentration and density. Diffusion of solute across the upper boundary forms a dense solution which is unstable to downwards convection. Over time, the concentration increases from $C^*_\text{-}$ towards $C^*_m$, and convection gradually shuts down.

The second and third systems, studied in the next chapter, form two different sorts of ‘free-interface’ system, in which the convective flux away from an interface causes the interface to move. These are typically two-component systems, which initially comprise a light fluid A overlying a dense fluid B. Dissolution of A into B creates fluid that is more dense than pure B. The system is thus unstable to convection, and the active interface between the two layers moves as A dissolves into B and convection transports the dense solution down into the lower layer. The concentration $C^*$ describes that of the solution of A in B, with pure A having concentration $C^*_-, and pure B having concentration $C^*_m < C^*_+$. Mathematically, this is related to the classical Stefan problem (see e.g. Hill 1987), and our approach to the modelling is similar to that used for convection in a (non-porous) fluid layer below a melting interface (e.g. Huppert & Sparks 1988a,b; Huppert 1989).

We shall investigate two qualitatively different free-interface systems, which correspond to immiscible and miscible fluids respectively. In the ‘immiscible’ system, A is only partially soluble in B, and, for simplicity, we assume that B is not at all soluble in A. The density is largest ($\rho^* = \rho^*_m$) at the maximum concentration of A in B, denoted by $C^*_m$. The concentration $C^*$ cannot lie in the range $C^*_m < C^* < C^*_+$, and, as such, there is a discontinuity in the concentration and density fields at the interface, which divides pure A above from a solution of A in B below. This behaviour can be seen in figure 5.1(b), which shows a typical density curve for the immiscible system, together with vertical profiles of the concentration and density.

In contrast, in the ‘miscible’ system A and B are fully soluble, and the equation
5. Convective shutdown I: fixed interface

of state \( \rho^*(C^*) \) is continuous, with a maximum at some intermediate concentration \( C_m^* \) as shown schematically in figure 5.1(c). There is a qualitative distinction here from the immiscible system, in that there is not a genuine interface between different fluids when the fluids are miscible. Instead, we define the interface to be equal to the contour of maximum density \( (\rho^* = \rho_m^*) \). This isopycnal separates stably stratified fluid above from unstably stratified fluid below, and is therefore an interface in the sense that it lies between regions of dynamically different fluid behaviour.

Both immiscible and miscible systems have important applications, most pertinently to the subject of CO\(_2\) sequestration. Supercritical CO\(_2\) and brine are immiscible, with CO\(_2\) being only 3–5\% soluble by weight in brine under typical storage conditions (van der Meer, 2005). In contrast, many experimental analogues of sequestration systems are based on mixtures of glycol and water, and form miscible systems (e.g. Neufeld et al. 2010; Backhaus et al. 2011).

We will develop a series of mathematical models which describe the different physical systems that we have introduced above. In this chapter, we examine the ‘fixed-interface’ system. In chapter 6, we examine both immiscible and miscible free-interface systems; first, under the assumption that the interface remains flat, and second, when this assumption is relaxed and the interface is free to deform. The layout of chapter 6 is discussed in §6.1.

The layout of this chapter is as follows. In §5.3, we present the governing equations, non-dimensionalization, and numerical scheme used to model these different one-sided systems. In §5.4, we present the results of high-resolution numerical calculations of the fixed-interface system. Motivated by these results, in §5.5 we derive a simple theoretical ‘box’ model of this system, which describes the shutdown of the solute flux over time using measurements of \( Nu(Ra) \) from a Rayleigh-Darcy cell. We compare the theoretical and numerical results in §5.6. We also show, in §5.7, that the dynamical structure of the flow in the one-sided system can be accurately predicted by measurements from a Rayleigh–Darcy cell. In §5.8, we summarize the main results.
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\[
\begin{align*}
\text{(a)} & \quad z^* = b_0^m, \quad C^* = C_m^m, \quad z = 1, \quad C = 0, \\
\text{(b)} & \quad z^* = b_0^l, \quad C^* = C_l^l, \quad z = 0, \quad C = -1,
\end{align*}
\]

Figure 5.2: A schematic showing the initial conditions in both dimensional and dimensionless variables: (a) the fixed-interface system with a stationary upper active boundary, which is the subject of this chapter; (b) free-interface systems (either immiscible or miscible) with an interfacial height that evolves in time, which are the subject of chapter 6.

5.3 Governing equations for chapters 5 and 6

5.3.1 Dimensional equations

In common with the previous chapters of this thesis, we consider the flow of a Boussinesq fluid in a two-dimensional, homogeneous, isotropic porous medium, with horizontal and vertical co-ordinates \( x^* \) and \( z^* \) respectively. We assume that the flow \( \mathbf{u}^* = (u^*, w^*) \) obeys Darcy’s law and is incompressible,

\[
\mathbf{u}^* = -\frac{K}{\mu} (\nabla p^* + \rho^* g \hat{z}^*), \quad \nabla \cdot \mathbf{u}^* = 0,
\]

where \( K \) is the permeability of the porous medium and \( \mu \) is the fluid viscosity, both of which are assumed to be constant, \( p^* \) is the pressure field, \( g \) is the acceleration due to gravity, and \( \hat{z}^* \) is a unit vector in the positive \( z^* \) direction. The density \( \rho^* \) is a function of the local concentration \( C^* \) (rather than temperature, as in previous chapters). The concentration \( C^* \) evolves in time \( t^* \) by advection and diffusion,

\[
\phi \frac{\partial C^*}{\partial t^*} = -\mathbf{u}^* \cdot \nabla C^* + \phi D \nabla^2 C^*,
\]

where \( \phi \) is the porosity of the porous medium and \( D \) is the diffusivity, both again assumed to be constant.

We consider here the boundary and initial conditions for both fixed-interface systems, which are the subject of this chapter, and free-interface systems, which are
the subject of chapter 6. The fixed-interface system has a stationary active upper boundary. The domain has height $h_0^*$ and width $L^*$, and the upper boundary has an imposed constant concentration $C^*|_{z^*=h_0^*} = C_m^*$ and no vertical velocity $w^*|_{z^*=h_0^*} = 0$. The lower and side boundaries have zero mass and buoyancy fluxes, $w^* = \frac{\partial C^*}{\partial z^*} = 0$ at $z^* = 0$, $u^* = \frac{\partial C^*}{\partial x^*} = 0$ at $x^* = 0, L^*$. (5.3a, b)

The medium is initially saturated with fluid at a concentration $C_0^* < C_m^*$. The initial and boundary conditions for this system are shown schematically in figure 5.2(a), and the equation of state is discussed below.

Free-interface systems (both immiscible and miscible) have an active interface that is located in the interior of the domain, and is free to move. The domain has a constant depth $H^*$ and width $L^*$, with zero mass and buoyancy fluxes on every boundary, $w^* = \frac{\partial C^*}{\partial z^*} = 0$ at $z^* = 0, H^*$, $u^* = \frac{\partial C^*}{\partial x^*} = 0$ at $x^* = 0, L^*$. (5.4a, b)

The medium is initially saturated with fluid in two layers (figure 5.2b): a lower layer of concentration $C_-,^*$, and an upper layer of concentration $C_+^* > C_-,^*$. The density of the lower layer $\rho_-^* = \rho^*(C_-^*)$ is greater than the density of the upper layer $\rho_+^* = \rho^*(C_+^*)$, and, as such, the system is stable to large-scale overturning. The initial height of the interface between the layers is given by $z^* = h_0^*$. For $t^* > 0$, the interfacial height is given by $z^* = h^*(x^*, t^*)$, which is defined to be the contour of maximum density $\rho^* = \rho_m^*$. The details of how the location of the interface is determined over time in each of the different model frameworks that we employ are discussed in §6.2 and §6.3.

For both fixed-interface and free-interface systems, we consider general power-law equations of state,

$$\rho^* = \rho_m^* \left[1 - b (C_m^* - C^*)^n\right],$$

where $b > 0$ is a constant coefficient and $n$ is a positive integer. The maximum density, given by the constant $\rho_m^*$, is attained at concentration $C_m^*$. For the fixed-interface system, the concentration $C^*$ is always less than $C_m^*$, and so $\rho^*(C^*) \leq \rho_m^*$.
irrespective of \( n \). For immiscible free-interface systems, the concentration above the interface is fixed at \( C^* = C_{m}^* \), while below the interface the concentration is again always less than \( C_{m}^* \). For miscible free-interface systems, however, (5.5) holds for \( C^* > C_{m}^* \), and so we require \( n \) to be an even (positive) integer in order to satisfy \( \rho^*_+ < \rho^*_m \). Representative equations of state for each system are shown in figure 5.1. In this work we focus primarily on either linear \((n = 1)\) or quadratic \((n = 2)\) equations of state.

### 5.3.2 Dimensionless equations

For all the systems considered, we define a density scale \( \Delta \rho^* = \rho^*_m b(C_m^* - C_\infty^*)^n \) to be the difference between the maximum density and the initial density of the lower layer, and a convective velocity scale \( U^* = Kg\Delta \rho_m^* / \mu \). We also define the dimensionless interfacial height \( h \), concentration \( C \) and density \( \rho \) to be

\[
    h = \frac{h^*}{h_0^*}, \quad C = \frac{C^* - C_m^*}{C_m^* - C_\infty^*}, \quad \rho = 1 + \frac{\rho^* - \rho_m^*}{\Delta \rho^*}. \tag{5.6a, b, c}
\]

The dimensionless concentration below the interface is then negative, and \( C = 0 \) at the interface where the density is maximum \((\rho = 1)\). We scale lengths with the initial interfacial height \( h_0^* \), velocities with \( U^* \), pressures with \( \mu U^* h_0^*/K \), and times with the convective time scale \( T^* = \phi h_0^*/U^* \).

Rescaling in this way gives dimensionless governing equations

\[
    \mathbf{u} = -[\nabla P - (-C)^n \hat{z}], \tag{5.7}
\]

\[
    \nabla \cdot \mathbf{u} = 0, \tag{5.8}
\]

\[
    \rho = 1 - (-C)^n, \tag{5.9}
\]

\[
    \frac{\partial C}{\partial t} = -\mathbf{u} \cdot \nabla C + \frac{1}{Ra_0} \nabla^2 C, \tag{5.10}
\]

with a reduced pressure \( P = p + z/[b(C_m^* - C_\infty^*)^n] \), and an initial Rayleigh number
5. Convective shutdown I: fixed interface

\[ Ra_0 = \frac{h_0 U^*}{\phi D^*} = \frac{h_0 K g \Delta \rho^*}{\phi D\mu}. \]  

(5.11)

For the fixed-interface system, the dimensionless initial condition is \( C(x, z, t = 0) = -1 \), and the upper boundary condition is \( C|_{z=1} = 0 \). For free-interface systems, the dimensionless initial concentration profile is given by

\[ C(x, z, t = 0) = \begin{cases} 
-1 & \text{for } 0 \leq z \leq 1, \\
C_+ & \text{for } 1 < z < H, 
\end{cases} \]  

(5.12)
as shown schematically in figure 5.2.

5.3.3 Numerical method

As in previous chapters, the requirement of incompressibility (5.8) can be satisfied by introducing a streamfunction \( \psi \), with \( (u, w) = (\psi_z, -\psi_x) \), and we can eliminate pressure by taking the curl of (5.7), to give

\[ \nabla^2 \psi = -\frac{\partial}{\partial x} (-C)^n. \]  

(5.13)

Equations (5.10) and (5.13) were solved numerically. The numerical method is briefly outlined here, and discussed in more detail in appendix A, §A.2.2. We anticipated a thin diffusive boundary layer below the interface \( z = h(x, t) \) and, in order to ensure that the dynamics near the interface are well resolved, we used a vertical co-ordinate transformation \( \zeta = f[z, h(t)] \). For the free-interface systems, this transformation is adaptive, and is recalculated once the interface has moved a sufficient distance to require it. The horizontal and temporal resolution are uniform.

We solved the Poisson equation (5.13) using a spectral method in the horizontal direction, and a compact fourth-order finite-difference operator for the vertical derivatives. The diffusion and advection operators in the transport equation (5.10) were discretized using standard second-order finite differences and flux-conservative techniques respectively, and the equation was solved using an alternating-direction implicit method (Press et al., 1989). The boundary condi-
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tions were imposed in such a way as to ensure that the numerical scheme retained second-order accuracy (see appendix A for details).

5.3.4 The flux

We have non-dimensionalized the variables with respect to the convective time scale $T^* = \phi h_0^*/U^*$. For the fixed interface, the dimensionless diffusive solute flux through the upper boundary is therefore given by $Ra_0^{-1} \partial C/\partial z|_{z=1}$ (from 5.10). However, we are aiming to compare the one-sided system with the Rayleigh–Darcy cell, where the dimensionless flux is more commonly defined with respect to the diffusive time scale (as in, for example, standard definitions of the Nusselt number used throughout this thesis; see (2.12)). It is thus helpful to consider a rescaled flux, which we define to be the actual dimensionless flux scaled by the flux $Ra_0^{-1}$ that would be given by diffusion down a unit linear concentration gradient in the absence of convection. The horizontally averaged rescaled flux $F(t)$ is therefore given by

$$F(t) = \frac{1}{L} \int_0^L \frac{\partial C}{\partial z} \bigg|_{z=1} \, dx.$$  (5.14)

Throughout this chapter, we measure and model the rescaled flux $F(t)$.

5.4 Numerical results

For the remainder of this chapter, we consider a fixed-interface system, in which the active interface is located at the stationary upper boundary $z = 1$. We begin with the results of high-resolution numerical calculations of the fixed-interface system. Numerical snapshots of the concentration field $C(x,z,t)$ are shown in figure 5.3, together with the horizontally averaged concentration profile $\bar{C}(z,t) = L^{-1} \int_0^L C \, dx$ at different times, for a linear equation of state ($n = 1$) and an initial Rayleigh number $Ra_0 = 10^4$. The corresponding average solute flux $F(t)$ (figure 5.4) will be discussed in detail at the end of this subsection.

Initially, a stable diffusive boundary layer grows below the upper boundary. After a critical time $t_c \sim Ra_0^{-1}$ (see, for example, Riaz et al. 2006; Daniel et al. 2013; Slim 2014), the boundary layer becomes unstable to short-wavelength instabilities.
leading to downward convection (figure 5.3a). At this point both the flux from the upper boundary and the convective dynamics are independent of the location of the lower boundary. At some time $t_1$, the first generation of convecting plumes reaches the base of the domain (figure 5.3b), while at some later time $t_2$, the return flow from this interaction reaches the upper boundary and the flux begins to decrease. For $t > t_2$ the system enters a different, ‘shutdown’, regime in which the flux $F(t)$ decreases as the interior of the domain becomes steadily more concentrated with solute. The times $t_1$ and $t_2$ are controlled both by the diffusive onset time scale $t_c \sim Ra_0^{-1}$ and the $O(1)$ convective time scale. Since $Ra_0 \gg O(1)$, we expect the convective time to dominate: thus $t_1$ can be assumed to be independent of $Ra_0$, and $t_2 \approx 2t_1$. We find numerically that $t_1 \approx 7.5$ and $t_2 \approx 15$, in broad agreement with the experimental results of Slim et al. (2013). For $t > t_2$, the horizontally averaged concentration $\overline{C}(z,t)$ is approximately independent of $z$ away from the boundary layer, and $\overline{C}$ increases steadily over time (figures 5.3c and d). These observations underpin the theoretical modelling in §5.5.

The dynamics in the shutdown regime, $t > t_2$, are dominated by persistent, descending megaplumes interleaved with a columnar return flow that rises towards the upper boundary. Instabilities in the thin boundary layer at the upper boundary drive the growth of small vigorous protoplumes, which carry dense fluid from the boundary layer into the larger descending megaplumes. As the interior becomes more concentrated, the dynamics of the flow become less vigorous; the depth of the boundary layer increases as the density contrast with the interior decreases; and the (differing) horizontal length scales associated with both protoplumes and megaplumes increase. The dynamical structure of the flow appears qualitatively very similar to that of the upper half of a Rayleigh–Darcy cell in the high-$Ra$ regime (see chapter 2). This similarity is discussed in §5.5.1.

The horizontally averaged solute flux (5.14) exhibits rapid chaotic fluctuations about a time-varying mean. Measurements of other variables from our numerical calculations also show some chaotic variation about time-varying average values. We typically ensemble-average our numerical results to reduce the fluctuations and to give clearer measurements for comparison with the theoretical modelling. The variables used in the theoretical sections of this work refer to the mean values. The number of repeat simulations used in an ensemble-average is given in the caption.
Figure 5.3: Snapshots of the concentration field $C$ in a fixed-interface system, from numerical simulations, for $n = 1$, $Ra_0 = 10^4$, and aspect ratio $L = 2$, together with plots of the horizontally-averaged concentration profile $\overline{C}(z,t) = L^{-1} \int_0^L C \, dx$: (a) time $t = 4$, before the first generation of plumes has reached the base of the domain; (b) $t = 8 \approx t_1$, when the descending plumes first reach the base; (c) $t = 32$, in the shutdown regime; (d) $t = 128$. The horizontally averaged concentration profile in (c) and (d) is approximately uniform away from the upper boundary. The horizontal spacing of the downwelling plumes increases over time. Note the different colour scales on the left.
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Figure 5.4: The horizontally averaged solute flux $F(t)$ (5.14), for a linear equation of state $n = 1$, aspect ratio $L = 2$, and $Ra_0 = 1 \times 10^4$ and $Ra_0 = 2 \times 10^4$ as marked: (a) measurements from one numerical simulation, showing the variability of $F$; and (b) measurements ensemble-averaged over eight numerical simulations (solid), together with the theoretical predictions (5.28) (dotted) as discussed in §5.5. The transition to the shutdown regime at $t = t_2$ is marked.

5.5 Theoretical box model

The numerical calculations showed that the horizontally averaged interior concentration is approximately uniform for $t > t_2$ (figures 5.3c and d), apart from in a thin boundary layer near the upper boundary. This observation provides the motivation for the development of a simple box model, using a well-mixed approximation. We assume that, outside the thin boundary layer, the horizontally
averaged concentration is independent of \( z \), so that

\[
\overline{C} = \Theta(t) \leq 0. \tag{5.15}
\]

As \( \Theta(t) \) increases towards zero, the strength of convection decreases. Based on the definition of the Rayleigh number in (5.11), we define a time-dependent Rayleigh number \( Ra(t) \) to be proportional to the current density difference between the upper boundary \( (C = 0) \) and the interior \( (C = \Theta(t) \leq 0). \) Thus

\[
Ra(t) = Ra_0 |\Theta(t)|^n. \tag{5.16}
\]

We further define a time-dependent Nusselt number \( Nu(t) \), by scaling the flux \( F(t) \) up to a unit concentration difference, which gives

\[
Nu(t) = \frac{F(t)}{|\Theta(t)|}. \tag{5.17}
\]

We expect \( Nu(t) \) to be given by some function of the current Rayleigh number, so that \( Nu(t) = N[Ra(t)] \). The functional form of \( N(Ra) \) is discussed in §5.5.2.

We integrate the transport equation (5.10) over the whole domain, and use the boundary conditions to obtain

\[
\frac{d}{dt} \int_0^1 \int_0^L C \, dx \, dz = \frac{1}{Ra_0} \int_0^L \frac{\partial C}{\partial z} \bigg|_{z=1} \, dx. \tag{5.18}
\]

Using (5.14) and the definition of the horizontally averaged concentration \( \overline{C}(z,t) \), (5.18) can be rewritten as

\[
\frac{d}{dt} \int_0^1 \overline{C} \, dz = \frac{F}{Ra_0}. \tag{5.19}
\]

Since under the well-mixed approximation (5.15) we are neglecting the area of the thin boundary layer, (5.19) can be combined with (5.15) and (5.17) to give

\[
\frac{d\Theta}{dt} = \frac{|\Theta|}{Ra_0} N[Ra(t)]. \tag{5.20}
\]
Equation (5.20) gives a theoretical prediction for the evolution of the shutdown regime, which we can solve for a given form of the Nusselt number $N(Ra)$. The model applies for $t > t_2$, and so (5.20) can be solved together with an initial condition for the interior concentration $\Theta(t_2)$. In fact, solutions can be extrapolated back to $t < t_2$, and (5.20) can thus be solved with an initial condition $\Theta(t_0) = -1$, where $t_0 < t_2$ is a virtual origin that allows for the differing dynamics of the system before it enters the shutdown regime. We find numerically that $t_0 = 0$ provides a very good approximation.

### 5.5.1 Relationship to the two-sided Rayleigh–Darcy cell

As noted earlier, the dynamical structure of one-sided flow in the shutdown regime (figure 5.3c and d) appears qualitatively very similar to half of the convective profile observed in a two-sided Rayleigh–Darcy (RD) cell (chapter 2). We now show that the Nusselt number $N_{RD}(Ra)$ measured in a RD cell is quantitatively applicable to shutdown in the one-sided system.

We consider first, for simplicity, the case of a linear equation of state ($n = 1$). Suppose a statistically steady RD cell has boundary conditions of constant concentration $C = 0$ on the upper boundary and $C = -1$ on the lower, and an average concentration $C_{iRD} = -1/2$ in the interior. As $n = 1$, the density difference $\Delta \rho_{RD}$ between the upper boundary and the interior is given by $\Delta \rho_{RD} = -C_{iRD} = 1/2$. In contrast, while the one-sided system also has a boundary condition of $C = 0$ on the upper boundary, it has a condition of no solute flux through the lower boundary, and an average interior concentration $C^i = \Theta(t)$. The density difference between the upper boundary and the interior is therefore given by $\Delta \rho = |\Theta(t)|$.

We compare the two systems by rescaling $Ra(t)$ to take account of the different boundary conditions and density differences between the upper boundary and the interior. Firstly, because of the different lower boundary conditions, we suggest that the one-sided system is related to the upper half of a RD cell of double the depth. Secondly, in order that the density difference should agree in the two systems, we require the total density difference across the RD cell to be scaled by a factor $\Delta \rho / \Delta \rho_{RD} = 2|\Theta|$. The factor $\Delta \rho = |\Theta|$ is already included in the definition of $Ra(t)$ (5.16), and we therefore define the effective Rayleigh number $Ra_e$ for the
equivalent RD cell to be \( Ra_e = 4Ra(t) \).

For the general case with a nonlinear equation of state \((n > 1)\), we can perform a similar analysis. However, there are two differences. Firstly the interior concentration \( C_{RD}^i \) of the Rayleigh–Darcy cell is a function of \( n \), as discussed in appendix 5.A. Secondly, the dimensionless density difference is not simply equal to the concentration difference, but is given by \( \Delta \rho_{RD} = |C_{RD}^i|^n \) and \( \Delta \rho = |\Theta|^n \). Therefore, the effective Rayleigh number is given by

\[
Ra_e = r(n)Ra(t), \quad \text{where} \quad r(n) = \frac{2}{\Delta \rho_{RD}},
\]

as, again, the factor \( \Delta \rho = |\Theta|^n \) is already included in the definition of \( Ra(t) \) (5.16). In appendix 5.A we provide numerical estimates of \( C_{RD}^i(n) \), and show that it can be well approximated by the empirical formula \( C_{RD}^i = -(n + 1)^{-1/n} \) for \( n \leq 5 \). Thus, \( \Delta \rho_{RD}(n) = 1/(n + 1) \), and the constant premultiplying factor \( r(n) \) reduces to

\[
r(n) = 2(n + 1).
\]  

5.5.2 The functional form of the Nusselt number

In a RD cell, the time-averaged Nusselt number \( Nu \) is a function of the Rayleigh number \( Ra \) only, and is given by the form \( N_{RD}(Ra) \). In chapter 2, we found that \( N_{RD} \) asymptotically scales linearly with \( Ra \). We also recall that the numerical measurements of \( N_{RD}(Ra) \) for \( 1300 < Ra < 4 \times 10^4 \) were extremely well fitted by an equation of the form

\[
N_{RD}(Ra) = \alpha Ra + \beta,
\]

(cf. (2.14)), where \( \alpha \approx 6.9 \times 10^{-3} \) and \( \beta \approx 2.75 \) are constants.

5.5.3 Analytic solution of the box model

The effective Rayleigh number \( Ra_e = r Ra_0 |\Theta|^n \), given by (5.16) and (5.21a), can be combined with (5.23) to give an expression for the Nusselt number in the
We use (5.25) to integrate (5.20) analytically. As discussed above, we take an initial condition \( \Theta(t_0) = -1 \), where \( t_0 < t_2 \) is a virtual time origin. The solution is given by

\[
\Theta(t) = -\frac{1}{\gamma} \left[ (1 + \gamma) e^{\alpha \gamma (t-t_0)} - 1 \right]^{-1/n},
\]

where \( \gamma = \beta / (\alpha r Ra_0) \).

If \( Ra_0 \) is sufficiently large \( (Ra_0 \gg 10^3) \) then \( \gamma \ll 1 \). In the limit \( \gamma \to 0 \), which corresponds to the simple asymptotic linear scaling \( N = \alpha r Ra \) in (5.25), (5.26) reduces to

\[
\Theta(t) = - [1 + \alpha n r (t - t_0)]^{-1/n},
\]

and the solute flux \( F(t) \), given by (5.17), becomes

\[
F(t) = \alpha r Ra_0 |\Theta|^{n+1} = \alpha r Ra_0 [1 + \alpha n r (t - t_0)]^{-(n+1)/n}.
\]

Thus, in the limit of large \( Ra_0 \) (\( \gamma \to 0 \)), the evolution of the interior concen-
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Concentration $\Theta(t)$ becomes independent of $Ra_0$, and the flux $F(t)$ is proportional to $Ra_0$ (as we might expect from the Nusselt number scaling), but otherwise evolves independently of $Ra_0$.

An important feature of these results is the length of time it takes for the convective flux to shut down. The rate at which the flux $F$ decreases is controlled by $\alpha$, the constant in the Nusselt number relationship (5.23). Since $\alpha \ll 1$, the time scales for the shutdown of convection are much greater than the $O(1)$ convective time scale.

The dependence on the equation of state (5.9) of both the flux and the interior concentration is different at early and late times (figure 5.5). Initially, the flux decreases more rapidly at larger values of $n$. This behaviour can be seen from leading-order expansions of (5.27) and (5.28) (with $t_0 = 0$), which show that

$$\Theta = - \left[ 1 - \alpha r t + O(\alpha^2 t^2) \right], \quad F = \alpha r Ra_0 \left[ 1 - (n + 1)\alpha r t + O(\alpha^2 t^2) \right].$$

Therefore, using (5.22), to leading order $d\Theta/dt \sim 2\alpha (n + 1)$ and $dF/dt \sim -4\alpha^2 (n + 1)^3$, both of which increase in magnitude with $n$. However, at late times (5.27) and (5.28) are dominated by different scalings with time: the model predicts that the interior concentration $\Theta(t)$ increases towards zero like $t^{-1/n}$, and the flux $F(t)$ decays like $t^{-(n+1)/n}$. Therefore, the increase of the interior concentration and the resulting decrease of the flux are both ultimately slower at larger $n$.

These differences can be understood by the shape of the density curve $\rho(C) = 1 - (-C)^n$ (5.9) for different values of $n$. At larger $n$, the gradient of the density curve near $C = -1$ is larger, and therefore the density difference $|\Theta|^n$ which drives convection initially decreases more rapidly. However, the different scaling behaviour of $\rho(C)$ near to the stationary point $C = 0$ means that the long-time scaling of $F(t)$ and $\Theta(t)$ has a weaker exponent at larger $n$. 

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Figure 5.6: Measurements from full numerical calculations (solid) together with theoretical predictions, for $Ra_0 = 10^4$ and aspect ratio $L = 2$: (a) the interior concentration $\Theta(t)$, ensemble-averaged over four calculations, for $n = 1$ and $n = 2$ as marked, together with the theoretical predictions from (5.26) (dotted); (b) the solute flux $F(t)$ for $n = 2$, ensemble-averaged over four calculations, together with the theoretical prediction from (5.17) and (5.26) (dashed), and the theoretical prediction in the asymptotic limit $\gamma \to 0$ from (5.28) (dotted). Numerical measurements of $F(t)$ for $n = 1$ are shown in figure 5.4.

5.6 Comparison of the box model and numerical results

In this section we compare the analytic solutions with numerical measurements. As previously noted, we find empirically that $t_0 = 0$ gives good agreement with the numerical results, and so we use this value throughout.

The interior average concentration $\Theta(t)$ is measured in the numerical simulations by defining a time-dependent boundary-layer depth, below which the concentration is averaged in both spatial directions. Figure 5.6(a) shows numerical measurements and theoretical predictions of $\Theta(t)$, for both a linear ($n = 1$) and a quadratic ($n = 2$) equation of state. The theoretical predictions from the box model (5.26) give very good agreement with the full numerical solutions.

Figure 5.6(b) shows numerical measurements of the solute flux $F(t)$ for a quadratic equation of state ($n = 2$). The theoretical solution derived from (5.26) and the simpler asymptotic solution (5.28) are also shown. These solutions are almost indistinguishable from each other except at late times. Both solutions give
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Figure 5.7: Numerical measurements of the average wavenumber $k$ of the downwelling megaplumes, for a linear equation of state $n = 1$, an aspect ratio $L = 2$, and $Ra_0 = 2 \times 10^4$, measured at $z = 0.5$ and plotted against the effective Rayleigh number $Ra_e = 4Ra_0|\Theta|$ (5.21): (a) measurements from one simulation, showing the typical variability of $k$; and (b) measurements ensemble-averaged over eight simulations (solid line), together with direct measurements of $k(Ra_e)$ in a RD cell (points) (adapted from figure 2.8).

excellent agreement with the numerical results.

These figures show that simple one-dimensional box models give a very good description of the evolution of the system in the shutdown regime. We have also shown that the results from a RD cell can be used both qualitatively and quantitatively to describe the average behaviour of the flux in the shutdown regime, and the corresponding evolution of the interior concentration $\Theta$. Moreover, these results suggest that the simple asymptotic linear scaling $N = \alpha r Ra$, with $\alpha = 6.9 \times 10^{-3}$ and $r(n)$ given by (5.22), is a very good approximation provided $Ra_0 > 10^3$.

5.7 Dynamical structure of shutdown: the horizontal wavenumber

The correspondence between one-sided and two-sided convection is further strengthened by a comparison of the dynamical structure of the flow. Figure 5.3 shows that in the shutdown regime the flow is dominated by long descending megaplumes, with an average horizontal wavenumber that decreases over time.
Based on the discussion above, we might expect the average horizontal wavenumber \( k(t) \), which will depend on the time-dependent Rayleigh number \( Ra(t) \), to be in agreement with the equivalent dependence \( k(Ra_e) \) from a RD cell.

We measured the average horizontal wavenumber \( k(t) \) by taking the Fourier transform of the concentration profile at \( z = 0.5 \), and calculating the average value of \( k \) from the Fourier spectrum. Figure 5.7 shows this measured \( k \) as a function of \( Ra_e = rRa(t) \), together with numerical results from chapter 2; figure 2.8 for \( k(Ra_e) \) in a RD cell. The good agreement seen in this figure provides further evidence that the one-sided system can be quantitatively compared to the upper half of a RD cell, and that the dynamical structures of the shutdown regime are well described by the results from a RD cell.

5.8 Conclusions

In this chapter, we have shown that measurements of the Nusselt number \( Nu(Ra) \) from the statistically steady two-sided Rayleigh–Darcy cell can be used to accurately predict the shutdown of the flux \( F(t) \) in one-sided convective systems. The relationship \( Nu(Ra) = \alpha Ra + \beta \), found in chapter 2, not only qualitatively describes the decay of the flux \( F(t) \) in the one-sided shutdown system, but can also be used to give very good quantitative agreement with the results of numerical calculations.

Furthermore, we have found that the dynamical structure of the flow in the shutdown regime can be accurately described by the structures of a Rayleigh–Darcy cell: the shutdown regime is dominated by downwelling megaplumes with an average horizontal wavenumber \( k(t) \), which decreases over time in quantitative agreement with the measurements of the wavenumber \( k(Ra) \) from a Rayleigh–Darcy cell.

We also characterized the effect of different power-law equations of state \( \rho = 1 - (-C)^n \) on the flux of solute, and thus on the time scale for shutdown. While the rate of shutdown is initially more rapid for larger values of \( n \), at late times the flux decreases more slowly. The initial linear rate of decrease of the flux scales like \( (n + 1)^3 \), while at long times the flux decreases like \( t^{-(n+1)/n} \). The time scale for shutdown \( (\sim \alpha^{-1}) \) is, irrespective of the form of the equation of state, much greater.
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Figure 5.8: Numerical measurements from a Rayleigh–Darcy cell, with $Ra = 10^4$: (a) the average concentration $\bar{C}(z)$ for different values of $n$ as marked; (b) estimated range of the interior concentration $C_{RD}^i(n)$ in the linear interior region, taken from the measurements in (a), together with an approximate analytic fit $C_{RD}^i = -(n + 1)^{-1/n}$ (dashed).

than the convective time scale ($\sim 1$). This observation is a result of the relative ‘inefficiency’ of the flux, as described by the small coefficient $\alpha$ in the relationship for the Nusselt number in a Rayleigh–Darcy cell (5.23).

In chapter 6, we develop this work by examining the shutdown of convection in ‘free-interface’ systems, which comprise two fluid layers with an interface that can move as a result of convection across it.

Appendix

5.A Discussion of the average interior concentration in a Rayleigh–Darcy cell

We consider a two-dimensional Rayleigh–Darcy cell in a porous medium, containing a fluid that satisfies a dimensionless power-law equation of state $\rho = 1 - (-C)^n$, as in (5.9). The cell has periodic (or no-flux) boundary conditions on the side walls,
and fixed concentrations on the upper and lower boundaries,

\[ C(x, z = 1) = 0, \quad (5.30) \]

\[ C(x, z = 0) = -1. \quad (5.31) \]

We consider the system in statistically steady state.

In chapter 2, we presented numerical results for the case of a linear equation of state \((n = 1)\). We showed that, close to the upper and lower boundaries of the domain, the horizontally averaged concentration profile \(\overline{C}(z)\) varies rapidly. However, in the interior of the domain \(\overline{C}(z)\) has a small linear gradient that decreases as the Rayleigh number \(Ra\) increases. In the limit \(Ra \to \infty\), the average concentration in the interior tends to a constant value, \(C_{RD}^{i} = -1/2\).

We have also carried out numerical calculations of (5.10) and (5.13) in a Rayleigh–Darcy cell for \(1 \leq n \leq 5\), at Rayleigh number \(Ra = 10^4\). Measurements of the interior concentration \(\overline{C}(z)\) from these calculations are shown in figure 5.8(a). Based on the results for \(n = 1\) discussed above, we make the assumption for \(n > 1\) that the gradient of \(\overline{C}(z)\) in the interior of the domain also decreases as \(Ra\) increases, and that, as \(Ra \to \infty\), the average concentration in the interior tends to a constant value \(C_{RD}^{i}(n)\). By extrapolating the linear interior gradient of \(\overline{C}(z)\) for each value of \(n\) from our measurements in figure 5.8(a), we generate estimates for the range of possible values of \(C_{RD}^{i}(n)\), as shown in figure 5.8(b). We find that an approximate analytic fit lying within this range is given by \(C_{RD}^{i} = -(n + 1)^{-1/n}\), which is also shown in figure 5.8(b). This curve provides a reasonable approximation for \(n < 5\), which includes the physically important cases, \(n = 1\) and \(n = 2\). We use this approximate form for \(C_{RD}^{i}\) throughout this chapter and the next.

\[ \text{In that chapter, concentration } C \text{ was replaced by temperature } T. \text{ As discussed in \(\S 1.2\), the governing equations for thermal and compositional convection are taken to be identical.} \]
5. CONVECTIVE SHUTDOWN I: FIXED INTERFACE
Chapter 6

Shutdown of convection in a porous medium II: free interface

The material contained in this chapter forms the second half of the paper ‘Convective shutdown in a porous medium’ (Hewitt et al., 2013a), which has been published in the Journal of Fluid Mechanics.

6.1 Introduction

In chapter 5, we explored the shutdown of convection in a one-sided ‘fixed-interface’ system, as defined in §5.2, and demonstrated the close link between such a one-sided system and the two-sided Rayleigh–Darcy cell. In this chapter, we will develop these ideas to model convective systems comprising two fluid layers, in which the flux of solute across an interface causes that interface to move. We examine the dynamics and evolution of these systems using a combination of simple theoretical box models, high-resolution numerical simulations, and laboratory experiments. These tools allow us to investigate and understand the similarities and differences between a variety of physical systems, as described in §5.2.

These different physical systems comprise two fluids that can be either immiscible or miscible (see §5.2): in an immiscible system, the upper fluid is only partially soluble in the lower, and (by assumption) the lower is not at all soluble in the upper; while in a miscible system, the upper fluid is fully soluble in the lower. For
both immiscible and miscible systems, dissolution of the upper fluid into the lower causes a change in the density of the solution, which drives convection. Typical equations of state, average concentration profiles, and average density profiles for immiscible and miscible systems can be seen in figures 5.1(b) and (c).

In this chapter, we develop two different mathematical models to describe free-interface systems. In §6.2, we consider both immiscible and miscible systems under the assumption that the moving interface can be approximated as remaining flat. Therefore, the interfacial height \( h \) is a function of time alone. This assumption allows us to use the results of the previous chapter to derive theoretical box models of each system, which are compared with direct numerical measurements. For the immiscible system (§6.2.1), we make the additional modelling assumption that the pore space is always fully saturated: there is no capillary retention of fluid in the pores of the medium, and as such the interface remains ‘sharp’. In the miscible system (§6.2.2), we recall that the ‘interface’ is defined by the isopycnal of maximum density. In §6.2.3, we summarize the main results of this section, and compare the two systems.

In §6.3, we relax the assumption of a flat interface, and present experimental and numerical results for the miscible system when the interface is free to deform. The experimental system consists of water overlying propylene glycol in a Hele-Shaw cell. Solutions of these fluids have a density curve that is qualitatively similar to that shown in figure 5.1(c). We find that the effects of interfacial deformation and entrainment can be considerable in the miscible system. In contrast, in §6.3.3 we argue that interfacial deformation is likely to be negligible in the immiscible system.

In §6.4, we summarize the main results of the chapter, and discuss the implications for the shutdown of convection in different physical settings. Estimates based on this work of the typical time scales for shutdown in current CO\(_2\) sequestration sites will be discussed in chapter 8, §8.2.

The relevant governing equations, variables, and non-dimensionalization for free-interface systems were introduced in §5.3. We recall that the system is initially stratified in two layers (figure 5.2b), with a lower layer \( 0 < z < 1 \) of concentration \( -1 \) and an upper layer \( 1 < z < H \) of concentration \( C_+ > 0 \). The maximum density is attained at \( C = 0 \). The density is given as a function of the concentration by
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(5.9).

6.2 Free-interface systems (a): Flat interface

If the interface is assumed to remain flat, then the interfacial height is a function of time alone, and is given by $z = h(t)$, with $h(0) = 1$.

As in §5.3.4, we consider the flux scaled by the diffusive flux in the absence of convection. Under the assumption of a flat interface, the scaled horizontally averaged flux $F(t)$ across the interface is given by

$$F(t) = \frac{1}{L} \int_0^L \frac{\partial C}{\partial z} \bigg|_{z=h(t)} \, dx. \quad (6.1)$$

The evolution of the interfacial height $h(t)$ can be calculated from conservation of solute over the entire domain, which gives

$$\int_0^H \int_0^L C(x,z,t) \, dx \, dz = L \left[ -1 + (H - 1) C_+ \right]. \quad (6.2)$$

The right-hand side of (6.2) is the result of evaluating the integral at $t = 0$.

6.2.1 Immiscible system

When the two fluids are immiscible (and, by assumption, the lower fluid is insoluble in the upper), the concentration $C_+$ above the interface $z > h(t)$ remains constant, as does the corresponding density $\rho_+ < 0$. Hence global conservation of solute (6.2) reduces to

$$\int_0^{h(t)} C \, dz = -1 + [h(t) - 1] C_+. \quad (6.3)$$

6.2.1.1 Theoretical box model

Following the analysis of §5.5, we use a well-mixed approximation for the interior of the system in $z < h(t)$: we assume that, below a thin boundary layer, the
horizontally averaged concentration $\bar{C}(z, t)$ is independent of $z$, and is given by

$$\bar{C} = \Theta(t) \leq 0.$$  \hfill (6.4)

Starting from the definition of the initial Rayleigh number (5.11), we now define the time-dependent Rayleigh number $Ra(t)$ to be

$$Ra(t) = Ra_0 \left|\Theta(t)\right|^n h(t),$$  \hfill (6.5)

which accounts for the changes in concentration and depth of the convecting layer. We further define a time-dependent Nusselt number $Nu(t)$, by scaling the horizontally averaged flux $F$ up to a unit concentration difference and height, which gives

$$Nu(t) = \frac{h(t)F(t)}{\left|\Theta(t)\right|}.$$  \hfill (6.6)

The Nusselt number is given by the functional form $Nu(t) = N[Ra(t)]$, as discussed in §5.5.2, and the flux $F(t)$ is given by (6.1).

As in §5.5, we integrate the transport equation (5.10) over the lower layer $z \leq h$, and use the boundary conditions together with (6.1) to obtain

$$\frac{d}{dt} \int_0^{h(t)} \bar{C} \, dz = \frac{F}{Ra_0}.$$  \hfill (6.7)

Under the well-mixed approximation (6.4), contributions to the area integral in (6.7) from the thin boundary layer below the interface are neglected. Equations (6.4), (6.6), and (6.7) can be combined to give

$$h \frac{d\Theta}{dt} = \frac{\left|\Theta\right|}{h Ra_0} N[Ra(t)].$$  \hfill (6.8)

Equation (6.8) can be compared to (5.20), which is the equivalent governing equation for the fixed-interface box model.

The well-mixed approximation (6.4) can also be combined with global conservation of solute (6.3) to give

$$h\Theta = -1 + (h - 1) C_+,$$  \hfill (6.9)
which can be rearranged to obtain the interfacial height,

\[ h(t) = \frac{C_+ + 1}{C_+ + |\Theta(t)|}. \]  

(6.10)

One could solve (6.8) and (6.10) numerically using any functional form of the Nusselt number \( N(Ra) \), including the numerical parameterization in (5.25). We have shown in chapter 5 that the asymptotic linear scaling \( N(Ra) = \alpha r Ra \), where \( \alpha = 6.9 \times 10^{-3} \) and \( r(n) \) is defined in (5.22), provides a very good approximation to (5.25) if \( Ra > 10^3 \), and we therefore use this scaling here. Equations (6.8) and (6.10), together with this linear scaling, give a simple ordinary differential equation for \( \Theta \),

\[ \left( \frac{C_+ + 1}{C_+ + |\Theta|} \right) \frac{d\Theta}{dt} = \alpha r |\Theta|^{n+1}. \]  

(6.11)

Equation (6.11) describes the evolution of \( \Theta(t) \) in the shutdown regime, \( t > t_2 \). In a similar manner to the analysis of §5.5, we extrapolate solutions back to \( t < t_2 \), and apply an initial condition \( \Theta(t_0) = -1 \), where \( t_0 < t_2 \) is a virtual origin. The solution to (6.11) is then given implicitly by

\[ \sum_{k=1}^{n} \left[ \frac{C_+^k}{k \Theta^k} \left( 1 - |\Theta|^k \right) \right] + \ln \left[ \frac{C_+ + |\Theta|}{|\Theta|(1 + C_+)} \right] = -\frac{\alpha r(-C_+)^{n+1}}{1 + C_+} (t - t_0). \]  

(6.12)
The height of the interface \( h(t) \) is related to the interior concentration \( \Theta(t) \) by (6.10). Using (6.6), the flux \( F(t) \) is related to \( \Theta(t) \) by

\[
F = \alpha r Ra_0 |\Theta|^{n+1}.
\]

Figure 6.1 shows solutions calculated from (6.12) for \( \Theta(t) \), \( F(t) \), and \( h(t) \). The concentration \( \Theta(t) < 0 \) increases monotonically towards \( \Theta(t \rightarrow \infty) = 0 \), while the corresponding interfacial height \( h(t) \) increases monotonically towards \( h(t \rightarrow \infty) = h_\infty = 1 + 1/C_+ \), independent of \( n \). In the limit of large \( C_+ \), which physically corresponds to the limit \((C_+^* - C_m^*) \gg (C_m^* - C_+^*)\), equation (6.12) reduces to the solution for a stationary interface (5.27), and the height \( h \) of the interface remains approximately constant for all time. For any value of \( C_+ \), the evolution of the system is ultimately given by the solution for a fixed interface (5.27) (up to an additional factor of \( 1/h_\infty \) multiplying \( t - t_0 \)), since \( h \rightarrow h_\infty \) at long times.

The predictions for a stationary interface from §5.5 are also shown for \( \Theta \) and \( F \) in figures 6.1(a) and (b). Given the relatively large change in the interfacial height \( h \) over time (figure 6.1c), it is surprising that the interior concentration \( \Theta \) (figure 6.1a) does not display a significant difference to the prediction for a stationary interface. This observation is related to the differences in the solute flux (figure 6.1b) between the predictions for a moving and a stationary interface: while the area of the domain below the interface (\( \propto h \)) is greater in the former case than in the latter, the flux \( F \) across the interface is also greater, and therefore the interior concentration \( \Theta \) is not significantly different. For larger values of \( C_+ \) (not shown here), we find that the solutions of (6.11) increasingly resemble those for a stationary interface.

The dependence of \( \Theta \) and \( F \) on \( n \) is also qualitatively similar to that for a stationary interface, which was discussed in §5.5.3. The interior concentration and the flux again have long-time behaviour \( \Theta \sim t^{-1/n} \) and \( F \sim t^{-(n+1)/n} \) to leading order, and the initial decay of the flux is again more rapid for larger \( n \).

### 6.2.1.2 Numerical results

We solved the full governing equations for the flat-interface immiscible system numerically as outlined in appendix A. These equations are (5.10) and (5.13) for
the convecting region $z < h(t)$, subject to boundary conditions $C = 0$ and $w = 0$ imposed at a flat interface $h(t)$, which is determined from (6.3).

Figure 6.2 shows measurements of the horizontally averaged concentration $\overline{C}(z,t)$ and the interfacial height $h(t)$ for both linear ($n = 1$) and quadratic ($n = 2$) equations of state. The upwards retreat of the interface is approximately linear at early times ($t < t_2$), while the downwelling plumes are descending through unmixed fluid. Once the system enters the shutdown regime ($t > t_2$), the behaviour of $h(t)$ changes. The interface moves more slowly for larger values of $C_+$, as there
is more solute per unit volume in the upper layer. The corresponding profiles of \( \overline{C}(z,t) \) show that the interior of the domain is well mixed for \( t > t_2 \), in agreement with the behaviour below a fixed interface (chapter 5) and with the well-mixed assumption (6.4). The predictions of the theoretical box model for the interfacial height \( h(t) \), which is based upon this well-mixed assumption, are also shown in figure 6.2, and give very good agreement with the numerical simulations.

6.2.2 Miscible system

When the two fluids are miscible, the relatively low concentration below the moving interface can affect the concentration field above the interface by diffusion. Since, by assumption, the interface \( z = h(t) \) remains flat, the concentration \( C \) is independent of \( x \) for \( z \geq h \). In this region, the governing transport equation (5.10) therefore reduces to a one-dimensional partial differential equation describing vertical diffusion away from the moving interface \( h(t) \). In the frame of reference moving with the interface, (5.10) becomes

\[
\frac{\partial C}{\partial t} - \frac{dh}{dt} \frac{\partial C}{\partial z} = \frac{1}{Ra_0} \frac{\partial^2 C}{\partial z^2}. \tag{6.14}
\]

6.2.2.1 Theoretical box model

The development of a theoretical box model for the miscible system follows similar reasoning to that for the immiscible system §6.2.1.1. The horizontally averaged interior concentration \( \Theta(t) \leq 0 \) (6.4), the time-dependent Rayleigh number \( Ra(t) \) (6.5), and the time-dependent Nusselt number \( Nu(t) \) (6.6) are all as defined in §6.2.1.1. The evolution equation for the average interior concentration \( \Theta(t) \) is again given by (6.8).

Unlike the immiscible system, the concentration above the interface does not remain constant. Instead, it evolves by diffusion (6.14), and varies over some length scale between \( C = 0 \) at the interface and \( C = C_+ \) (as shown schematically in figure 5.1c). In order to generate a simple box model that approximates the
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Figure 6.3: Theoretical predictions for the immiscible (dashed) and miscible (solid) systems, with \( n = 2, \ C_+ = 2, \ t_0 = 0, \) and \( Ra_0 = 2 \times 10^4 \): (a) the average concentration \( \Theta(t) \), for which the two predictions are almost indistinguishable; (b) the solute flux \( F(t) \); (c) the interfacial height \( h(t) \), which has qualitatively different late-time behaviour in the two systems.

solution of (6.14), we define a diffusive boundary-layer depth

\[
\delta(t) = \frac{2}{C_+} \int_h^H (C_+ - C) \, dz,
\]

which is an integral measure of the length scale of the concentration profile in \( z > h \). We then approximate (6.14) by assuming that the evolution of \( \delta \) can be described by a simple ordinary differential equation of the form

\[
\frac{d\delta}{dt} = \frac{a_1}{Ra_0} - \frac{a_2}{Ra_0} \frac{dh}{dt},
\]

where \( a_1 \) and \( a_2 \) are numerical coefficients. Equation (6.16) is motivated by the physical balances that control the boundary-layer depth \( \delta \): the first term on the right hand side of (6.16) describes the diffusive growth of a boundary layer with a flux proportional to the diffusivity \( Ra_0^{-1} \) and the concentration gradient, while the second term describes the advection of the interface.

The constants \( a_1 \) and \( a_2 \) in (6.16) are chosen so that the total solute \( \delta C_+/2 \) contained in the boundary layer gives a good approximation to that in the full solution of (6.14). We find \( a_1 \) and \( a_2 \) by comparing solutions of (6.16) with analytic solutions of (6.14) in two limits. In the limit where \( dh/dt \) is negligible, the pure-diffusion solution of (6.14) has the form \( C \sim \text{erf}[(z - h) \sqrt{Ra_0/4t}] \), and (6.16) gives \( \delta = \sqrt{2a_1 t/Ra_0} \). Similarly, in the steady limit in which advection balances
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diffusion, the solution of (6.14) has the form \( C \sim \exp [-\dot{h} Ra_0 (z - h)] \), where \( \dot{h} = dh/dt \), while (6.16) gives \( \delta = a_1/a_2 \dot{h} Ra_0 \). We use (6.15) to equate each of these solutions at leading order, which gives \( a_1 = 8/\pi \), and \( a_2 = a_1/2 = 4/\pi \).

Including the contribution from the diffusive upper boundary layer, global conservation of solute (6.2) gives

\[
h (C_+ + |\Theta|) = (1 + C_+) - \frac{\delta C_+}{2}. \tag{6.17}
\]

After rearranging (6.8), (6.16), and (6.17), we extract coupled evolution equations for the concentration \( \Theta \), the height of the interface \( h \), and the diffusive boundary layer depth \( \delta \),

\[
\frac{d\Theta}{dt} = \frac{|\Theta| N}{h^2 Ra_0}, \tag{6.18}
\]

\[
\left( |\Theta| + C_+ - \frac{a_2 C_+}{2} \right) \frac{dh}{dt} = \frac{a_1 C_+}{2 \delta Ra_0} + \frac{|\Theta| N}{h Ra_0}, \tag{6.19}
\]

\[
\left( |\Theta| + C_+ - \frac{a_2 C_+}{2} \right) \frac{d\delta}{dt} = \frac{a_1 (C_+ + |\Theta|)}{\delta Ra_0} - \frac{a_2 |\Theta| N}{h Ra_0}. \tag{6.20}
\]

Equations (6.18)–(6.20) give a theoretical prediction for the evolution of shutdown in a miscible flat-interface system. We integrate these equations numerically using the functional form \( N(Ra) \) in (5.25).

The solutions for the interior concentration \( \Theta \) and the flux \( F \) from this model (figures 6.3a,b) are almost indistinguishable from those for the immiscible system. However, the interfacial height \( h \) for the miscible system exhibits qualitatively different behaviour at long times (figure 6.3c). The diffusion of solute above the interface slows the upward motion of the interface, and eventually leads to a decrease in the isopycnal that defines \( h \). Equation (6.19), together with (6.6), give an equation for \( dh/dt \), which shows that the height of the interface will decrease when

\[
F < \frac{a_1 C_+}{2\delta}, \tag{6.21}
\]

i.e. the height of the interface will decrease when the flux of solute into the lower layer (\( F \)) is less than the diffusive flux into the upper layer (\( \sim C_+/\delta \)).

In a finite system with no-flux boundaries, the final steady state must have a
uniform concentration $C_\infty$, which is determined by conservation of solute (6.2) to be

$$C_\infty = -\frac{1}{H} + \left(\frac{H-1}{H}\right)C_\pm.$$

(6.22)

If $C_\infty < 0$, then the interface $z = h(t)$ must reach the upper boundary $z = H$, and (6.21) is never satisfied. Conversely, if $C_\infty > 0$ the interface must eventually descend, and approaches the base of the domain by diffusion. From (6.22), $C_\infty > 0$ if $H > 1 + 1/C_\pm$. This condition is satisfied for all the results presented in this chapter.

6.2.2.2 Numerical results

We solved the full governing equations for the miscible system numerically (see appendix A). These equations are (5.10) and (5.13) for $z < h(t)$, and (6.14) for $z > h(t)$, together with conservation of solute (6.2), and the flat-interface assumption $w = 0$ at $z = h(t)$.

Figure 6.4 shows measurements of the horizontally averaged concentration $\overline{C}(z, t)$ and the interfacial height $h(t)$, with a quadratic equation of state $n = 2$. As
in the case of the immiscible system (figure 6.2), the rate of upwards retreat of the interface is approximately constant for $t < t_2$, and then decreases once the system enters the shutdown regime ($t > t_2$). Unlike the immiscible system, however, the concentration field above the interface evolves in time (figure 6.4). This evolution becomes very significant at long times, and results in an eventual decrease of the interfacial height $h(t)$ (figure 6.4b). The time at which the interface begins to descend decreases with increasing $C_+$, as predicted by (6.21). The predictions of the box model are also shown in figure 6.4b, and accurately capture both the slowing of the interface and its eventual descent.

6.2.3 Conclusions for immiscible and miscible systems with a flat interface

The results in figures 6.2 and 6.4 show that the theoretical box models give excellent predictions for the shutdown of free-interface systems, under the assumption that the interface remains flat. These figures also highlight the main difference between the immiscible and miscible systems: the long-time evolution of the interfacial height $h(t)$, which continually increases in the immiscible system, but eventually decreases in the miscible system. Given this qualitative difference in the interfacial behaviour, it is remarkable that the solute flux $F(t)$ and the interior concentration $\Theta(t)$ are so similar between the two systems (figure 6.3). The timescales for the shutdown of convection in the two systems are therefore roughly equal, even though observations of the interfacial height $h(t)$ might suggest otherwise. In the limit of large $C_+$, we find that the predictions of the box models for these free-interface systems can be well approximated by the solution in §5.5 for a fixed interface.

These results apply when the assumption of a flat interface is appropriate. In the next section, we examine miscible systems with a deformable interface, and show that the removal of the flat-interface approximation can lead to very different rates of shutdown.
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6.3 Free-interface systems (b): Deformable interface

In this section we relax the flat-interface assumption. Therefore, the interface is free to 'deform', and solute can be entrained across it.

In §6.3.1 we present numerical results for the miscible system. In §6.3.2, to test the validity of the numerical results in a physical system, we compare with measurements from an experimental miscible system in a Hele-Shaw cell. In §6.3.3, we consider the validity of the flat-interface approximation for miscible systems and discuss the anticipated effects of a deformable interface on immiscible systems.

6.3.1 Numerical results for the miscible system

We solved the governing equations (5.10) and (5.13) over the whole domain, with an initial condition given by (5.12) and a quadratic equation of state ($n = 2$) (see appendix A for numerical details). As discussed in §5.2, the interfacial height $z = h(x,t)$ is defined by the contour of maximum density $\rho = \rho_m$, which is a function of horizontal position. We therefore define the average interfacial height $\bar{z}(t)$ to be the height at which the horizontally averaged density is maximum (which corresponds to the height at which $\bar{C}(z,t) = 0$).

Snapshots of the concentration field (figure 6.5a) show that there can be significant interfacial deformation in the miscible system. The extent of the deformation decreases with increasing $C_+$. The dominant wavelength of the deformed interface appears to be set by the lateral spacing of the descending megaplumes. The average interfacial height $\bar{h}(t)$ and the interior concentration $\Theta(t)$ are compared with predictions from the miscible box model under a flat-interface approximation in figures 6.5(b) and (c). Both variables increase significantly more rapidly than the box model predicts, which suggests that the total solute flux $F(t)$ is initially much greater than with a flat interface. Measurements of $F(t)$ from the numerical simulations (not shown here) suggest that the initial flux is approximately 3 times larger than with a flat interface when $C_+ = 1.2$, and approximately 2 times larger when $C_+ = 2$. 

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Figure 6.5: Numerical results at $Ra_0 = 2 \times 10^4$, domain width $L = 2$ and height $H = 2$, and a quadratic equation of state $n = 2$: (a) snapshots of the concentration profile at $t = 5$, for $C_+ = 1.2$ and $C_+ = 2$, showing significant deformation of the interface; (b) the average interfacial height $\overline{h}(t)$ (solid) for $C_+ = 1.2$ and $C_+ = 2$, together with the height predicted by the miscible theoretical box model (dashed); (c) the interior concentration $\Theta(t)$ (solid) for $C_+ = 1.2$, together with the prediction of the miscible theoretical box model (dashed).

6.3.2 Experimental results for the miscible system

In order to explore the effects of a deformable interface further, and to corroborate the numerical results of §6.3.1, we conducted an experiment in a Hele-Shaw cell using two miscible fluids: propylene glycol (PPG) and water. Backhaus et al. (2011) used these fluids to examine the onset of convection and the evolution of the
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Figure 6.6: Relationship between density and concentration for the propylene glycol–water system. Concentration $C^* = 1$ corresponds to pure water. Symbols denote measurements made in a densitometer, of which the curve is a cubic fit $\rho^* = f^*(C^*) = \rho_0^- (1 + 0.077 C^* - 0.173 C^{*2} + 0.062 C^{*3})$, with $\rho_0^- = 1.036 \text{ g/cm}^3$.

initial convective plumes. Neufeld et al. (2010) used a similar system, composed of water with a mixture of methanol and ethylene-glycol, to examine the convective flow for $t_c < t < t_2$. Here, in contrast, we examine the long-time evolution of the system in the shutdown regime.

The experimental system consists of two glass sheets, separated by a shim of thickness $l = 0.41 \text{ mm}$. The cell has width $L^* = 40 \text{ cm}$ and height $80 \text{ cm}$. The flow in the gap satisfies Darcy's law (5.1a), with an effective permeability $K = l^2 / 12 = 1.4 \times 10^{-4} \text{ cm}^2$ and porosity $\phi = 1$. PPG, of density $\rho_0^- = 1.0367 \text{ g/cm}^3$, filled the lower layer of the cell up to a depth $h_0^* = 32.5 \text{ cm}$. The PPG was overlain by a layer of water, of density $\rho_+^* = 0.9995 \text{ g/cm}^3$, up to a total depth $H^* = 66 \text{ cm}$. We define the concentration $C^*$ to be the proportion of water by weight, so that the concentration of pure PPG is $C^- = 0$ and that of water is $C_+^* = 1$. Measurements of the density for different concentrations are shown in figure 6.6, together with a cubic fitting equation $\rho^* = f^*(C^*)$. The maximum density is obtained at $C_m^* \approx 0.25$, and is given by $\rho_m^* = 1.0451 \text{ g/cm}^3$. The diffusivity of PPG in water varies a little with concentration, but is roughly constant between $C^- = 0$ and $C_m^* = 0.25$, with an approximate value $D = 2.5 \times 10^{-6} \text{ cm}^2/\text{s}$ (Wang et al., 2010).

We measured the average interfacial height $\bar{h}^*(t)$ and the interior concentration $\Theta^*(t)$ by the addition of blue dye to the water. The ambient temperature varied by less than $2^\circ \text{C}$ for the duration of the experiment ($\approx 3 \text{ weeks}$). The experiment
was set up by injecting both fluids into the cell from the top: the cell was first filled with the layer of PPG, which was allowed to settle; the overlying layer of water was then added over a period of some tens of seconds. Setting the experiment up in this way led to some initial local mixing and interfacial deformation, the effects of which decayed over about 10 mins; from then onwards the flow was dominated
by downwelling fingers spread uniformly across the cell, and the interface was horizontal, except for the local deformation. This time over which the start-up transients decayed is much less than the time taken for the plumes to reach the base of the cell ($t^*_1 \approx 8 - 9$ hours).

We also performed numerical simulations to compare with the experimental results (figure 6.7). In order to make a fair comparison, we estimate the effects of two physical processes in the experimental system. Firstly, the viscosity of aqueous PPG depends strongly on concentration. Pure PPG has viscosity $\mu \approx 0.05$ Pa s, while the solution with the maximum density has viscosity $\mu \approx 0.015$ Pa s (Sun & Teja, 2004). Therefore the average viscosity below the interface will decrease over time as the average concentration increases. Secondly, experimental measurements of the velocity of the downwelling plumes suggest that Taylor dispersion (Taylor, 1953) will act to increase the effective diffusivity by a factor of $2 - 3$. An estimate of both of these effects, together with the parameters presented above, gives an initial Rayleigh number $Ra_0 \approx 2 \times 10^4$, and a convective time scale $T^* \approx 2.2$ hours. The numerical simulations used this initial value of $Ra_0$, together with the equation of state $\rho = f(C)$ (figure 6.6) and an upper concentration $C_+ = 3$.

In order to give a simple approximation of the change of viscosity over time, we assume that the relevant viscosity scale is given by the average viscosity of all the fluid below the interface, and that the viscosity varies linearly with $1/\Theta^*(t)$. Since $Ra_0$ is inversely proportional to the viscosity, the value of the Rayleigh number $Ra_0$ in the simulations was changed over time, such that it increased linearly with the average concentration $\Theta(t)$. This simple approximation is not intended to reproduce the exact evolution of the experimental system, but rather to provide a reasonable qualitative estimate of the effects of viscosity variation.$^1$

The dynamical structure of the flow and the profile of convection in the experimental system are very similar to those in the numerical simulations (figures 6.7a and b). The average interfacial height $\bar{h}(t)$ and the interior concentration $\Theta(t)$ (figures 6.7c and d) similarly show excellent agreement between the experimental and numerical measurements. The transition to the shutdown regime can be

$^1$Note that the variation of viscosity (and also, weakly, of diffusivity) with concentration indicates that the Prandtl number $Pr = \nu/\kappa$ varies. However, unlike pure-fluid convection, $Pr$ plays no role in the convective flow, and so we only need to account for variations in $Ra$. 

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observed at \( t_2 \approx 8 \) by the change in behaviour of the average interfacial height \( \bar{h} \) (figure 6.7c): before this time the upward retreat of the interface is approximately linear. At much later times, both the experimental and numerical measurements show that the interface slows down and eventually the height starts to decrease.

The initial linear upward retreat of the interface agrees qualitatively with the numerical observations in §6.2.2.2, and the eventual decrease of the interface agrees qualitatively with the predictions from the miscible box model in §6.2.2.1. We note, however, that the time \( t_2 \approx 8 \) is much earlier than the predictions and numerical measurements of \( t_2 \) in §6.2, because of the enhanced solute flux through the deformable interface here.

### 6.3.3 Discussion of systems with a deformable interface

The above results show that the effects of a deformable interface can be very significant for the miscible system. The excellent agreement between the numerical and experimental results with a deformable interface corroborates this observation.

We suggest that the removal of the flat-interface assumption leads to a significantly larger solute flux for two main reasons. Firstly, interfacial deformation results in the sloping of isopycnals below the interface, which leads to a baroclinic generation of lateral flow along the sloping boundary layer, and so an enhancement of the diffusive flux through the interface. (The simple increase in the length of the interface due to deformation is too small to account for the significant increase in flux.) Secondly, there is a contribution to the flux from material transport: positively buoyant fluid from above the interface can be entrained down across the interface. As the fluid loses solute by diffusion to its surroundings, its density increases because of the non-monotonic equation of state, and it continues to descend. It is difficult to quantify the relative importance of these two effects to the increase of the solute flux.

The interface deforms due to the competing effects of the stabilizing density gradients above the interface and the density gradients between upwelling and downwelling plumes that drive convection below the interface. If the stabilizing density gradient is much greater than the driving density gradients, then we expect both the interfacial deformation and any entrainment across the interface to be
small. This prediction is given credence by the numerical results of §6.3.1, which show that the interfacial deformation, and the corresponding enhancement of the solute flux, are less at larger values of $C_+$. These observations suggests that the approximation of a flat interface is likely to be more appropriate for larger $C_+$ in the miscible system.

We have not examined the immiscible system with a deformable interface in this chapter. In order to model this system numerically, we would need a different approach from that used in the rest of this thesis, as the free interface would need to be tracked in both space and time, and the domain over which the equations were to be solved would no longer have a flat upper boundary.

We can, however, consider the expected effects of a deformable interface in an immiscible system. At the interface, there is a constant stable density jump $1 + |\rho_+|$, which is always greater than the typical density differences ($<1$) between upwellings and downwellings that drive convection. We therefore anticipate that the interface will remain approximately planar, and that the approximation of a flat interface will be appropriate for immiscible systems, particularly if $|\rho_+|$ is large. This observation highlights an important difference between the immiscible and miscible systems.

### 6.4 Conclusions

One-sided porous convection at high Rayleigh number bears many of the dynamical signatures of the statistically steady two-sided Rayleigh–Darcy cell. We have used this observation to develop theoretical box models which describe the shutdown of complex one-sided convective systems, by coupling the evolution of the interior concentration with the flux through the boundary layer. These theoretical models, together with our numerical and experimental tools, have allowed for the examination of a variety of different physically motivated systems, in which the active interface is either fixed or is free to move.

In this chapter, we used the techniques developed in chapter 5 to consider two different free-interface systems, comprising immiscible or miscible fluids. In §6.2, we examined both of these systems under the assumption that the interface, as defined in §5.2, remained flat. Our models predict very similar behaviour for the
flux over time between the immiscible and miscible systems. In the limit of large $C_+$, the models can be very reasonably approximated by the solution for a fixed interface. Physically, this limit corresponds to the case when the concentration of maximum density $C_m^*$ is much closer to the concentration of the lower layer $C_-^*$ than to that of the upper $C_+^*$.

We have shown, however, that the evolution of the interfacial height $h(t)$ in the two systems is qualitatively different at long times: in the immiscible system the height increases for all time, while in the miscible system it eventually decreases, provided $H$ is sufficiently large, even although the flux of solute across the interface into the lower layer remains positive. This observation provides an important difference when comparing the two systems, as discussed below.

In §6.3, we relaxed the assumption of a flat interface. We presented numerical simulations of the miscible system, which show that the interfacial height eventually decreases, in qualitative agreement with the predictions of our theoretical box model. However, the solute flux is much larger than the box model predicts. This observation was corroborated by experimental results from a Hele-Shaw cell, which show excellent agreement with full numerical simulations. We suggest that the enhancement of the flux in the miscible system is due to entrainment across the interface and sloping isopycnals below the interface, as discussed in §6.3.3. These effects are the result of a balance between the stabilizing density gradients above the interface and the driving density gradients between the interleaving plumes below the interface.

In immiscible systems, however, these density gradients are not comparable, as there is a stabilizing discontinuity in the density $(1 + |\rho_+|)$ across the interface which will dominate, particularly if $|\rho_+|$ is large. Therefore, we anticipate that the interface will remain approximately planar and entrainment across it will be negligible, in agreement with the assumptions of a flat interface.

The relative applicability of the flat-interface approximation, and the long-time behaviour of the interfacial height $h(t)$, each provide an important difference between the immiscible and miscible systems, and suggest that care should be taken when modelling immiscible systems with a miscible analogue, or vice versa. For example, Neufeld et al. (2010) and Backhaus et al. (2011) each use miscible experimental systems to model the convective dissolution of CO$_2$ in a deep saline.
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aquifer, which is an immiscible system. In the miscible experimental systems, we anticipate that the effects of interfacial deformation and entrainment would lead to a significant enhancement ($\approx 200 - 300\%$) of the solute flux. In contrast, in the CO$_2$ sequestration system, the stabilizing density difference between supercritical CO$_2$ and brine ($\sim 300$ kg/m$^3$) is very much larger than the density contrasts that drive convection ($\sim 10 - 20$ kg/m$^3$), and therefore we anticipate that interfacial deformation and entrainment would be negligible.

Under the assumption that capillary retention in the pore space can be ignored, and thus that the interface is ‘sharp’, the convective dissolution of CO$_2$ can be well described by our immiscible box model with a moving flat interface and a linear equation of state $n = 1$, presented in §6.2.1. In addition, since CO$_2$ is only very weakly soluble in brine (3 – 5% by weight), the value of $C_+$ for this system would be very large ($\sim 20 - 30$), and the flux would be well approximated by the solution for a fixed interface (5.28). In dimensional form, the total horizontally averaged solute flux for the fixed-interface system with $n = 1$ is given by

$$F^*(t) = \frac{4\alpha \phi h_0^* T^* (C_m^* - C_+^*)}{(T^* + 4\alpha t)^2},$$  \hspace{1cm} (6.23)$$

where $T^*$ is the convective time scale, given by $T^* = \phi h_0^* \mu / (K g \Delta \rho_m^*)$, and $\alpha = 6.9 \times 10^{-3}$. In §8.2, we consider an illustrative example of convection in a high-permeability aquifer, and use (6.23) to estimate typical time scales for shutdown in CO$_2$ sequestration systems.

I am very grateful to Mark Hallworth for invaluable help with the experimental work contained in this chapter.
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Chapter 7

Three-dimensional Rayleigh–Darcy convection at high Rayleigh number

The material contained in this chapter has been published in the Journal of Fluid Mechanics, under the title ‘High Rayleigh number convection in a three-dimensional porous medium’ (Hewitt et al., 2014b).

7.1 Introduction

Thus far in this thesis we have been concerned with two-dimensional flow. In this chapter, we present a numerical investigation of three-dimensional high-$Ra$ Rayleigh–Darcy convection in a porous medium, which remains largely unstudied except at low values of $Ra$. This chapter forms a three-dimensional analogue of much of the work in chapter 2, and, as we shall see, reveals a number of similarities, and some interesting differences, between two-dimensional and three-dimensional Rayleigh–Darcy convection at high $Ra$.

Most previous numerical studies of three-dimensional Rayleigh–Darcy convection have focussed on steady convection for $Ra \leq 300$. As in two-dimensions, there is no flow for $Ra < 4\pi^2$, while for $4\pi^2 \leq Ra \leq 4.5\pi^2$ the only unstable mode is purely two dimensional (Holst & Aziz, 1972). The two-dimensional mode con-
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tinues to give the largest heat flux for $Ra \lesssim 97$ (Straus & Schubert, 1979), while for $97 \lesssim Ra \lesssim 300$ the flux is maximized by a steady three-dimensional planform (Schubert & Straus, 1979). Multiple possible steady states exist across this range of $Ra$ (Straus & Schubert, 1981). Schubert & Straus (1979) found unsteady solutions for $Ra \gtrsim 300$, and some of the dynamics of the flow for $300 \lesssim Ra \lesssim 740$ were investigated by Kimura et al. (1989). We are not aware of any numerical studies of the statistically steady system that explore the dynamics of the flow for $Ra > 740$. More recent numerical studies have explored transient (rather than statistically steady) porous convection in three-dimensions, driven by a buoyancy source on one boundary only (Pau et al., 2010; Fu et al., 2013). The latter authors explored the dynamics of the flow for $Ra \leq 6400$ and identified cellular structures of plumes near to the active boundary, which coarsened and were entrained into larger, more persistent, plumes. The spatial scale of the plume structures near the boundary scaled approximately with $Ra^{-1}$.

Laboratory experiments of statistically steady three-dimensional porous convection have also provided measurements of both the heat flux and the dominant planform of the flow (Elder, 1967; Lister, 1990). The detailed experiments of Lister (1990) are particularly interesting as they provide observations of the structure of the flow for $Ra = O(1000)$: the flow consisted of ‘a significant number of dendritic downwellings’ which fed into larger plumes, and measurements suggested that the lateral scale of the large plumes decreased like $(Ra + c)^{-0.5}$, for some constant $c$.

In this chapter, we investigate in detail the flow in a three-dimensional Rayleigh–Darcy cell for $Ra \leq 2 \times 10^4$, using high-resolution numerical simulations. In §7.2, we outline the governing equations and numerical scheme used in the chapter. In §7.3.1, we briefly describe some features of the flow for $4\pi^2 \leq Ra \lesssim 1750$. In §7.3.2, we explore in detail the dynamical structure of the flow and the buoyancy flux $Nu(Ra)$ in the ‘high-Ra’ regime ($Ra \gtrsim 1750$). In §7.4, we summarize and discuss the main results of this work.
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7.2 Governing equations and numerical scheme

7.2.1 Dimensionless equations

We consider a three-dimensional cell of height $H$ containing a fluid-saturated homogeneous and isotropic porous medium. The cell is heated at the lower boundary and cooled at the upper boundary, such that a temperature difference $\Delta T$, which gives rise to a density difference $\Delta \rho$, is imposed across the cell. The flow $\mathbf{u} = (u, v, w)$ in the medium is assumed to be Boussinesq and incompressible, and satisfies Darcy’s law. The equation of state $\rho(T)$ is linear, and the temperature field $T$ evolves by advection and diffusion. In dimensionless variables, these equations are given by

$$\nabla \cdot \mathbf{u} = 0, \quad \mathbf{u} = - (\nabla p - T \hat{z}), \quad (7.1a, b)$$

$$\frac{\partial T}{\partial t} = - \mathbf{u} \cdot \nabla T + \frac{1}{Ra} \nabla^2 T, \quad (7.2)$$

where $p$ is the pressure. The Rayleigh number $Ra$ is given by

$$Ra = \frac{\Delta \rho gKH}{\phi \kappa \mu}, \quad (7.3)$$

where $g$ is the gravitational acceleration, $K$ is the permeability, $\phi$ is the porosity, $\kappa$ is the thermal diffusivity, and $\mu$ is the viscosity of the fluid, all of which are assumed to be constant.

In dimensionless variables, the Rayleigh–Darcy cell has unit height with boundary conditions on the upper and lower boundaries given by

$$w = 0, \ T = 1 \quad \text{on} \quad z = 0, \quad w = T = 0 \quad \text{on} \quad z = 1. \quad (7.4)$$

The cell is periodic in the two horizontal directions, with period $L$ (figure 7.1).

The average dimensionless flux is given by the Nusselt number,

$$Nu = \langle nu(t) \rangle = \left\langle \frac{1}{L^2} \int_0^L \int_0^L \left. - \frac{\partial T}{\partial z} \right|_{z=0} \, dx \, dy \right\rangle, \quad (7.5)$$
where the angle brackets $\langle \rangle$ denote a long-time average, and $nu(t)$ is the instantaneous horizontally averaged Nusselt number.

### 7.2.2 Numerical method

The constraint of incompressibility (7.1a) can be satisfied by the introduction of a vector potential $\Psi = (\psi_x, \psi_y, \psi_z)$ which obeys $u = \nabla \wedge \Psi$. The potential is determined by this relationship only up to the addition of $\nabla \xi$, for any scalar $\xi$. To constrain this gauge freedom, we consider the curl of (7.1b), which gives

$$\nabla \wedge u = \nabla (\nabla \cdot \Psi) - \nabla^2 \Psi = \left( \frac{\partial T}{\partial y}, -\frac{\partial T}{\partial x}, 0 \right).$$  \hspace{1cm} (7.6)

Equation (7.6) reduces to a set of simple Poisson equations for the components $\psi_{x,y,z}$ of the vector potential if the gauge condition is chosen to be

$$\nabla \cdot \Psi = 0,$$  \hspace{1cm} (7.7)

(cf. the Lorentz gauge condition in electrodynamics). Equation (7.6) then reduces to

$$\nabla^2 \psi_x = -\frac{\partial T}{\partial y}, \quad \nabla^2 \psi_y = \frac{\partial T}{\partial x}, \quad \nabla^2 \psi_z = 0.$$  \hspace{1cm} (7.8a, b, c)
It is straightforward to show (see E & Liu 1997) that the gauge condition (7.7) is satisfied throughout the domain provided that is satisfied on the boundaries. Since the domain is periodic in both \( x \) and \( y \), both the gauge condition (7.7) and the velocity boundary conditions in (7.4) are satisfied by setting

\[
\psi_x = \psi_y = \frac{\partial \psi_z}{\partial z} = 0, \quad \text{on} \quad z = 0, 1. \tag{7.9a, b, c}
\]

Equations (7.8c) and (7.9c) combine to give \( \psi_z = 0 \) everywhere. The velocity \( \mathbf{u} \) is determined by the Poisson equations (7.8a,b) for \( \psi_x \) and \( \psi_y \), with boundary conditions (7.9a,b).

We solved (7.2) and (7.8a,b) numerically. The numerical scheme is briefly outlined here, and discussed in detail in appendix A, §A.3. As with the two-dimensional simulations of chapter 2, we used a coordinate transformation \( \zeta(z) \) to fully resolve the thin diffusive boundary layers near the upper and lower boundaries of the domain. The Poisson equations (7.8a,b) were solved using fast Fourier transforms for the \( x \) and \( y \) derivatives, and second-order finite differences for the vertical derivatives. The transport equation (7.2) was solved using an unconditionally stable three-dimensional alternating-direction implicit method devised by Brian (1961). As in two dimensions, we spatially discretized the diffusion terms using second-order finite differences, and used a flux-conservative approach for the advection operator. A midpoint method was used for the time derivatives to give second-order temporal accuracy. The numerical scheme was parallelized using a hybrid of open multi-processing (OpenMP) and message-passing interface (MPI) specifications.

Except for some simulations described in §7.3.1, the initial condition was given for completeness, we note that there is a more efficient method for calculating \( \mathbf{u} \), which is not used in this work. It is straightforward to show that any flow \( \mathbf{u} \) with vanishing vertical vorticity, as in (7.6), and vanishing divergence, as in (7.1a), can be written in the form

\[
\mathbf{u} = \nabla \wedge (\nabla \wedge \eta \hat{z}) = \eta_{xz} \hat{x} + \eta_{yz} \hat{y} - (\eta_{xx} + \eta_{yy}) \hat{z}, \tag{7.10}
\]

for some function \( \eta(x, y, z) \), using the gauge freedom in the curl operator. With the form (7.10), the curl of Darcy’s law reduces to \( \nabla^2 \eta = T + f(z) \), for arbitrary \( f(z) \) which can be set to zero w.l.o.g. (as the velocity components in (7.10) all contain a derivative of \( \eta \) with respect to \( x \) or \( y \)). The velocity is therefore determined by just one Poisson equation rather than by two as in (7.8). I am grateful to Mike Proctor for bringing this approach to my attention.
by a linear vertical temperature gradient, \( T(x, y, z) = 1 - z \), with a spatially random perturbation of magnitude \( 2.5 \times 10^{-3} \). We refer to this initial condition as IC1.

7.3 Numerical results

The primary focus of this chapter is to explore three-dimensional flow in the ‘high-\( Ra \)’ regime, which will be taken here to be the range \( Ra \gtrsim 1750 \). In order to provide a context for these results, we begin in §7.3.1 with a brief outline of the dynamics of the flow for \( Ra \lesssim 1750 \). A more detailed study of the variety of interesting dynamical structures, bifurcations, and pattern formation exhibited by the flow in this ‘moderate-\( Ra \)’ regime is left for future work. In §7.3.2, we investigate the high-\( Ra \) regime in detail.

7.3.1 Overview of the flow dynamics for moderate values of \( Ra \)

Two sets of simulations for moderate \( Ra \) were undertaken with aspect ratio \( L = 2 \). The first set comprised independent simulations in which the initial conditions were given by a small random perturbation to a linear base state (IC1). The second set was a sequence of simulations in which the final state of one simulation was used as the initial condition for the next and \( Ra \) was increased by a factor of \( 6/5 \) (IC2). In each case, the simulations were allowed to run until the flow had evolved to a steady or statistically steady state.

Figure 7.2(a) shows measurements of \( Nu(Ra) \) from these simulations. It can be seen that there is some variability, both between repeated simulations with IC1 at the same value of \( Ra \), and between the two sets of simulations at comparable values of \( Ra \). This variability is due to the flow having evolved to different spatial structures in different simulations, rather than to insufficient averaging of the heat flux in a given simulation.

In the simulations with IC1 (figure 7.2a, circles), the spatial structure of the flow was as follows. For \( 45 \lesssim Ra \lesssim 100 \), the flow evolved to a steady planform of rolls inclined with either the \( x \) or \( y \) axis (figure 7.2b; i). For \( 100 \lesssim Ra \lesssim 225 \), the
Figure 7.2: (a) Calculations of $Nu(Ra)$ from the onset of convection at $Ra = Ra_{crit} = 4\pi^2$ to the ‘high-Ra’ regime. Data are from simulations with initial conditions IC1 (black circles) and IC2 (blue dots), as described in the text. All simulations with $Ra \leq 1750$ have aspect ratio $L = 2$; those with $Ra \geq 1750$ are discussed in §7.3.2. The relationship $Nu(Ra)$ from a two-dimensional cell (with $L = 2$ and IC2) is included for comparison (red line; from chapter 2). (b)–(c) Snapshots of the temperature field at depth $z = 30/Ra$, just above the lower boundary, for a selection of values of $Ra$, corresponding to the small arrows in (a). The snapshots in (b) are of simulations with IC1 (down arrows), and those in (c) are of simulations with IC2 (up arrows). Each snapshot is copied four times to show a $4 \times 4$ horizontal domain.
flow evolved to a steady planform of inclined rolls (figure 7.2b; ii), where ‘inclined’ means not aligned with either axis. For $225 \lessgtr Ra \lessgtr 400$, the flow evolved to a steady planform of inclined square cells (figure 7.2b; iii). At $Ra = 400$, one simulation again evolved to a steady planform of inclined squares, while another evolved to an unsteady planform of aligned squares.

For $400 \lessgtr Ra \lessgtr 1750$, the flow was unsteady, and we found a variety of spatial structures in this range. In most simulations (e.g. figure 7.2b; iv,vi), the flow evolved to a regular background planform of convective cells on which were superposed unsteady sheet-like ‘dripping’ disturbances arising in the boundary layers. In a few simulations (e.g. figure 7.2b; v), the flow appeared more disordered and a regular background planform was not evident. For $Ra \gtrsim 1750$, we did not observe any regular planform. In addition, as can be seen in figure 7.2(a), for $Ra \gtrsim 1750$ we did not find any significant variability in $Nu$ between different simulations with IC1. Henceforth, we refer to the range $Ra \gtrsim 1750$ as the high-$Ra$ regime.

We found some significant differences in the spatial structure of the flow between the simulations with IC1 and simulations with IC2 at comparable values of $Ra$. In the simulations with IC2 (figure 7.2a, dots), the spatial structure was as follows. For $50 \leq Ra \leq 215$, the planform of the flow was a steady roll aligned with the $y$ axis (figure 7.2c; i). At $Ra = 258$ the flow evolved to an unsteady state which oscillated periodically between two rectangular cells (figure 7.2c; ii) and one inclined square cell. For $310 \leq Ra \leq 924$, the planform was a steady array of four square cells (figure 7.2c; iii). For $1109 \leq Ra \leq 2300$, the flow took the form of unsteady perturbations to these regular background cells, and the structure of the flow appeared to be increasingly disordered as $Ra$ was increased through this range (figure 7.2c; iv-vi).

Comparison of the two sets of simulations outlined above indicates that hysteresis can affect both the flow structure and the value of $Nu$ for $Ra \lessgtr 1750$. The results also suggest that the bifurcation structure and the dynamical behaviour of the system are highly complex in this moderate-$Ra$ regime, and would require a detailed further study to disentangle. For example, for each of the different spatial structures of the flow identified in the simulations with IC1, a branch of solutions could presumably be followed for increasing or decreasing $Ra$ as in the simulations.
7.3.2 The high-$Ra$ regime

As discussed above, for $Ra \geq 1750$ we found that there is no significant variation in $Nu$ between different simulations with IC1 at the same $Ra$, and the flow structure did not exhibit any regular background planform. In this section, we investigate the flow in the high-$Ra$ regime in detail. All the simulations presented in the remainder of this chapter have initial conditions IC1.

7.3.2.1 Structure of the flow

Figure 7.3 shows snapshots of the temperature field in the high-$Ra$ regime at different depths $z$ and different values of $Ra$, and figure 7.4 shows snapshots from the same simulations at fixed $x = L/2$. The flow has many analogues with two-dimensional Rayleigh–Darcy flow at high $Ra$; in particular, there are clear visual parallels between the vertical slices in figure 7.4 and snapshots of the flow in two dimensions (Otero et al. 2004, and chapter 2, figure 2.2). The flow can be divided into three regions of differing dynamics. The interior region appears to be dominated by roughly vertical and fairly large-scale exchange flow in distinct columns of hot rising fluid and cold sinking fluid, which we refer to as megaplumes. At the upper and lower boundaries of the domain there are thermal boundary layers which are almost too small to distinguish in figure 7.4. Between the boundary layers and the interior flow is a region dominated by the growth and interaction of long, thin, sheet-like plume structures that arise from time-dependent boundary-layer instabilities (figure 7.3). The sheet-like plumes are the three-dimensional analogue of two-dimensional protoplumes of chapter 2, and so we refer to this region as the protoplume region. The protoplume sheets erupt from the boundary layers and are laterally entrained into the large-scale megaplume flow. Visual inspection of figure 7.3 suggests that the spatial scale of the protoplumes decreases roughly like $Ra^{-1}$ (note the different spatial scales in the figure), while the dominant lengthscale of the interior megaplumes has a much weaker dependence on $Ra$ (see §7.3.2.4 below).
Figure 7.3: Snapshots of the temperature field at heights of \( z = 30/Ra \) near to the lower boundary, (left), \( z = 0.5 \) in the interior of the flow (centre), and \( z = 1 - 30/Ra \) near to the upper boundary (right). (a) \( Ra = 4000 \) and \( L = 2 \); (b) \( Ra = 8000 \) and \( L = 1 \); and (c) \( Ra = 1.6 \times 10^4 \) and \( L = 0.5 \). Note the different scales on the axes for each subfigure.

### 7.3.2.2 The Nusselt number \( Nu(Ra) \)

In a statistically steady state in the high-\( Ra \) regime, the time-dependent Nusselt number, \( nu(t) \), exhibits chaotic fluctuations about the time-averaged value \( Nu \).
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Figure 7.4: Snapshots of the temperature field (from the same simulations as in figure 7.3) at \( x = L/2 \), for (a) \( Ra = 4000 \) and \( L = 2 \); (b) \( Ra = 8000 \) and \( L = 1 \); and (c) \( Ra = 1.6 \times 10^4 \) and \( L = 0.5 \).

The amplitude of the fluctuations is notably smaller than that measured for two-dimensional porous convection at the same values of \( Ra \) (figure 7.5), which is likely a reflection of the additional spatial dimension over which the flux is averaged.

The time-averaged Nusselt number \( Nu = \langle nu \rangle \) is estimated numerically by time-averaging \( nu(t) \) until the uncertainty in the mean is less than 0.25%.

Measurements of \( Nu(Ra) \) for different aspect ratios \( L \) in the high-\( Ra \) regime are shown in figure 7.6, together with the least-squares power-law and linear fits to the data. The best-fit power-law scaling is \( Nu \sim Ra^{0.94} \), but we find that the data is much more accurately described by the linear fit, which takes the form

\[
Nu = \alpha_3 Ra + \beta_3; \quad \alpha_3 = 9.6 \times 10^{-3}, \quad \beta_3 = 4.6.
\] (7.11)
Figure 7.5: The instantaneous horizontally averaged Nusselt number \( n_u(t) \) for \( Ra = 10^4 \) and \( L = 1 \): (a) together with \( n_u(t) \) from numerical simulations of two-dimensional Rayleigh–Darcy convection at \( Ra = 10^4 \) (lower line); and (b) individual data points separated by five time steps \( \Delta t \), which illustrates the high temporal resolution of the calculations.

The good fit given by (7.11) strongly suggests that, as in two dimensions, the classical linear scaling \( Nu \sim Ra \) is attained asymptotically.

While (7.11) has an analogous form to the linear fit found in two dimensions (chapter 2), perhaps the most important practical observation from these measurements is that the flux \( Nu(Ra) \) is much larger than in two dimensions. A comparison of the pre-factor \( \alpha_3 = 9.6 \times 10^{-3} \) from (7.11) with the pre-factor \( \alpha = 6.9 \times 10^{-3} \) from the two-dimensional fit (2.14) gives \( \alpha_3/\alpha \approx 1.4 \), which indicates that the flux in the high-\( Ra \) regime is approximately 40% larger in three dimensions.

The slight variation in the measurements shown in figure 7.6 is likely a reflection of some long-timescale variability in the structure of the flow in the interior of the domain. It is possible that the structure is affected by mode restriction from the horizontal periodicity of the domain, although the relatively good agreement between measurements at different aspect ratios in figure 7.6 suggests that any effects of mode restriction on \( Nu \) are small. We return to this point when we investigate the dominant horizontal length scales of the flow in §7.3.2.4 below.

7.3.2.3 Three-dimensional heat-exchanger solution

Movies of the flow through the interior of the domain reveal that the large-scale exchange flow is almost quasi-steady: the upwelling and downwelling plumes are
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Figure 7.6: The time-averaged Nusselt number scaled by $Ra$, in the high-$Ra$ regime, for aspect ratio $L = 2$ (green squares), $L = 1$ (black circles), $L = 0.75$ (red stars), and $L = 0.5$ (blue dots). The best-fit power law $Nu = 0.018Ra^{0.94}$ (dashed line) does not capture the trend in the data as $Ra$ is increased; instead, a very good fit is provided by $Nu = \alpha_3 Ra + \beta_3$ (solid line) for $\alpha_3 = 9.6 \times 10^{-3}$ and $\beta_3 = 4.6$.

Figure 7.7: The temporally and horizontally averaged temperature profile $\langle T \rangle$, for $Ra = 4000$ (red solid), $Ra = 8000$ (green dashed), and $Ra = 1.6 \times 10^4$ (blue dot-dashed). The profiles are approximately linear through the interior of the domain, and the gradient increases with $Ra$. In contrast, for two-dimensional Rayleigh–Darcy convection the gradient decreases with $Ra$ (figure 2.6).

`persistent`, in that their locations do not vary appreciably over either the timescale for eruption and entrainment of sheet-like protoplumes, or over the timescale for vertical advection across the domain.

As in two dimensions (chapter 2), there are steady ‘heat-exchanger’ solutions to the governing equations (7.1)–(7.2) which can be used as a model for the ex-
change flow in the interior of the domain. Heat-exchanger solutions comprise a steady balance between vertical advection along a background temperature gradient and horizontal diffusion between interleaving columns of a given planform. The simplest such three-dimensional heat-exchanger model, with a square columnar planform, is given by

\[ T = A \cos kx \cos ky - \frac{2k^2}{Ra}z, \quad u = v = 0, \quad w = A \cos kx \cos ky, \quad (7.12a, b, c) \]

and consists of square columns with amplitude \( A \) and wavenumber \( k \) in both \( x \) and \( y \) directions.

Measurements of the temporally and horizontally averaged temperature \( \langle T \rangle \) (figure 7.7) show that the background temperature is roughly linear throughout the interior region, in agreement with the prediction of (7.12a). However, unlike in two dimensions where the gradient decreases with \( Ra \) (see figure 2.6, chapter 2), here we observe that the magnitude of the weak negative gradient increases as \( Ra \) is increased. We return to this observation in §7.3.2.5.

We measure the amplitude using the root-mean-squared (rms) temperature perturbations and velocities, \( T_{\text{rms}}, u_{\text{rms}}, v_{\text{rms}}, \text{ and } w_{\text{rms}} \). Analytic calculation of the
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rms values from (7.12) shows that, in the heat-exchanger model, $T_{\text{rms}} = w_{\text{rms}} = A/2$ and $u_{\text{rms}} = v_{\text{rms}} = 0$. Numerical measurements of the rms quantities at $z = 0.5$ indicate an increasing agreement with the model predictions as $Ra$ is increased (figure 7.8a). The horizontal velocities decrease with $Ra$, and the vertical velocity and temperature appear to tend to the same constant value, which yields an estimate of $A = 2T_{\text{rms}} \approx 0.2$. As a consistency check, this measurement can be used with the heat-exchanger theory to estimate the flux $Nu(Ra)$, as follows. As $Ra \to \infty$, vertical advection dominates the flux through the interior of the domain, and the vertical advective flux given by (7.12) is $Nu = A^2 Ra/4$. Using the measured estimate of $A$ gives a prediction of $Nu \approx 0.01Ra$, which is reassuringly close to the asymptotic prediction from the directly measured relationship (7.11) of $Nu = 9.6 \times 10^{-3} Ra$.

Figure 7.8(b) shows the vertical variation of the rms measurements at different values of $Ra$. The figure indicates that the rms quantities are increasingly uniform throughout the interior of the domain as $Ra$ is increased, in agreement with the heat-exchanger model. In contrast, near the upper and lower boundaries the rms quantities vary appreciably. These measurements reflect the fact that the heat-exchanger model breaks down near the boundaries where the flow is dominated by the strongly time-dependent growth and entrainment of sheet-like protoplumes.

These measurements all indicate that a heat-exchanger model provides an increasingly good description as $Ra \to \infty$ of the flow throughout the interior region of a three-dimensional Rayleigh–Darcy cell. As in two dimensions, the interior flow becomes increasingly ordered as $Ra \to \infty$ into columns of steady exchange flow, although the planform of this flow is not yet clear. Some indication of the lateral structure is provided by measurements of the dominant horizontal wavenumber $k_x$ which are presented in the next section.

7.3.2.4 The average horizontal wavenumber $k(Ra)$

In order to extract a measure of the average horizontal wavenumber $k(Ra)$ from the numerical calculations, we measured the power in each mode by taking a double Fourier transform of the temperature field. Figure 7.9(a–c) shows snapshots of the resultant power spectra as a function of the horizontal wavenumbers $k_x$.
and $k_y$, both at $z = 0.5$ (in the interior region) and at $z = 30/Ra$ (taken as a rough estimate of a depth in the protoplume region). The spectra reveal that the power $P(k_x, k_y)$ depends predominantly on the magnitude of the wavevector, or the ‘radial wavenumber’ $k_r = (k_x^2 + k_y^2)^{1/2}$, rather than on the angle $\theta = \tan^{-1}(k_y/k_x)$, which indicates that the flow is isotropic.

Measurements of the radial power $\tilde{P}(k_r) = \int P k_r d\theta$ at $z = 0.5$ (figure 7.9d) show a clear peak in the spectra, which indicates that the flow in the interior of the cell has a well-defined dominant horizontal lengthscale. This lengthscale corresponds to the megaplume spacing. For larger radial wavenumbers, there is a rapid exponential decay in the radial power. Measurements of $\tilde{P}$ at $z = 30/Ra$ (figure 7.9e) again show a peak at the same wavenumber as in the interior, which is the
signal from the roots of the megaplumes. For larger radial wavenumbers, however, there is a plateau in the radial power and then a much slower exponential decay than in the interior. These features are due to the high wavenumber sheet-like plumes that dominate the flow in the protoplume region. The decay in the radial power also displays a different dependence on $Ra$ in the protoplume region and in the interior of the cell. In the protoplume region (figure 7.9e), the measurements collapse as a function of $k_r/Ra$, while in the interior (figure 7.9d) the dependence on $Ra$ is much weaker. The different scaling with $Ra$ of the decay in the power can also be observed in the snapshots of $P(k_x, k_y)$ in figure 7.9(a–c), where the typical radii of the spectra increase more rapidly with $Ra$ in the protoplume region (right-hand column) than in the interior region (left-hand column).

We measured the average dominant wavenumber $k$ at a given height $z$ by taking the expected value of $k_r$ over two dimensions, and averaging over time, to give

$$k = \left\langle \frac{\int k_r \tilde{P}(k_r) \, dk_r}{\int \tilde{P}(k_r) \, dk_r} \right\rangle = \left\langle \frac{\int \int \sqrt{k_x^2 + k_y^2} P(k_x, k_y) \, dk_x \, dk_y}{\int \int P(k_x, k_y) \, dk_x \, dk_y} \right\rangle.$$

(7.13)
Measurements of \( k(Ra) \) from (7.13) at \( z = 0.5 \) are shown in figure 7.10(a). A least-squares power-law fit to the data gives a scaling of

\[
k \approx 0.17 Ra^{0.52},
\]

with 95% confidence intervals for the exponent giving a range of 0.52±0.05. Equation (7.14) can be compared with the fit \( k \approx 0.48Ra^{0.4} \) to the average wavenumber from two-dimensional Rayleigh–Darcy convection (see chapter 2): while the magnitude of the wavenumbers is similar over the range of \( Ra \) for which we have measurements, the three-dimensional wavenumber displays a distinctly stronger scaling with \( Ra \) (figure 7.10a).

Measurements of \( k(Ra) \) at \( z = 30/Ra \) (in the protoplume region), which we denote \( k_{pp} \), are shown in figure 7.10(b). The inset reveals a linear scaling \( k_{pp} \sim Nu \), which, from (7.11), implies that \( k_{pp} \sim Ra as Ra \to \infty \). This result suggests that the horizontal lengthscale of the sheet-like protoplumes scales with the boundary-layer depth \( \sim 1/Nu \). It also confirms that the average horizontal lengthscale of the flow has a much stronger scaling with \( Ra \) near to the upper and lower boundaries than in the interior, in agreement both with the different decay of the spectra in figure 7.9 and with visual comparison of the snapshots in figure 7.3. In addition, the result agrees with previous suggestions for the \( Ra^{-1} \) scaling of protoplume structures in transient three-dimensional convection with only one active boundary (Fu et al., 2013).

In order to constrain the numerical cost, we needed to reduce the aspect ratio \( L \) as \( Ra \) was increased. It might, therefore, be possible that mode restriction due to the relatively small aspect ratios could have affected the structure of the flow, and thus the measurements of \( k \) at \( z = 0.5 \) in figure 7.10(a). To investigate the effect of mode restriction, we undertook multiple calculations at different aspect ratios across a range of \( Ra \). The good agreement between the corresponding measurements of \( k \) (figure 7.10a) suggests that any effects of mode restriction are small. As an additional check, we undertook two simulations in cells with rectangular, rather than square, horizontal cross-sections, and found no statistically significant difference in the measurements of \( k \); these simulations were at \( Ra = 2500 \) with horizontal aspect ratio 2 \( \times \) 1, and \( Ra = 5000 \) with horizontal aspect ratio 1 \( \times \) 0.5.
Owing to the high computational cost of simulations at the largest values of $Ra$, we have been unable to check the results for $Ra \geq 1.2 \times 10^4$ at different aspect ratios; however, the data agrees with the trend of the measurements at lower $Ra$, which again suggests that mode restriction does not play a major role. We note that there is some variability in the data between the different simulations, which does not appear to have a systematic dependence on aspect ratio, and which we attribute to very long-timescale variation in the dominant wavenumber. Similar variability is observed in two-dimensional convection (chapter 2, figure 2.8).

### 7.3.2.5 The vertical temperature gradient

In figure 7.7, we observed that the magnitude of the linear background temperature gradient increased with $Ra$, particularly between $Ra = 4000$ and $Ra = 8000$. Figure 7.11(a) shows direct measurements of the background temperature gradient $\partial \langle T \rangle / \partial z$. The measurements can be approximately divided into two regions of different behaviour: for $Ra \lesssim 5000$ the magnitude of the gradient increases with $Ra$, while for $Ra \gtrsim 5000$ the gradient is roughly independent of $Ra$.

The heat-exchanger framework (7.12) indicates that the background tempera-
ture gradient is related to the horizontal wavenumber $k$ by

$$\frac{\partial \langle T \rangle}{\partial z} = -\frac{2k^2}{Ra}.$$  

(7.15)

Therefore, based on (7.15), the roughly constant temperature gradient for $Ra \gtrsim 5000$ is consistent with the measured scaling $k \sim Ra^{0.52 \pm 0.05}$ for the wavenumber. Indeed, a direct comparison of the measurements of $k$ and measurements of the gradient using (7.15) gives very good agreement for $Ra \gtrsim 5000$ (figure 7.11b). This agreement provides further evidence that the interior flow is increasingly well-described by the heat-exchanger model.

The precise trend in the measurements of the background temperature gradient as $Ra \to \infty$ is not clear from the data in figure 7.11(a). However, we would not expect a positive asymptotic scaling, since the gradient should not diverge as $Ra \to \infty$. Given the good agreement between the measurements and the heat-exchanger model, this expectation corresponds, via (7.15), to a constraint that the asymptotic exponent for the scaling of the wavenumber $k$ is no greater than 0.5. It should be noted that 0.5 lies well within the 95%-confidence interval for the exponent in (7.14), and so an asymptotic scaling of $k \sim Ra^{0.5}$ is consistent with the measurements presented here. Measurements at higher values of $Ra$ would be required to confirm this scaling.

### 7.4 Conclusions and discussion

In this chapter, we have presented the first measurements of statistically steady three-dimensional convection in a porous medium at high $Ra$. Measurements of the flux over the range $1750 \leq Ra \leq 2 \times 10^4$ are very well fitted by an expression of the form $Nu = \alpha_3 Ra + \beta_3$, for $\alpha_3 = 9.6 \times 10^{-3}$ and $\beta_3 = 4.6$. This fit, which has the same form as the analogous fit for two-dimensional high-$Ra$ porous convection (chapter 2), indicates that the flux attains the classical linear scaling asymptotically. The flux is roughly 40% larger than in two dimensions, and this difference has evident importance for physical applications.

The structure of the flow for $Ra \gtrsim 1750$ is dominated in the interior by persistent columnar exchange flow. Instabilities in the thin thermal boundary layers
near the upper and lower boundaries give rise to eruptions of long, thin, sheet-like protoplume structures, which are entrained laterally into the interior exchange flow. Measurements of the wavenumber in the protoplume region show that the lateral lengthscale of the thin sheet-like plumes scales with $Nu^{-1}$, and thus with $Ra^{-1}$ as $Ra \to \infty$.

Measurements of the interior flow indicate that it is increasingly well described by a steady three-dimensional heat-exchanger flow as $Ra$ is increased. The flow consists of a steady balance of vertical advection in interleaving columns along a background linear temperature gradient and horizontal diffusion between the columns. While we considered a specific heat-exchanger model with a square planform, it is difficult to discern a distinct horizontal planform of the exchange flow from snapshots of the interior flow (figure 7.3). The increasing agreement between the measurements and heat-exchanger theory as $Ra$ is increased suggests that the planform might become more distinct at higher values of $Ra$. Measurements of the interior flow reveal a distinct average horizontal wavenumber $k$ which is fitted over the range $1750 \leq Ra \leq 2 \times 10^4$ by $k \sim Ra^{0.52\pm 0.05}$. This scaling is much weaker than the scaling in the protoplume regions, but is also distinctly stronger than the analogous scaling of $k \sim Ra^{0.4}$ in two dimensions. The fairly good agreement between simulations at different aspect ratios suggests that mode restriction does not have a significant effect on this scaling. In addition, measurements of the background temperature gradient for $Ra \gtrsim 5000$ are consistent with the measurements of $k$, based on heat-exchanger theory.

As discussed in §7.3.2.5, based on the good agreement between measurements of the interior flow and the predictions of heat-exchanger theory, we expect the asymptotic exponent for the scaling $k(Ra)$ to be bounded above by 0.5. Otherwise, horizontal diffusion ($\sim k^2/Ra$) would become stronger than vertical advection asymptotically, and the convective heat transfer would vanish as $Ra \to \infty$. A plausible prediction based on the measurements in this chapter is therefore that the asymptotic scaling is $k \sim Ra^{0.5}$, although calculations at higher values of $Ra$ would be required to confirm this. Certainly, the scaling appears to be stronger than the two-dimensional scaling of $k \sim Ra^{0.4}$, and the question remains as to why this difference exists. One theory that has been suggested for the physical control of the wavenumber $k(Ra)$ is that $k$ is determined by the smallest length...
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scale, or ‘minimal flow unit’, for which the flux remains independent of aspect ratio (Wen et al., 2013) (see chapter 3). Interestingly, this theory predicts a scaling of $k \sim Ra^{0.5}$ for steady two-dimensional convection (Corson, 2011). In chapter 3, we suggested that the reason the measured scaling in two dimensions is weaker than this is because it is constrained by the stability of the interior columnar flow. It seems likely, therefore, that a stability analysis of the three-dimensional heat-exchanger flow could shed light on the reason for the different scalings for $k$ in two and three dimensions. Such an analysis, as discussed at the end of chapter 3, is left for future work.

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Chapter 8

Conclusions, and implications for CO$_2$ sequestration

8.1 Conclusions

In this thesis we have studied a range of problems involving convection in a fluid-saturated porous medium at high Rayleigh number $Ra$.

In chapter 2, we presented a detailed numerical investigation of the statistically steady flow in a two-dimensional Rayleigh–Darcy (porous Rayleigh–Bénard) cell at high $Ra$. Rayleigh–Darcy convection undergoes a transition at $Ra \approx 1300$ from predominantly large-scale quasi-periodic rolls to vigorous columnar exchange flow driven by unsteady plume formation in boundary layers. Our measurements of the convective flux, as described by the Nusselt number $Nu$, in this ‘high-$Ra$’ regime reveal that, contrary to some previous indications, the classical linear scaling $Nu \sim Ra$ is attained asymptotically. The measurements of $Nu(Ra)$ for $1300 < Ra \leq 4 \times 10^4$ are extremely well described by $Nu = \alpha Ra + \beta$, for $\alpha = 6.9 \times 10^{-3}$ and $\beta = 2.75$.

The structure of the flow is characterised in the interior by vertical columnar exchange flow of ‘megaplumes’ across the height of the cell at a (statistically) regular and $Ra$-dependent horizontal wavenumber. Near the boundaries, the flow is instead dominated by short-wavelength boundary-layer instabilities, which give rise to the rapid growth of protoplumes. The protoplumes are driven laterally
and entrained into the interior megaplume flow. We found that the interior flow is increasingly well described as $Ra \to \infty$ by a simple, steady, columnar heat-exchanger model with a single horizontal wavenumber $k(Ra)$ and a linear background temperature field. The flow, therefore, becomes increasingly ‘ordered’ as $Ra$ is increased, in clear contrast to the turbulent interior dynamics of pure-fluid Rayleigh–Bénard convection for $Ra \gg 1$. The dominant horizontal wavenumber $k$ of the interior flow increases as $Ra$ is increased, and numerical measurements of $k(Ra)$ for $1300 < Ra \lesssim 4 \times 10^4$ are roughly fitted by $k \sim Ra^{0.4}$, although there is some suggestion of a weaker scaling at the highest values of $Ra$. An investigation of the dynamics of protoplumes near the upper and lower boundaries of the cell suggested that the columnar wavenumber is not controlled directly by the vigorous dynamics near the boundaries.

In chapter 3, we examined the hypothesis that the columnar flow-structure of high-$Ra$ porous convection is instead determined by the stability of the columnar flow. We tested this hypothesis by examining the linear stability of an unbounded columnar heat-exchanger solution, which is governed by the parameter $A = \hat{A}Ra/k$, where $\hat{A}$ is the amplitude of the flow. The flow is always unstable; for $A \lesssim 17.2$ the instability takes the form of a large-scale overturning associated with the background unstable linear temperature gradient, while for $A \gtrsim 17.2$, the instability takes the form of vertically propagating pulses on the background columns. A matched asymptotic expansion in the limit of strong columnar flow or large $Ra$ (i.e. $A \gg 1$) showed that the growth rate $\text{Re}\{\sigma\}$ asymptotes to $\text{Re}\{\sigma\} = 0.2308A^{4/9}$ as $A \to \infty$. Direct numerical simulations indicated that the evolution of the instability in the non-linear regime results in a coarsening of the columnar flow.

We applied the results of the stability analysis to the columnar flow in a Rayleigh–Darcy cell, by balancing the time scales for growth of the most unstable perturbation and vertical propagation across the domain. This balance suggests that the columnar flow is unstable for wavenumbers $k$ greater than $k \sim Ra^{5/14}$, as $Ra \to \infty$. A correction to this scaling for non-asymptotic values of $Ra$ predicts a slightly stronger dependence on $Ra$ for $Ra \lesssim 4 \times 10^4$, in good agreement with the trend of the numerical measurements presented in chapter 2. This result supports the hypothesis that the physical mechanism controlling the horizontal scale of
columnar convection is the stability of the columnar flow. Under this hypothesis, the interior flow in a Rayleigh–Darcy cell is forced at small lengthscales \( \sim Ra^{-1} \) by protoplumes near the upper and lower boundaries, but the flow coarsens and the horizontal lengthscales increase until the flow becomes stable, at a lengthscale \( \sim k^{-1} \sim Ra^{-5/14} \) as \( Ra \to \infty \).

In chapter 4, we examined the implications for high-\( Ra \) convection of heterogeneity in the porous medium, specifically when the heterogeneity takes the form of thin low-permeability horizontal layers. We presented a numerical study of statistically steady convection in a cell containing a thin low-permeability horizontal layer in its centre. When both the height \( h \) and the relative permeability \( \Pi \) of the interior low-permeability layer are small, the flow is governed solely by their ratio \( \Omega = h/\Pi \), the impedance. We studied the flow in this limit, and analysed the dependence of both the convective flux \( Nu \) and the dynamical flow-structure on \( \Omega \).

There are two particularly striking features of this system. First, as \( \Omega \) is increased from zero (the limit of homogeneous Rayleigh–Darcy convection), the flow develops a cellular structure and the horizontal lengthscale \( \lambda \) of the cells increases dramatically (roughly like \( \lambda \sim \Omega^{1/2} \)). Second, the flux \( Nu \) can increase as \( \Omega \) is increased from zero (i.e. as the permeability of the inner layer is decreased, for fixed \( h \ll 1 \)), before decreasing significantly for larger values of \( \Omega \). At \( Ra = 2500 \), for example, \( Nu \) attains a maximum at \( \Omega \approx 0.3 \) that is roughly 30\% larger than the Nusselt number for homogeneous convection. For larger values of \( Ra \), the increase in \( Nu \) with \( \Omega \) is weaker. For larger values of \( \Omega \) (\( \Omega \gtrsim 5 \)), there is a transition in the flow structure as the impedance to flow across the interior layer is so large that diffusion, rather than advection, becomes the dominant transport mechanism there. We demonstrated that both the qualitative decrease of the flux with \( \Omega \) in the advection regime and the flux in the diffusive regime can be described with simple reduced models. The model in the advection regime also predicts an increase in the wavelength of \( \lambda \sim \Omega^{1/2} \), in agreement with the numerical data. The curious increase in \( Nu \) with \( \Omega \) for small \( \Omega \) is not described by these simple models.

The work contained in chapters 2–4 was concerned primarily with statistically steady ‘two-sided’ convection. In chapters 5 and 6, we instead studied ‘one-sided’ porous convection, driven by a source of density on one boundary only. We devel-
oped theoretical, numerical, and experimental models of the shutdown of high-$Ra$ convection in a range of one-sided porous systems with different physical applications. In chapter 5, we found a close dynamical relationship between the slowly evolving one-sided shutdown system and the two-sided Rayleigh–Darcy cell. Our results showed that measurements of $Nu(Ra)$ from a Rayleigh–Darcy cell can be used to give excellent quantitative agreement with the evolution of the flux in the shutdown regime. We used this observation to develop simple reduced theoretical models of the shutdown of convection, which give excellent predictions of the evolution of the convective flux when compared with direct numerical simulations. The dynamical structure of the flow in the shutdown regime is dominated by persistent columnar megaplumes that extend across the height of the domain, and the horizontal spacing of these plumes changes with the evolving average density in very good quantitative agreement with measurements from a Rayleigh–Darcy cell. This work was extended to consider the effect of general power-law equations of state.

In chapter 6, we developed the ideas of the previous chapter to investigate systems comprising two fluid layers, separated by an active interface which can move as a result of the convective flux across it. We separately examined the case of two immiscible fluids and the case of two miscible fluids. Under the assumption that the interface remains flat as it moves, we developed reduced theoretical models of each system, which give excellent agreement with measurements of the evolution of the flux and the height of the interface from direct numerical simulations. In the case of miscible fluids with an interface that is free to deform, we also found good agreement between laboratory experiments in a Hele–Shaw cell and numerical simulations. These investigations showed that the flux could be dramatically enhanced by interfacial deformation. For immiscible fluids like CO$_2$ and water, we argued that interfacial deformation was unlikely to be important owing to the stabilizing density jump at the interface; this observation highlights an important difference between immiscible and miscible systems.

In common with the majority of previous studies of porous convection, the work in chapters 2-6 concerned two-dimensional flow. In chapter 7, the results of fully resolved numerical simulations of the statistically steady flow in a three dimensional Rayleigh–Darcy cell for $Ra \lesssim 2 \times 10^4$ were presented. An overview
of the flow for $Ra < 1750$ revealed a range of interesting and largely unexplored convective dynamics. In the high-$Ra$ regime ($Ra \gtrsim 1750$), measurements of the convective flux were very well described by $Nu = \alpha_3 Ra + \beta_3$, for $\alpha_3 = 9.6 \times 10^{-3}$ and $\beta_3 = 4.6$. This fit both implies that the classical linear scaling $Nu \sim Ra$ is attained asymptotically, and also indicates that the convective flux is roughly 40% larger than the corresponding flux in the two-dimensional cell, measured in chapter 2.

There are certain clear analogues between the three-dimensional flow structure in the high-$Ra$ regime and the two-dimensional structure characterized in chapter 2. The statistically steady three-dimensional flow for $Ra \gtrsim 1750$ consists of large-scale persistent columnar exchange flow in the interior of the domain. Instabilities in the thin thermal boundary layers near to the upper and lower boundaries of the domain give rise to time-dependent bursts of long, thin, sheet-like protoplumes, which are driven laterally and entrained into the interior exchange flow. The spatial scale of the sheet-like protoplumes scales with $Nu^{-1}$, and thus with $Ra^{-1}$ as $Ra \to \infty$. The interior exchange flow is increasingly well described by a steady heat-exchanger model, characterized by a linear background temperature gradient and a dominant horizontal wavenumber $k$. Measurements of the wavenumber were fitted over the range $1750 \leq Ra \leq 2 \times 10^4$ by $k \sim Ra^{0.52 \pm 0.05}$, which gives a distinctly larger exponent than the equivalent expression for two-dimensional convection (roughly $k \sim Ra^{0.4}$; chapter 2). Based on the good agreement with the heat-exchanger framework, we expect the asymptotic scaling to be bounded above by $k \sim Ra^{0.5}$ (as discussed §7.4), which lies well within the confidence interval of the measured scaling.

## 8.2 CO$_2$ sequestration

### 8.2.1 Implications and discussion

The primary motivation for this work, as discussed in §1.1, was to model and understand the convective dissolution of geologically sequestered CO$_2$ in saline aquifers. In this thesis, we have measured flux laws, analysed the dynamical structure of convection, and developed simple reduced models of convection that
can be used in geophysical settings. We consider the implications of some of these results here.

For the sake of this discussion we will use illustrative parameter values from a relatively high permeability aquifer, such as the Utsira sand reservoir at Sleipner (Ennis-King & Paterson, 2005; Bickle et al., 2007). We take: permeability $K = 5 \times 10^{-12}$ m$^2$; porosity $\phi = 0.3$; $g = 10$ m/s$^2$; driving density contrast between dense CO$_2$ solution and brine $\Delta \rho^* = 15$ kg/m$^3$; viscosity of brine $\mu = 5 \times 10^{-4}$ Pa s; and diffusivity of CO$_2$ $D = 10^{-9}$ m$^2$/s. The equation of state for CO$_2$ and brine is linear ($n = 1$ in the terminology of chapters 5 and 6). We consider an aquifer of depth $H = 100$ m. The convective time scale $T^*$ for this system is given by $T^* = \phi H \mu / (\Delta \rho^* g K) \approx 0.6$ years, and, for comparison, the diffusive time scale is $H^2 / D \approx 3 \times 10^5$ years. The Rayleigh number for this illustrative aquifer, which is the ratio of these time scales, is $Ra \approx 6 \times 10^5$.

In chapter 2, we determined the flux law $Nu = \alpha Ra + \beta$ for two-dimensional statistically steady convection. For $Ra > O(10^4)$, this expression can be very well approximated by setting $\beta = 0$. The horizontally averaged dimensional flux $F^*$ (i.e. the volume flux per unit area) is then given by the expression

$$F^* = \frac{\alpha b g K (C^*_m - C^*_n)^2}{\mu},$$

(8.1)

where $b$ is the coefficient in the linear equation of state $\rho(C)$ (5.5). The flux is thus independent of both the height $H$ of the aquifer and the diffusivity $D$. The expression $(C^*_m - C^*_n)$ denotes the difference in the concentration of CO$_2$ between the dense CO$_2$-saturated solution ($C^*_m \approx 0.05$) and pure brine ($C^*_n = 0$); the fact that this driving concentration difference is small reflects the weak solubility of CO$_2$ in brine ($\sim 5\%$ by weight).

The parameter values above give $F^* \approx 5 \times 10^{-10}$ m$^3$/s. Using a density of 700 kg m$^{-3}$, this value gives a mass flux of supercritical CO$_2$ of about 11 thousand tons per year, per kilometre squared of the CO$_2$–brine interface. For comparison, roughly one million tons of CO$_2$ are injected at Sleipner each year. Estimates from simple gravity-current models of a CO$_2$ plume spreading under gravity (Lyle et al., 2005) suggest that the areal extent of the injected current scales with the square root of the rate of injection, and will increase linearly with time during
injection. For the parameter values above, the areal extent of the current would reach 1 km$^2$ after approximately 50 years of injection. These estimates indicate that dissolution will typically take place over much longer timescales than those of injection.

The typical lengthscales of the flow can also be calculated: based on the parameters above, together with the observed scalings from chapter 2, the width of a megaplume would be roughly 3 m, while protoplumes would be approximately 5 cm wide.

These estimates are based on measurements from statistically steady two-dimensional two-sided convection. A comparison of measurements of the flux at early times in a one-sided system (e.g. figure 5.4) with measurements from a Rayleigh–Darcy cell (figure 2.4), shows that the flux in the one-sided system is more than double that in the two-sided system. Thus, in an unbounded aquifer (i.e. a one-sided system), we would expect the values of the flux to be at least double the estimates given above. Moreover, the results are for two-dimensional convection; based on the results of chapter 7, we would expect the flux to be roughly 40% larger again in a physical (i.e. three-dimensional) unbounded aquifer.

If, however, the aquifer were closed, the convective flux would shut down over time. The dissolution of CO$_2$ in this situation can be well described by our immiscible box model with a moving flat interface, as discussed in §6.4. Using the values above (with the initial height of the CO$_2$-brine interface at $h_0^* = 100$ m), together with the observations in chapters 5 and 6, we would expect the transition to the shutdown regime to occur after roughly $t^* \approx 10$ years. The subsequent evolution of the horizontally averaged flux is determined from our box models and given by (6.23), which can be rewritten as:

$$F^*(t) = \frac{4 \alpha b g K (C_m^* - C_s^*)^2}{\mu (1 + 4 \alpha t/T^*)^2},$$

(8.2)

where $T^* = \phi h_0^* \mu / (\Delta \rho^* g K) \approx 0.6$ years is the convective time scale, and $\alpha = 6.9 \times 10^{-3}$. Based on our immiscible box model, after 20 years, the solute flux would have halved. After 75 years, it would be one tenth of its initial value. In this time, the interface would have retreated by nearly 4 metres (4% of the original...
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depth), and about 0.8 million tons of CO₂ would have dissolved for every square kilometre of the CO₂-brine interface. We again note that these results are for two-dimensional convection; based on the results of chapter 7, we would predict that the values of the flux would be roughly 40% larger in the shutdown regime in a three-dimensional system. We also note that these illustrative results apply to laterally confined aquifers, and, while the physical processes that we examined in chapter 5 and 6 are still relevant, the time scales and dynamics of shutdown in laterally unconfined aquifers may differ substantially.

We can briefly also consider the effects of heterogeneous layering in the medium. Suppose that the exemplar aquifer, of total depth $H = 100$ m, contains a thin horizontal layer of depth $h^* = 1$ m. The magnitudes of these values are consistent with observations of thin mudstone layers at Sleipner (Bickle et al., 2007). The permeability of the layers could range from $10^{-1000}$ times smaller than the main aquifer, which gives rise to values of the impedance $\Omega$ in the range $0.1 \lesssim \Omega \lesssim 10$. Neufeld & Huppert (2009) used an example value for the permeability ratio at Sleipner of $\Pi \approx 0.05$, which gives $\Omega \approx 0.2$. In this case, the results of chapter 4 suggest that the low-permeability layers would have little negative effect on the rate of dissolution. If, however, the permeability contrast were much larger, the flux would be considerably lower. In such a case it is likely that lateral migration along the top of the low-permeability layer or leakage through fractures in the layer would dominate the dynamics (see, e.g. Pritchard et al. 2001; Neufeld & Huppert 2009), rather than convection across the layer.

The representative values and time scales given here correspond to relatively high-permeability aquifers like that at Sleipner. Some potential storage sites have permeabilities that are $2 - 3$ orders of magnitude smaller than that considered here, in which case the flux would be extremely weak; even the transition to the shutdown regime would take thousands of years. In such aquifers, we would not expect convective dissolution to provide a significant trapping mechanism.

8.2.2 Directions

An important future direction for understanding the dynamics of CO₂ sequestration systems is the integration of these models of convection into dynamic models.
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of flow in porous media. In particular, current parameterizations of convection assume that the injected CO$_2$ is stationary, whereas, in general, the current will either be rising as a plume or laterally migrating as a gravity current. Since the density difference between supercritical CO$_2$ and brine ($\sim 300$ kg m$^{-3}$) that drives this migration is many times stronger than the density difference driving convection ($\sim 10 - 20$ kg m$^{-3}$), it is possible that the motion of the current would have an appreciable effect on the rate of dissolution, particularly if the current was flowing up a background slope in the caprock. The study of convection in the presence of flow (or, analogously, convection forced with an imposed velocity), provides the next step for the modelling presented in this thesis. A fuller understanding of the effect of flow on the strength of convection would allow for a more accurate comparison of the timescales of dissolution with those of spreading (e.g. Lyle et al. 2005; Vella & Huppert 2006) or leakage (e.g. Pritchard 2007; Neufeld et al. 2011). In some recent laboratory experiments using miscible fluids, Macminn & Juanes (2013) have begun to look at this coupled problem of spreading and dissolution.

In common with previous studies of porous convection, throughout this thesis we have made the assumption that capillary retention in the pore space can be neglected, and thus that the interface between CO$_2$ and brine is ‘sharp’. Capillary retention will have two main effects: first, isolated pockets of CO$_2$ will be retained and trapped in the pores, in the wake of the migrating CO$_2$ current (this effect provides another secure trapping mechanism for CO$_2$; see §1.1 and Hesse et al. 2008); and second, a ‘capillary fringe’ of partially saturated CO$_2$ and brine will form at the interface. The extent of the capillary fringe depends on the capillary forces and pore-size distribution of the rock. Golding et al. (2011) used measurements of the capillary pressure to estimate that the depth of the partially saturated region lies in the range $0.1 - 100$ m (high-permeability aquifers, which thus have weaker capillary pressures, are likely to have depths towards to lower end of this range). In contrast, the illustrative values quoted above give an estimate of the boundary-layer depth of $O(1)$ cm. This comparison suggests that the effects of partial saturation may be important for convective dissolution, and warrant further investigation.

It should be noted that, from the point of view of laboratory experiments, an examination of the interaction between convective dissolution and the effects of
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partial saturation is not straightforward. Most analogue fluids used in previous experiments of convective dissolution are miscible (such as, for example, the fluids used in chapter 6), and so there are no capillary effects. Similarly, there is no partial saturation in a Hele–Shaw cell, which provides a useful setup for experiments as it is easy to observe the flow. Nevertheless, the development of a viable experimental setup that exhibits both partial saturation and convective dissolution would be useful, since a theoretical approach is also complicated. A possible theoretical approach could involve the modelling of both effects on the pore scale and the development of a parameterization which could be incorporated into continuum (numerical) models.

For a fuller understanding of the effect of dissolution on sequestered CO$_2$, comparison with reservoir-scale experiments and field observations is also required. The complex geometry and heterogeneity of most aquifers indicates that care must be taken with models developed for idealised systems, and comparison with field data provides a meaningful check on the accuracy of model predictions. Such comparison for simple models of spreading under gravity has been ongoing using seismic data at the Sleipner site (Bickle et al., 2007; Boait et al., 2012). It would be interesting to extend the modelling of this thesis to compare the effects of dissolution more directly with field measurements, both from natural CO$_2$ reservoirs (Gilfillan et al., 2009) and from sequestration sites like Sleipner.
Appendix A

Numerical Method

The governing equations for Boussinesq convection in an ideal porous medium are given by incompressibility, Darcy’s law, an equation of state, and an advection-diffusion transport equation for the temperature or concentration field. In this appendix, we discuss the techniques used throughout this thesis to solve these equations numerically. All the numerical code was written in the Fortran 90 programming language.

Throughout the appendix, superscript indices with index $n$ refer to temporal discretization with timestep $\Delta t$, while the subscript indices $i$, $j$, and $k$ refer to spatial discretization in the $x$, $y$, and $z$ directions, respectively.

A.1 Two-dimensional Rayleigh–Darcy convection

As discussed in chapter 2, the governing equations for two-dimensional Rayleigh–Darcy convection with a linear equation of state are given by

\begin{equation}
\nabla^2 \psi = -\frac{\partial T}{\partial x},
\end{equation}

\begin{equation}
\frac{\partial T}{\partial t} + \nabla \cdot \mathbf{u} T = \frac{1}{Ra} \nabla^2 T,
\end{equation}
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Figure A.1: (a) The coordinate transformation $z(\zeta)$ for $Ra = 2 \times 10^4$. The grid points shown are separated by five (uniform) vertical steps $\Delta\zeta$. (b) The horizontally and temporally averaged temperature profile $\langle T \rangle$ for $Ra = 2 \times 10^4$ near to the lower boundary $z = 0$, showing the high density of grid points in the boundary layer (each dot represents one grid point).

(cf. §2.2). The boundary conditions on the upper and lower boundaries of the domain are given by

$$T = 1, \; w = 0 \quad \text{at} \quad z = 0, \quad \text{and} \quad T = 0, \; w = 0 \quad \text{at} \quad z = 1, \quad (A.3a, b)$$

and the domain is periodic at $x = 0, L$.

In this section, we discuss the numerical methods used to solve $(A.1)$–$(A.3)$.

A.1.1 Coordinate transformation and grid spacing

Based on a balance between advection and diffusion in $(A.2)$, the diffusive boundary-layer depth is expected to scale with $Ra^{-1}$. At high $Ra$, we therefore anticipate extremely thin vertical boundary layers at the upper and lower boundaries, in contrast with much larger vertical scales throughout the interior of the domain. In order to accurately resolve the boundary layers with a vertically uniform grid, we would therefore over-resolve the interior. We dramatically reduced the computational cost of the calculations by using a vertical coordinate transformation $\zeta(z)$ which maps points from the boundary layer into the interior.
The transformation from $\zeta \in [0,1]$ to $z \in [0,1]$ is given by

$$z = \frac{1}{2} \left[ 1 + \frac{\tanh [\eta (\zeta - 1/2)]}{\tanh (\eta/2)} \right], \quad (A.4)$$

where $\eta$ is an adjustable parameter. For a given value of $Ra$, $\eta$ is defined implicitly by the requirement that

$$\left. \frac{\partial T}{\partial \zeta} \right|_{z=0} \approx O(1). \quad (A.5)$$

An example of this coordinate transformation $z(\zeta)$ with $\eta \approx 8.3$ for $Ra = 2 \times 10^4$ is shown in figure A.1(a). The extremely high spatial resolution that we are able to employ in the boundary layers is demonstrated in figure A.1(b), which shows the horizontally averaged temperature profile near to the bottom boundary.

The governing equations (A.1) and (A.2) were transformed analytically to $(x, \zeta)$ coordinates and then solved on a uniform rectangular grid using horizontal and (transformed) vertical resolution $\Delta x$ and $\Delta \zeta$ respectively. The temperature and streamfunction were calculated on a staggered grid in $(x, \zeta)$ coordinates (see figure A.2). This discretization both arises naturally from the flux-conservative nu-
A. NUMERICAL METHOD

The numerical method that we employ, which is discussed below, and it also aids the implementation of the boundary conditions. The temperature field was calculated at the centre of every grid square, which equates to points with coordinates \( ([n + 1/2] \Delta x, [m + 1/2] \Delta \zeta) \) for integer \( n \) and \( m \). The streamfunction was calculated at the vertices of the grid, which equates to points with coordinates \( (n \Delta x, m \Delta \zeta) \). In order to implement second-order boundary conditions for the temperature field, we also stored an additional temperature point half a grid cell outside the domain on every side, as shown in figure A.2.

A.1.2 The Poisson equation

The Poisson equation (A.1) was solved using a fast-Fourier transform in the horizontal \((x)\) direction, and a simple tridiagonal finite difference method in the vertical. This technique is useful for periodic problems without rapid variation between gridpoints, and is cheaper and quicker than relaxation methods.\(^1\)

After taking the Fourier transform and changing variables, (A.1) becomes

\[
\frac{\partial \zeta}{\partial z} \frac{\partial}{\partial \zeta} \left( \frac{\partial \zeta}{\partial z} \frac{\partial \tilde{\psi}}{\partial \zeta} \right) - k^2 \tilde{\psi} = -i k \tilde{T}, \tag{A.6}
\]

where a tilde signifies a Fourier transform in the \(x\) component, and \( k \) is the horizontal wavenumber. Given \( \tilde{T}(k, z) \), (A.6) is discretized using standard second-order finite difference operators, \( \tilde{\psi}(k, z) \) is determined by inverting the resulting tridiagonal equation, and the solution \( \psi(x, z) \) is determined by an inverse Fourier transform of \( \tilde{\psi} \). Therefore, at a fixed time \( t \), we can calculate \( \psi \), and so the velocity field, from the temperature field \( T \).

The standard real Fourier transform enforces periodic boundary conditions on the flow at \( x = 0, L \). Alternatively, boundary conditions of zero heat flux (as in chapters 5 and 6) can be enforced by using a Fourier sine transform, in which case the single spatial derivative on the right-hand side of (A.6) is given by a cosine transform.

\(^1\)We also developed a successive over-relaxation (SOR) method and a multi-grid method to solve the Poisson equation, but, based on a comparison of speed, accuracy and ease of implementation, particularly with respect to the periodic boundary conditions, we used a spectral method in all the simulations presented in this thesis.
A.1.3 The transport equation

Equation (A.2) was discretized using an alternating-direction implicit (ADI) method (e.g. Press et al. 1989), centred on the half time step to give second-order accuracy in time. The temporal discretization takes the semi-implicit form

\[
\frac{T^{n+1} - T^n}{\Delta t} = \frac{1}{2} \nabla \cdot (u^{n+1/2} \left[ T^{n+1} + T^n \right]) + \frac{1}{2 Ra} \nabla^2 \left( T^{n+1} + T^n \right) + O(\Delta t^2). \tag{A.7}
\]

The diffusion terms in (A.7) were spatially discretized using standard second-order finite-difference operators. The advection operator was discretized using a flux-conservative representation, which matches the advective fluxes into and out of grid squares and retains second-order spatial accuracy by using the velocities at the boundaries of the grid cells (as in figure A.2). The spatial discretization of the advection operators thus takes the form

\[
\left[ \frac{\partial}{\partial x} (uT) \right]_i = \frac{1}{\Delta x} \left[ u_{i+1/2} \left( \frac{T_{i+1} + T_i}{2} \right) - u_{i-1/2} \left( \frac{T_i + T_{i-1}}{2} \right) \right] + O(\Delta x^2), \tag{A.8}
\]

\[
\left[ \frac{\partial}{\partial z} (wT) \right]_k = \frac{1}{\Delta \zeta} \left( \frac{\partial \zeta}{\partial z} \right)_k \left[ w_{k+1/2} \left( \frac{T_{k+1} + T_k}{2} \right) - w_{k-1/2} \left( \frac{T_k + T_{k-1}}{2} \right) \right] + O(\Delta \zeta^2). \tag{A.9}
\]

The ADI scheme involves the recasting of (A.7) into two coupled discrete equations, each of which is implicit in one spatial direction and explicit in the other. The equations were solved by inverting a cyclic tridiagonal matrix in the \(x\) direction, and a regular tridiagonal matrix in the \(\zeta\) direction. The ADI scheme is unconditionally stable, and the time step \(\Delta t\) was selected to satisfy the Courant condition, as discussed in §A.1.6 below.

A.1.4 Combining the equations

There are various methods for calculating \(u^{n+1/2}\) given the temperature and velocity at previous time steps. For the sake of compactness, we used a midpoint method rather than an extrapolation method (like the Adams–Bashforth method).
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The midpoint method updates $T^n$ to $T^{n+1}$ as follows. First, the velocity field $u^n$ is calculated using (A.6). Second, this velocity field is used as an approximation of $u^{n+1/4}$ in the transport equation (A.7) with half the time step, to give an approximation of the temperature at the half time step $T^{n+1/2}$. Third, this temperature field is used to calculate the velocity at the half time step $u^{n+1/2}$ using (A.6) again. Finally, given the velocity at the half time step, (A.7) is used to evolve the original temperature field $T^n$ forward one time step to give $T^{n+1}$.

A.1.5 Boundary conditions

The arrangement of grid points shown in figure A.2 means that the vertical velocity $w$ is stored at points along the upper and lower boundaries of the domain, so that it is very straightforward to impose no-flow boundary conditions there. The fixed-temperature conditions at these boundaries in (A.3) are slightly more complicated to impose, as the temperature is not calculated exactly on the boundary (see figure A.2). In order to retain second-order spatial accuracy, we use a quadratic extrapolation of the nearest three grid points to the boundary. For example, if we desire $T = \Xi$ at $z = 0$ in the simple case of no vertical coordinate transformation ($\zeta(z) = z$), quadratic extrapolation gives

$$T_{-1/2} = -2T_{1/2} + \frac{T_{3/2} + 8\Xi}{3} + O(\Delta z^2).$$

(A.10)

In the general case with a coordinate transformation ($\zeta(z) \neq z$), we can generate a similar, but more involved, expression for the temperature $T_{-1/2}$.

Since all the heat flux into the domain is diffusive, the heat flux at the upper or lower boundary is easily measured using the temperature points on either side of the boundary. For example, the heat flux at the lower boundary is given by

$$\left. \frac{\partial T}{\partial z} \right|_{z=0} = \left. \left( \frac{\partial \zeta}{\partial z} \right) \right|_{z=0} \frac{T_{1/2} - T_{-1/2}}{\Delta \zeta} + O(\Delta z^2).$$

(A.11)

A.1.6 Verification of numerical scheme

We have compared our solutions of both (A.6) and (A.7) against known analytic solutions of the Poisson and transport equations, to confirm that the code gives
Figure A.3: The time-dependent Nusselt number \( \nu(t) = L^{-1} \int \partial T/\partial z \big|_{z=0} \, dx \) at \( Ra = 2 \times 10^4 \). The data points shown are separated by ten time steps \( \Delta t \).

second-order spatial and temporal errors. With the full combined code, we have observed the well-known onset of convection at \( Ra = 4\pi^2 \), and found good agreement with weakly non-linear theory for slightly larger values of \( Ra \) (Nield & Bejan, 2006). We have recovered the results of Graham & Steen (1994) for moderate values of \( Ra \leq 1300 \), and of Otero et al. (2004) for \( Ra < 10^4 \), as shown in figure 2.4 in chapter 2.

In the high-\( Ra \) regime, the smallest horizontal scales are found in thin boundary-layer instabilities (protoplumes), and the horizontal resolution is chosen to ensure that the thinnest points of these structures contain at least ten grid points. These horizontal scales appear to decrease like \( Ra^{-1} \) (see chapter 2, §2.4.2). For all but the highest decade of \( Ra \) data, we have confirmed that our results are sufficiently well resolved by doubling both the horizontal and vertical (\( \zeta \)) resolution and recovering statistically identical results. For the highest decade, we used a resolution that is consistent with the observed spatial scalings at lower values of \( Ra \), giving us confidence that all our results are well resolved. Typical values of the horizontal and (transformed) vertical discretization range from \( \Delta x = (256)^{-1} \) and \( \Delta \zeta = (180)^{-1} \) at \( Ra = 2500 \), to \( \Delta x = (4096)^{-1} \) and \( \Delta \zeta = (450)^{-1} \) at \( Ra = 4 \times 10^4 \).

The time step \( \Delta t \) is chosen to be smaller than the Courant time scale \( \Delta x/\max|u| \), which corresponds to the physical requirement that fluid is not advected further than one grid cell in one time step. At \( Ra_0 = 2 \times 10^4 \), the time step was \( \Delta t = (1400)^{-1} \). Figure A.3 shows the horizontally averaged time-dependent
Nusselt number $\nu(t)$ at $Ra = 2 \times 10^4$; the points shown are separated by ten time steps, and the fluctuations are well resolved.

### A.2 Extensions of numerical scheme in two dimensions

In this section we outline the manner in which the numerical scheme discussed above can be extended to model the different systems that we have considered in this thesis.

#### A.2.1 Convection with a low-permeability layer: chapter 4

In chapter 4, we developed the numerical scheme discussed above to model high-$Ra$ convection in a Rayleigh–Darcy cell with a low-permeability interior layer in the region $z_1 < z < z_2$. We developed both ‘full simulations’, in which the low-permeability layer was fully resolved, and ‘reduced simulations’, in which the low-permeability layer was parameterized by a jump condition for the horizontal velocity (4.12).

The basic numerical scheme is very similar to that described above; the main difference lies in the choice of coordinate transformation $\zeta(z)$ needed to resolve both the dynamics at the upper and lower boundary layers and the dynamics near to the interior layer. For the ‘full simulations’, we used a rather convoluted coordinate transformation from $\zeta \in [0, 1]$ to $z \in [0, 1]$ of the form

$$z(\zeta) = \frac{\mathcal{T}(\zeta, 0.25 + \nu, \eta_1) + \mathcal{T}(\zeta, 0.75 - \nu, \eta_1) + \varepsilon \mathcal{T}(\zeta, 0.5, \eta_2)}{\mathcal{T}(1, 0.25 + \nu, \eta_1) + \mathcal{T}(1, 0.75 - \nu, \eta_1) + \varepsilon \mathcal{T}(1, 0.5, \eta_2)}, \quad (A.12)$$

where

$$\mathcal{T}(x, y, \eta) = \tanh [\eta (x - y)] + \tanh (\eta y), \quad (A.13)$$

and $\eta_1$, $\eta_2$, $\nu$ and $\varepsilon$ are specified parameters that depend on the thickness of the low-permeability layer $h$ and the Rayleigh number $Ra$. These parameters were chosen to ensure that sufficient grid points lay both in the boundary layers near $z = 0$ and $z = 1$, and in the regions near $z = z_1$ and $z = z_2$. 

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For the ‘reduced simulations’, we used a simpler transformation of the form

\[ z(\zeta) = \frac{\mathcal{T}(\zeta, 0.25 + \nu, \eta) + \mathcal{T}(\zeta, 0.75 - \nu, \eta)}{\mathcal{T}(1, 0.25 + \nu, \eta) + \mathcal{T}(1, 0.75 - \nu, \eta)}, \tag{A.14} \]

where \( \mathcal{T} \) is defined in (A.13), and \( \eta \) and \( \nu \) are again parameters that control the stretching, and depend on \( \Omega \) and \( Ra \). The parameters were chosen to ensure the dynamics near \( z = 0, z = 0.5, \) and \( z = 1 \) are fully resolved.

In the full simulations, both the transport equation and the Poisson equation were solved across the whole domain. In the reduced simulations, we instead solved a jump condition for the horizontal velocity at \( z = 0.5 \), given by

\[ \Omega \frac{\partial w}{\partial x} = [u]_{z=0.5_+} - [u]_{z=0.5_-}, \tag{A.15} \]

(cf. (4.12)). In order to incorporate (A.15) into the numerical scheme, it can be written in terms of the streamfunction \( \psi \). The horizontal Fourier transform of the resultant equation takes the form

\[ \Omega k^2 \tilde{\psi} = \frac{\partial \tilde{\psi}}{\partial z} \bigg|_{z=0.5_+} - \frac{\partial \tilde{\psi}}{\partial z} \bigg|_{z=0.5_-}. \tag{A.16} \]

Equation (A.16) replaces the usual transformed Poisson equation (A.6) for the value of \( \tilde{\psi} \) at \( z = 0.5 \). Numerically, the expression for \( \tilde{\psi}_k \) at \( z = 0.5 \) is replaced by the discretized form of (A.16), which depends on \( \tilde{\psi}_{k \pm 1} \); the system thus remains tridiagonal and can be solved as before. In addition, since temperature \( T \) is continuous at \( z = 0.5 \), the transport equation can again be solved across the whole domain, just as in §A.1.3.

### A.2.2 One-sided convection: chapters 5 and 6

In chapters 5 and 6, we developed numerical schemes to describe both fixed-interface and free-interface one-sided convection, with immiscible fluids and a flat interface, and miscible fluids and both flat and deformable interfaces.

In chapter 5, the governing equations (5.10) and (5.13) were solved throughout the domain \( 0 \leq z \leq 1 \). Similarly, in §6.3 the same equations were solved through-
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out the domain \(0 \leq z \leq H\). In §6.2, however, the equations (5.10) and (5.13) were solved below the interface \(0 \leq z \leq h(t)\) only, in order to impose a flat interface at \(z = h(t)\). Above the interface, the concentration either remains constant (immiscible system) or satisfies a one-dimensional advection-diffusion equation (6.14) (miscible system).

As in previous chapters, in order to accurately resolve the dynamics near to the interface \(z = h\), we used a vertical-coordinate transformation \(\zeta(z, h)\). In chapter 5 and in §6.2, the transformation from \(\zeta \in [0, h]\) to \(z \in [0, h]\) was given by

\[
z = h \left[ 1 + \frac{\tanh[\eta (\zeta - h/2)]}{\tanh[\eta h/2]} \right],
\]

where \(\eta(Ra_0)\) is a stretching parameter that was chosen to ensure that sufficient points lay in the boundary layer below the interface. In §6.3, the governing equations were solved over the whole domain, and the interface was located in the interior. A more complex transformation was required to accurately resolve the boundary layers on either side of the interface, without dramatically increasing the computational cost. We employed a transformation of the form

\[
z = \frac{H}{A_1 + A_2} \left\{ A_1 \frac{\tanh(a_1 \eta \zeta)}{\tanh(H a_1 \eta)} + A_2 \left[ 1 + \frac{\tanh(a_2 \eta (\zeta - H))}{\tanh(H a_2 \eta)} \right] \right\}
\]

where \(\eta(Ra_0)\) is again a constant stretching parameter, and \(A_1, A_2, a_1\) and \(a_2\) are specified functions of the average interfacial height \(\overline{h}(t)\), which were chosen to increase the resolution in a region centred on \(z = \overline{h}\), and wider than the range of any interfacial deformations. To reduce the computational cost, the transformation \(\zeta(z, \overline{h}(t))\) was not re-calculated at every time step, but only when the interface \(z = \overline{h}\) had moved a sufficient distance to require it. After each calculation of a new vertical discretization \(\zeta(z, \overline{h})\), the variables were mapped from the previous discretization to the new grid using quadratic interpolation.

The governing equations (5.10) and (5.13) were again solved using a fast-Fourier transform and an ADI method, as described above in §A.1.2 and (A.1.3). In §6.2 (free-interface systems with a flat interface), the location of the interface \(h(t)\) was found by global conservation of solute (6.2) at each time step. For the miscible system with a flat interface (§6.2.2), the one-dimensional transport equation (6.14)
was solved at each time step using standard second-order finite-difference operators on a uniform grid above the interface.

### A.3 Three-dimensional Rayleigh–Darcy convection: chapter 7

In chapter 7, we presented results for three-dimensional Rayleigh–Darcy convection in the high $Ra$ regime. The governing equations consist of two Poisson equations for the non-zero components of the vector potential $\Psi = (\psi_x, \psi_y, 0)$, and a transport equation for the temperature $T$ (see §7.2). These equations, introduced in (7.8a,b) and (7.2), respectively, are given by

$$
\nabla^2 \psi_x = -\frac{\partial T}{\partial y}, \quad \nabla^2 \psi_y = \frac{\partial T}{\partial x}, \quad \frac{\partial T}{\partial t} = -\mathbf{u} \cdot \nabla T + \frac{1}{Ra} \nabla^2 T. \quad (A.19a, b, c)
$$

The velocity $\mathbf{u} = (u, v, w)$ is given from $\Psi$ by

$$
(u, v, w) = \nabla \times \Psi = \left(-\frac{\partial \psi_y}{\partial z}, \frac{\partial \psi_x}{\partial z}, \frac{\partial \psi_y}{\partial x} - \frac{\partial \psi_x}{\partial y}\right). \quad (A.20)
$$

The boundary conditions on the upper and lower boundary of the domain are given by

$$
\psi_x = \psi_y = 0, \quad T = 1 \quad \text{on} \quad z = 0, \quad \psi_x = \psi_y = T = 0 \quad \text{on} \quad z = 1, \quad (A.21)
$$

where the cell is periodic in both $x$ and $y$ directions, with period $L$.

#### A.3.1 Coordinate transformation and grid spacing

As for two-dimensional convection, we employed a vertical coordinate transformation $\zeta(z)$ to fully resolve the thin diffusive boundary layers near to $z = 0, 1$. The transformation was identical to that used for the two-dimensional simulations, discussed in §A.1.1.

The governing equations (A.19) were transformed to $(x, y, \zeta)$ coordinates and discretized on a uniform cuboidal grid. The three variables $(\psi_x, \psi_y, T)$ are calcu-
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Figure A.4: (a) A schematic showing one cuboid of the numerical grid, with the locations at which \( \psi_x \) and \( \psi_y \) are calculated. The components of the velocity, given by (A.20), are thus determined at the centre of each face of the cuboid as shown. The temperature is calculated at the centre of each cuboid. (b) Measurements of the average temperature \( \langle T \rangle \) near to the lower boundary, which demonstrate that the boundary layer is well resolved.

lated on a staggered grid, which is a requirement of the flux-conservative scheme and helps to facilitate implementation of the boundary conditions: the temperature is calculated at the centre of each grid cuboid, while \( \psi_x \) and \( \psi_y \) are calculated around the cuboid in such a manner that \( u, v \) and \( w \) are determined in the centre of the relevant faces of the cuboid (see figure A.4a). The boundary conditions for \( \psi_x \) and \( \psi_y \) on \( z = 0,1 \) from (A.21) are straightforward to impose with this staggered layout.

A.3.2 The equations

The two Poisson equations (A.19a,b) were solved using fast-Fourier transforms in both the \( x \) and \( y \) directions, and second-order finite differences to discretize the resultant tridiagonal system in the \( \zeta \) direction.

The transport equation (A.19c) was solved using a three-dimensional ADI scheme, following Brian (1961), which is discussed below. As in §A.1.3, the diffusion operator was discretized using standard two-dimensional finite-difference operators. The advection operator was discretized using a flux-conservative formulation, such that the velocity into and out of every grid cell is calculated (as in
Second-order ADI methods are closely related to second-order semi-implicit (Crank–Nicholson) methods (Douglas, 1962; Press et al., 1989). Given an equation like (A.19c), a second-order ADI method involves the recasting of the equation into multiple coupled discretized equations, each of which is implicit in some spatial directions and explicit in others. By reformulating these coupled equations back into one equation, it can be shown that the set of ADI equations is equivalent, up to second order in $\Delta t$, to the semi-implicit discretization of the original equation.

While the ADI scheme is unconditionally stable in two spatial directions, in three dimensions it is not necessarily (Douglas, 1962). In particular, the ‘natural’ choice of three-dimensional ADI scheme, which has three coupled discretized equations, each of which advances an interval $\Delta t/3$ and is implicit in one direction and explicit in the others, is only conditionally stable, and the requirements of stability give a restrictively small value of $\Delta t$. There are, however, a multitude of possible sets of coupled discrete equations which, when combined, give the same semi-implicit equation up to second order in $\Delta t$. This fact has given rise to a number of different three-dimensional ADI schemes, which have different stability properties. The method that we have used is unconditionally stable, and is attributable to Brian (1961) and Douglas (1962).

As in two dimensions, we used a midpoint method to determine the velocity at the half time step, and so to retain second-order accuracy for the time derivative. We parallelized the code using a hybrid scheme involving both open multi-processing (OpenMP) and message-passing interface (MPI) specifications.

### A.3.3 Verification of numerical scheme

We verified our numerical scheme by reproducing published measurements of $Nu(Ra)$ for low values of $Ra$. We observed the onset of convection with a two-dimensional mode at $Ra = Ra_c = 4\pi^2$ (Holst & Aziz, 1972). We recovered the results of Schubert & Straus (1979) for $Ra < 300$, including the transition at $Ra \approx 97$ to fully three-dimensional convection.

As discussed above in §A.1.6, we chose a horizontal resolution to fully resolve the smallest horizontal scales, which appear to decrease like $Ra^{-1}$. The vertical
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scale was chosen to ensure that multiple grid points lay inside the thin boundary layers near the upper and lower boundaries of the domain, the depth of which is also anticipated to scale with $Ra^{-1}$. In order to reduce the numerical cost, we used slightly fewer points in the vertical direction than for the two-dimensional simulations discussed in §A.1; however, the simulations remain well resolved in the vertical direction (see figure A.4b). Typical values of the horizontal and (transformed) vertical discretizations range from $\Delta_x = \Delta_y = (128)^{-1}$ and $\Delta_\zeta = (150)^{-1}$ at $Ra = 1000$, to $\Delta_x = \Delta_y = (2048)^{-1}$ and $\Delta_\zeta = (220)^{-1}$ at $Ra = 2 \times 10^4$. We tested simulations with double the horizontal resolution and with both larger and smaller vertical resolutions at $Ra = 2000$ and recovered statistically identical results.
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