Exploring the effects of an obstruction on the evolution of the Rayleigh-Taylor Instability

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Declaration

This dissertation is the result of my own work and includes nothing which is the outcome of work done in collaboration except as declared in the Preface and specified in the text. It is not substantially the same as any that I have submitted, or, is being concurrently submitted for a degree or diploma or other qualification at the University of Cambridge or any other University or similar institution except as declared in the Preface and specified in the text. I further state that no substantial part of my dissertation has already been submitted, or, is being concurrently submitted for any such degree, diploma or other qualification at the University of Cambridge or any other University or similar institution except as declared in the Preface and specified in the text.

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Christopher Brown
April 2018
“If you’re going through hell, keep going.”
Winston Churchill
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Abstract

This thesis discusses the effect of an obstruction on the evolution of the Rayleigh-Taylor instability in a confined geometry at low Atwood numbers. Laboratory experiments are the principal method of investigation, though these data are supplemented with implicit large eddy simulations (ILES). The laboratory data are captured using an innovative laser scanning system which is able to simultaneously record density and velocity data in 3D. A new approach for calculating density data from laser induced fluorescence measurements is developed and demonstrated. The technique is used to improve the accuracy of the density measurement from laser induced fluorescence, by correcting for the damage to dye caused by the laser.

The introduction of an obstacle at the height of the initial interface results in dramatic changes to the dynamics of mixing, even when this obstacle is only a few percent of the domain width. Two obstructed scenarios are considered. In both of these an obstruction is placed on the interface between an upper heavy layer and lower light layer. In the first case, a single horizontal opening connects the upper and lower layers. A bidirectional flow exchanges fluid through the opening, establishing a circulation cell in each layer. These cells exist quasi-steadily for long periods, constantly recirculating and mixing the fluid in each layer. This acts to increase the time required for mixing compared with the classical unobstructed case, but results in a more uniformly mixed final stratification.

The second case has two horizontal openings, one either side of the obstruction. This results in markedly different dynamics. The flow through each of the openings switches back and forth between being bidirectional (as with the single opening case) and unidirectional, with unidirectional exchange reversing direction with a constant period. These results are consistent with the ILES data.

For both of these cases a wide range of analytical techniques are used to connect the new obstructed dynamics with previously conducted research, such as calculating the molecular mixing fraction, energetics and mixing efficiency. A multistage mixing process is identified, unique for cases with an obstruction. For the single opening case a hierarchy of models are developed that accurately capture the density change of each layer for both the experimental and numerical data. The effect of changing the aspect ratio of the domain is investigated using ILES, from which different dynamical regimes are observed, discussed and analysed.
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Chapter 1

Introduction and previous work

1.1 Motivation

Turbulence is one of the most important unsolved problems remaining in classical physics today (Feynman et al., 1963). The existence and importance of turbulence in a wide range of phenomena, from industrial processes to oceanic mixing, has resulted in a concerted effort over the past half century to understand the dynamics, mixing processes and fundamental underpinnings of turbulence.

This thesis will focus on the turbulent mixing and dynamics resulting from the growth of a classical instability, the Rayleigh-Taylor instability (RTI). The RTI is fundamental to some of the key problems faced in physics today, from the very large scale astrophysics seen in supernova (e.g. Cook et al. (2004)), to developing a new clean sustainable energy source using inertial confinement fusion (ICF), where capsules of deuterium and tritium are imploded with an array of lasers (e.g. Petrasso (1994)). The intention is for the implosion to compress the capsules to such high pressures that nuclear ignition occurs. However, the imperfect container, asymmetry in the drivers and differing densities of the fuels enable hydrodynamical instabilities to grow, observed to be dominated by the RTI. These instabilities mix cooler, outer-shell substances with the hot core, preventing nuclear ignition from occurring (Weber et al., 2014).

Whilst substantial work has been done studying the growth of the RTI in Newtonian fluids, little has been done to investigate its growth in other media. The original proposition of this thesis is to understand some of the fundamental questions relating to the growth of the RTI in materials with strength, such as shear thickening fluids, through laboratory research. The first and simplest step in understanding how the RTI might develop in a material with strength is to investigate how the RTI interacts with a solid object. This interaction has not previously been studied from a RTI perspective. Such a solid object could be theoretically imagined as pertaining to part of the fluid which has solidified or not yet yielded.
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The experimental equipment used to investigate the growth of the RTI is a perspex tank with the upper and lower layer halves separated by a solid steel barrier that is removed at the start of each experiment. Similar experimental setups have been used by Dalziel et al. (1999); Linden et al. (1994) and Davies Wykes and Dalziel (2014), amongst others. Thus, the simplest way a solid obstruction can be created within the flow is to only partially remove the removable barrier at the start of an experiment, see figure 1.1 for a schematic.

The experimental setup, representing the simplest first step in understanding how a solid object may interfere with the growth of the RTI in a confined environment, is analogous to problems arising in numerous natural environments. For example, continuing the discussion of the ICF problem, it is possible that the initial shell containing the fluid is not completely ablated, such that fragments of solid shell may enter the core and modify the expected dynamics from that of the classical, unobstructed RTI. Geological examples include mixing in the mantle, where, due to temperature or chemical variations, part of the mantle may become solid and interfere with expected dynamics. There are, additionally, possible applications to industrial mixing and natural ventilation problems (e.g. in an environment containing mezzanines).

It is with these motivations in mind, combined with the interesting and unexpected dynamics that resulted from preliminary investigations of only partially withdrawing the removable steel barrier, that this thesis focuses on understanding the different dynamics of mixing that occur from the inclusion of a solid obstruction to the classical RTI. This will be achieved through a

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Fig. 1.1 Diagram showing the tank setup. The size of the opening is indicated by $γL$. 

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The RTI grows from perturbations in a density gradient, $\nabla \rho$, when it is accelerated by a pressure gradient, $\nabla p$, acting in the opposite direction such that $\nabla p \cdot \nabla \rho < 0$ (Rayleigh, 1883; Taylor, 1950). The classical case, and that investigated in this thesis, occurs when a heavy layer of fluid of density $\rho_U$ rests on top of a lighter layer of fluid of density $\rho_L$ such that $\rho_U > \rho_L$ under the presence of gravitational acceleration $g$. A diagram showing the mechanism of growth of the RTI is shown in figure 1.2. We can see that when the density interface is perturbed, baroclinic vorticity, $\omega$, is generated on the interface between the two fluids due to a misalignment of pressure and density gradients. This is highlighted in the inviscid, variable density vorticity equation (derived by taking the curl of the momentum equation)

$$\frac{D\omega}{dt} - (\omega \cdot \nabla) u = -\frac{1}{\rho^2} \nabla \rho \times \nabla \rho,$$  \hspace{1cm} (1.1)
where $\omega$ is the vorticity, $u$ the velocity, $\rho$ the density, $p$ the pressure field and the $\nabla \rho \times \nabla p$ is the baroclinic term. Whilst the vorticity is originally located on the interface due to generation by the $\nabla \rho \times \nabla p$ term, in miscible fluids the region of large density gradients can grow, increasing the size of the vorticity generating region and, with it, reducing the $\nabla \rho \times \nabla p$ term.

Initial perturbations on the interface between these two fluids grow rapidly and ultimately mix the two layers together. Youngs (1984) identified three key regimes in the growth of the instability. In the first regime, initially investigated by Rayleigh (1900) and later by Taylor (1950), the instability grows exponentially. This can be shown by considering two layers of fluid of infinite extent with an interface perturbed by some small height as given by

$$z_0 = \eta \cos(kx),$$

(1.2)

where $z_0$ is the height of the initial perturbation at $x$, $\eta$ is the maximum amplitude and $k$ is the wavenumber of the applied perturbation. Following Chandrasekhar (1961), for an inviscid fluid, the amplitude of this interface is governed by

$$\ddot{\eta}(t) = n^2(k)\eta(t),$$

(1.3)

with

$$n^2 = k \left( g \frac{\rho_U - \rho_L}{\rho_U + \rho_L} - \frac{k^2 \sigma}{\rho_U - \rho_L} \right),$$

(1.4)

where $\sigma$ is the surface tension between the interfaces. The solution for two fluids initially at rest is

$$\eta(t) = \eta(0) \cosh(nt).$$

(1.5)

We see that for the case $\sigma = 0$, $g > 0$ and $\rho_U > \rho_L$, $n$ is real and the interface grows exponentially. If $g < 0$, then $n$ is imaginary and we recover stable gravity waves on the interface. The effect of surface tension is to stabilise the interface, such that perturbations shorter than a critical wavelength,

$$\lambda_c = \sqrt{\frac{\sigma}{g(\rho_U - \rho_L)}},$$

(1.6)

are stabilised. We can see that, when surface tension is included, and by differentiating equation (1.4) with respect to $k$, the dominant mode of growth is given by

$$\lambda_m = \sqrt{3}\lambda_c.$$

(1.7)
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By including kinematic viscosity, $\nu$, Youngs (1984) found an approximate form for the dominant growth rate,

$$\lambda_m \approx 4\pi \left( \frac{\nu^2 \rho_U + \rho_L}{g \rho_U - \rho_L} \right)^{1/3}.$$  

(1.8)

After the very earliest stages of growth, when the amplitude of the perturbation has grown to be in the range $(0.1 - 0.4) \lambda_m$, it was observed that the linear theory overestimates the growth of the instability (Sharp, 1984). In this second regime, the exponential growth is succeeded by the power law time dependency of the weakly non-linear regime. In this stage the longer wavelength perturbations grow fastest, believed to be caused by a non-linear enhancement and interaction of higher order modes (Abarzhi, 2010). It was believed that memory of the initial conditions was lost at this stage, however, recent results seem to suggest that this is not the case, with, in some cases, the influence of the initial condition existing throughout the mixing (Dalziel et al., 1999; Mueschke et al., 2006).

The third stage of growth was predicted by Youngs (1984) to be quadratic in time. In this final stage, assuming knowledge of the initial conditions has been forgotten and viscosity is not important, the only length-scale in the problem is $gt^2$. These assumptions allowed Youngs (1984) to derive a self-similar relationship for the penetration of light fluid into dense, giving the height of the mixing region (turbulent mixing zone)

$$h = \alpha Agt^2,$$

(1.9)

where $\alpha$ is a constant and $A$ is the Atwood number,

$$A(t) \equiv \frac{\rho_U(t) - \rho_L(t)}{\rho_U(t) + \rho_L(t)}.$$  

(1.10)

The Atwood number is an important non-dimensional number that characterises the growth of the RTI. The initial Atwood number $A(t = 0)$ will be known as $A_0$ and is often the primary Atwood number used when describing the setup of most cases. For large density differences, such that $A_0 > 0.5$, the heavy fluid forms sharp spikes as it penetrates into the light fluid. Conversely, the light fluid forms blunt bubbles as it rises into the heavy fluid (Andrews and Dalziel, 2010). For small density differences, $A_0 \lesssim 0.1$, in a fluid that may be considered Boussinesq (i.e. where differences in inertia are negligible but gravity is sufficiently strong to make the specific weight non-negligible), the instability is symmetric with the spikes and bubbles from each layer appearing similarly blunt, and ‘mushroom’ shaped, like that seen in figure 1.3. Youngs’ prediction of quadratic growth was confirmed experimentally by Read
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Fig. 1.3 The experimental growth at a Rayleigh-Taylor unstable interface growing from a perturbation caused by the wake of a steel barrier being removed at the start of a solid barrier experiment.

(1984), finding $\alpha \approx 0.07$. Rearranging equation (1.9) we have that the time scale of turbulent mixing by the RTI is $\tau_T = \sqrt{H/Ag}$, where $H$ is the height of the domain. This enables us to define the non-dimensional time $\tau = \sqrt{Ag/\dot{H}t}$.

1.2.1 Experimental investigation

The first experimental investigations undertaken to understand the RTI were by Rayleigh (1883). In his experiment a layer of warm buoyant salty water was suspended by a porous membrane above cold fresh water. The membrane limited the heat exchange between the two layers such that the majority of heat was lost to the atmosphere. When sufficiently cooled (dense), the upper layer flowed through the membrane into the lower layer in thin vertical fingers. These fingers, Rayleigh believed, were the result of baroclinically driven instability growth of the RTI. However, he had inadvertently discovered a double diffusive instability known today as salt fingering (Schmitt, 1995).

The earliest experimental work to accurately capture the RTI was done by Lewis (1950), in an attempt to verify the model suggested by Taylor (1950). In these experiments, small 0.1 m containers with stable stratifications of water were accelerated vertically downwards using air cannons. The apparatus only allowed early two-dimensional growth to be measured, but this was sufficient to confirm the work of Taylor.

The RTI was not investigated again for another 30 years until the development of the rocket-rig experiments by Read (1984). These experiments used solid fuel rockets to accelerate tanks filled with light fluid over heavy vertically downwards. Typically, the fluids were immiscible with a large Atwood number, $A > 0.2$. The very rapid acceleration, up to 50 g, created an unstable Rayleigh-Taylor (RT) interface that was able to grow three-dimensionally. However,
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the rapid acceleration meant observations were difficult, short and limited to high Atwood numbers. These experiments found $\alpha = 0.07$.

The desire to investigate small Atwood number RTI lead Andrews and Spalding (1990) to develop an overturning tank, rotating a stable stratification of fluid by 180°, and thus placing the heavy fluid above the light. However, the tank needed to be narrow to prevent the interface from becoming sloped during overturning. This resulted in limiting the RTI to just two dimensions. The finite time required to rotate the tank, and the inviscid response to overturning, resulted in a broad initial mixing region which hid the early growth. The variable nature of the rotation also introduced several small perturbations that limited the repeatability of the data.

At a similar time the removable barrier experiments of Linden and Redondo (1991) were developed to investigate low Atwood number RT growth. The experiments involved separating a heavy layer of fluid above a lighter layer using a removal aluminium barrier. At the start of the experiment the barrier was removed and the two layers were able to mix through RTI. This experimental setup is similar to the one used in the thesis with modifications made to the tank and barrier.

The simplicity of this setup comes with significant drawbacks. These will be discussed in further detail in section 2.2. The two most significant drawbacks are the finite time taken to withdraw the barrier and the perturbation its removal produces. Viscous boundary layers in the upper and lower layers, produced by the movement of the barrier, leave behind a wake with a strong regular two-dimensional perturbation. The mechanical peeling of these boundary layers as the barrier is removed from the tank leaves behind strong vortices that propagate vertically away from the barrier. Despite this, the initial two-dimensional perturbation quickly transitions to three dimensions and the growth appears to approach that of equation (1.9), with Linden and Redondo (1991) finding $\alpha = 0.07$, later revised to $\alpha = 0.044$ after accounting for long wave disturbance (Linden et al., 1994).

The viscous wake and mechanical peeling behaviour was addressed by Dalziel (1993) using a composite barrier comprised of two plates wrapped in nylon fabric. When the nylon sheets were removed, the plates were removed concurrently, at half the speed. This confined the shear to be between the plates and the nylon, leaving the fluid unaffected and effectively eliminating the viscous boundary layers. However, the increased thickness of the composite barrier resulted in a larger void being left which was filled asymmetrically by upper layer fluid. This resulted in an inviscid method for generating a two-dimensional vortex sheet.

The removal of a finite volume of fluid, caused by the removal of the barrier, produces a strong jet that propagates down the side of the tank on which the barrier was first opened. This is due to the asymmetrical filling of the volume left by the barrier with fluid from the upper layer (Dalziel et al., 1999). Mitigation of this effect was attempted by Davies Wykes
and Dalziel (2014) by inflating a bladder at the bottom of the tank as the barrier was removed. Whilst they succeeded in reversing the direction of the jet the complexity involved with timing the filling of the bladder resulted in larger errors than were caused by the initial jet.

The advantages of a statistically steady RT experiment saw Snider and Andrews (1994) develop the water tunnel experiment, where a stream of cold (dense) water is brought into contact with a warm (light) stream beneath it. The two streams flow off the end of a splitter plate at the same speed, such that a RT mixing zone grows downstream according to

\[ h = \alpha Ag[(x - x_0)/U]^2, \]

with a virtual origin, \( x_0 \), upstream of the splitter plate and \( U \) the speed of the laminar flow. Snider and Andrews (1994) found \( \alpha = 0.07 \). These experiments showed that, outside the mixing region, the flow was unchanged and remained at rest in a frame moving at speed \( U \). These experiments were continued by Ramaprabhu and Andrews (2004) and Mueschke et al. (2009), though in both cases the density difference was created by varying concentrations of salt rather than temperature differences.

Recent experiments performed by Tsiklashvili et al. (2012) begin with in an unstable stratification of paramagnetic salts that are contained by magnetic fields. When the electromagnet is switched off at the start of the experiment the fluids are able to mix through the RTI. This experimental setup allowed Tsiklashvili et al. (2012) to control initial conditions more carefully, where they found \( 0.07 < \alpha < 0.16 \) depending on the initial conditions used.

In her thesis Davies Wykes (2014) conducted experiments in which two stably stratified layers, with an unstable density difference at their interface, were initially separated by a solid steel barrier. This barrier was withdrawn half way at the start of each experiment, allowing the two layers to mix. Initially the mixing region developed normally in the opening. Fluid was observed to flow from above and below the barrier into the mixing region, forming an oscillating interface that grows due to the RTI. At later times Davies Wykes (2014) observed that a large-scale circulation was established in each of the layers. The late time development was very similar to that seen in other stratified experiments when the barrier was fully withdrawn. By measuring the final density profile it was observed that the central region was more stratified than that for an experiment where the barrier was fully withdrawn, however, there had been greater mixing in the outer region.

1.2.2 Numerical work

As computing power has developed and become more readily accessible, numerical simulations have become an increasingly useful tool in understanding the RTI, particularly in scenarios that
are not as easily attainable in laboratory experiments. The earliest numerical simulations of
the RTI were conducted by Youngs (1984), in which he predicted the quadratic growth of the
mixing region at late times.

As the resolution of simulations increased with time, there became increasing concern on the
regularly lowering value of $\alpha$ found in simulations, $0.01 < \alpha < 0.07$ compared to the reasonably
constant value of $\alpha \approx 0.07$ found in experiments. To address these mounting concerns an
international collaboration was established, the ‘Alpha Group’ (Dimonte et al., 2004). The
group ran a series of well-defined test scenarios using a large number of numerical solvers to
try to pin down the value of $\alpha$. The results were consistent, finding $\alpha = 0.0256 \pm 0.003$ for the
majority of simulations and confirming that the variations in $\alpha$ were not algorithmic.

Two possible explanations have been proposed for the discrepancy between the experimental
and numerical value of $\alpha$. The first is due to a dependence on the initial conditions. In
experiments this can be quite complicated and difficult to measure, with knowledge of the
largest mode, of order the size of the tank, ever present throughout the experiment (Dalziel,
1993; Snider and Andrews, 1994). In contrast, simulations are usually initialised with small-
scale random noise. Olson and Jacobs (2009) found smaller values of $\alpha$ when experiments
were initiated with complex small-scale initial conditions similar to what was typically used in
simulations. Similarly, Dalziel et al. (1999) found that when simulations were initiated with
similar initial conditions to removable barrier experiments the value of $\alpha$ for the simulations
increased such that there was a much better agreement between experimental and numerical
estimates.

The second possible explanation is due to a difference in the Schmidt number, $Sc = \nu/D$, where $\nu$
the kinematic viscosity and $D$ is the mass diffusivity. Experiments typically have $Sc \sim O(10^3)$,
whereas many simulations have $Sc \sim O(1)$, thus diffusion will play a much more
significant role in smoothing out density differences in the numerics. This effect varies with
the size of the Reynolds number, $Re = uL/\nu$, where $u$ and $L$ are the characteristic velocity and
length scale respectively. With a low Reynolds number, a high Schmidt number will reduce
molecular mixing, whereas at high Reynolds number the effect of the Schmidt number is
believed to be minor due to the generation of small scales by turbulent mixing.

When attempting to simulate the growth of the RTI, accurately resolving all the scales is
incredibly difficult. As the instability grows, the Reynolds number increases with the largest
structures in the flow, whilst the length scale of the smallest eddy decreases. At early times in
simulations these scales become inadequately resolved. Direct Numerical Simulations (DNS)
try to resolve all of the scales, but with this vast range in scales makes these simulations
prohibitively expensive for most researchers.
From the desire to reduce computational cost and increase algorithmic efficiency, a large body of research has concentrated on understanding the effects of under-resolving the small scales when attempting to simulate RTI. These range from local eddy-viscosity models (Smagorinsky, 1963) to models with no explicit small scale modelling as in Implicit Large Eddy Simulations (ILES) (Margolin et al., 2006). The lack of explicit small scale modelling in ILES results in highly efficient computational calculations, and, in certain applications, can produce accurate results (Lawrie and Dalziel, 2011; Ramaprabhu et al., 2013).

1.3 Mixing and mixing efficiency

Whenever there are concentration gradients in a flow, diffusion will act to reduce them. By introducing turbulence this process can be enhanced. Turbulent motion stretches concentration interfaces, increasing the area over which diffusion acts. For typical density differences and length scales of the setups considered in this thesis the timescale of laminar diffusion scales as $T_D \sim H^2/D \sim 10^9$ s, where $H$ is the height of the domain and $D$ is the diffusion coefficient. In contrast, turbulent diffusion for the RTI scales as $T_T \sim \sqrt{H/(Ag)} \sim 10$ s. Thus, turbulent diffusion is a significantly faster process than laminar diffusion.

Winters et al. (1995) considered the problem where mixing is defined as a change in the probability density function (pdf) by molecular mixing in a closed system, one where there are no heat or mass losses across the boundaries. This formalism assumes a Boussinesq incompressible fluid with a linear equation of state, due to temperature changes from dissipation and latent heat being negligible. It should be noted, however, that a linear equation of state is not always an appropriate assumption, particularly when applied outside the laboratory environment such as on oceanic scales (Tailleux, 2009).

A useful measure to aid the understanding of turbulent mixing is the mixing efficiency. Mixing efficiency attempts to identify the energy used in irreversible mixing versus that which is dissipated by viscosity. This thesis will follow the definition of Winters et al. (1995), by partitioning gravitational potential energy,

$$E_p = g \int_V z \rho \, dV, \quad (1.12)$$

into that which is able to do work and a background potential energy,

$$E_b = g \int_V z \rho_{sort} \, dV. \quad (1.13)$$
Here $\rho_{\text{sort}}$ is the sorted density profile that would occur if every fluid particle were allowed to rise or fall adiabatically (i.e. without heat or mass transfer between the system and its surroundings) until the system were in its lowest potential energy state. The available potential energy, $E_a$, is energy that would be released if the system were able to be sorted adiabatically

$$E_a = E_p - E_b = g \int \frac{1}{V} z(\rho - \rho_{\text{sort}}) \, dV. \quad (1.14)$$

The kinetic energy, $E_k$, is also energy available for mixing, such that the total energy available for mixing at any time is

$$E_T = E_a + E_k = \int \frac{1}{V} g z(\rho - \rho_{\text{sort}}) + \frac{\rho |\mathbf{u}|^2}{2} \, dV. \quad (1.15)$$

A commonly used definition for the mixing efficiency is that of a cumulative mixing efficiency, which is the energy difference between the initial and final state

$$\eta = \frac{E_b(t_{\text{final}}) - E_b(t_{\text{initial}})}{E_T(t_{\text{final}}) - E_T(t_{\text{initial}})}. \quad (1.16)$$

If we assume that the system both starts and finishes at rest, then this simplifies to

$$\eta = \frac{E_b(t_{\text{final}}) - E_b(t_{\text{initial}})}{E_a(t_{\text{final}}) - E_a(t_{\text{initial}})}. \quad (1.17)$$

This definition is commonly used when referring to RTI mixing efficiencies (Dalziel et al., 2008; Davies Wykes and Dalziel, 2014) and will be used throughout this thesis.

### 1.4 Buoyancy exchange flows

The introduction of an obstruction in the development of the RTI has connections to the work done in understanding the ventilation in buildings. Historically, buildings were created on an ad hoc basis, growing organically to their occupant’s needs. The lack of precision building methods and materials resulted in buildings which were essentially leaky. The pollutants created by the inhabitants, from fires and respiration for example, are naturally dispersed from the building through temperature exchange or the pressure of wind against the building. It was only in the latter half of the last century that buildings were designed to be spaces that are truly sealed from the outdoors, efficient at conserving their heat. This resulted in buildings
Introduction and previous work

becoming poorly ventilated, such that pollutants are now contained inside buildings and need to be actively removed.

The simplest method of exchange is through the opening of windows, however, this may not always be appropriate and can be costly in terms of heat loss in winter. The other main method used in warmer climates is to use an air conditioning (or comfort cooling) unit that exchanges the interior air with filtered temperature controlled air drawn from outside. Such units are extremely costly to run and in many places can result in extreme temperature contrasts within the buildings that are uncomfortable for inhabitants.

As urban areas become more densely populated, the vertical space occupied by buildings becomes greater. This results in a large number of rooms and spaces that are all vertically connected, whether this be via a central atrium or stair well. As a result there can be significant pressure variations throughout buildings (Peppes et al., 2001). Situations can arise where there are large density differences between storeys, such as in building fires (Karlsson and Quintiere, 1999). It is these situations, where there is a vertical exchange through a horizontal opening, that are most relevant to the research presented in this thesis.

The first mathematical investigation of buoyancy driven flow through a horizontal opening was by Brown (1962). He used two large reservoirs of air at different temperatures such that the coolest air was above the warmest. The two reservoirs were connected via a horizontal square opening with side lengths $D$ and thickness $L$. Brown’s experiments considered the range $0.0825 < L/D < 0.66$, with one of the major results being that the mass transfer rate increased with $L/D$. However, Brown’s experimental setup provided no insight into the mechanisms of exchange between the two reservoirs.

Epstein (1988) used different concentrations of brine to create a buoyancy gradient. This has the advantage, over using heat, that the experimental area does not need to be lined with insulation, allowing the exchange area to be more easily visualised. Epstein’s experiments consisted of two large reservoirs connected by a small circular horizontal opening at their centre with thickness $L$ and diameter $D$, both much smaller than the size of the reservoirs. A range of different exchange sizes were considered, $0.01 < L/D < 10$, with four different flow regimes identified as the ratio increased.

The experiments presented in this thesis consider cases with $0.005 < L/D < 0.05$, which is within the range of Epstein’s so called oscillatory exchange with very small $L/D$ and $L \to 0$. Epstein observed the growth of what he described as upward (and downward) fingers or plumes of fresh (and saltwater) which periodically broke from the surface.

Epstein then used theory from Taylor (1950) for the 2D growth of RTI to develop his own model for the exchange. Epstein, with his circular opening, assumed an initial one-dimensional
1.5 Filling box

With the surface of the interface, \( \eta \), growing as

\[
\eta = \eta_0 e^{nt} \cos \left( \frac{\pi r}{D} \right),
\]

(1.18)

where \( r \) is the radial distance from the centre, \( t \) the time from the initial disturbance and the growth rate \( n \) is

\[
n = \sqrt{\frac{\pi gA}{D}},
\]

(1.19)

where \( A \) is the Atwood number across the opening. Epstein used observations to deduce that the growth on the interface breaks off and disperses within the rest of the layer when the growth has reached a size comparable to the size of the opening,

\[
\eta = D \cos \left( \frac{\pi r}{D} \right),
\]

(1.20)

with the volume of the finger given by

\[
V = \int_0^D \pi r^2 \, d\eta = \left( 1 - \frac{2}{\pi} \right) D^3.
\]

(1.21)

The time required to reach the break-off height is

\[
t_b = \frac{1}{n} \ln \left( \frac{D}{\eta_0} \right).
\]

(1.22)

Then, using experimental results of Lewis (1950), Epstein showed that the wave-like nature of the interface transitioned to finger-like protrusions when \( \ln(\eta/\eta_0) \sim 5 \). Epstein used his observation that \( \eta \sim D \) at break off to calculate an exchange flux through the opening,

\[
Q = \frac{V}{2t_b} = 0.028 \sqrt{D^3 gA},
\]

(1.23)

which was only slightly below the experimental value measured.

1.5 Filling box

As will be seen later, the dynamics from introducing an obstruction establishes two buoyant plumes that transport fluid from the interface vertically to upper and lower boundaries. Once at these boundaries, the plumes propagate horizontally, mix with the ambient and overturn when
they interact with the other vertical sidewall. This motion is comparable with the dynamics studied in ‘filling boxes’, which typically consider buoyant plumes in a contained box.

Baines and Turner (1969) were the first to introduce the filling-box model that examined the stratification that developed over time from a single plume in a closed cylinder. They found that a plume, from a localised buoyancy source at the bottom of the domain, rose to the top and spread laterally. This created a buoyant layer that was continuously fed by buoyant fluid from the base. The influx of buoyant fluid caused the layer to deepen and expand downwards towards the bottom.

Their model worked well for cases where the domain was much wider than it was tall, however, for narrower boxes their model was less useful. The issue was that their model was unable to take account of a plume colliding with the vertical sidewalls, overturning and mixing with the ambient. Baines and Turner (1969) were able to demonstrate that there was negligible overturning when $H/R < 1$, with $H$ the height of the domain and $R$ the radius. This result was verified by Manins (1979) who derived a full analytic solution for the motion in the box exterior to the plume.

In his thesis, Barnett (1992) studied domains which had height much larger than their width, $H/R > 1$. Barnett found that there is a critical balance between the upflow of the plume and the downflow. For large enough aspect ratios the plume is prevented from reaching the top of the domain by shear induced turbulence between it and the downflow.

Kaye and Hunt (2007) sought to quantify the extent of overturning in a cylindrical box when the horizontal spreading along the upper boundary from a plume collides with the vertical side wall of the domain. By modelling the overturning plume as a wall fountain, they were able to derive a model for the extent of vertical overturning, $h_O$, as a function of the aspect ratio, $R/H$, and confirmed this experimentally. They found that for $R/H < 0.25$ there was no overturning, the plume being blocked. For $0.25 < R/H < 0.66$ the overturning region scaled as $h_O/H \approx 0.33 (R/H)^{-1/3}$, which they called the ‘rolling mode’. Then for $R/H > 0.66$ the overturning region was a constant $h_O/H \approx 0.38$ and this was called the ‘slumping mode’. In the rolling mode the flow rolled over on itself, engulfing fluid as it fell back. In the slumping mode there was little to no entrainment of fluid but waves were observed on the interface.

1.6 Thesis outline

This thesis aims to introduce and explain the new dynamics produced from the introduction of an obstruction between two layers of fluid which are RT unstable. This will be achieved by using an innovative experimental setup which accurately captures both the density and velocity fields in 3D for the full depth of the tank. These data will be combined with computational
simulations to attempt to bed these new obstructed dynamics within the well developed RTI and stratified turbulence fields. In addition to this, a hierarchy of models will be developed and presented that accurately predict the density change with time for a range of openings.

The structure of the thesis is as follows. The experimental and numerical methods are discussed in chapters 2 and 3 respectively. In chapter 4 a time series of experimental LIF data for a classical unobstructed and obstructed domain are presented to introduce the reader to the qualitative differences between the two cases. After this, a hierarchy of improved diagnostic methods are derived in chapter 5, which improve the quality and accuracy of the LIF data.

A domain where there is only one opening, so called ‘singly connected’, is presented in chapter 6. Here experimental data will be supplemented with numerical data to contrast obstructed cases against classical unobstructed results. Thereafter domains where there are two openings connecting the layers, so called ‘multiply connected’, will be presented in chapter 7. Finally, conclusions and proposed future research are presented in chapter 8.
Chapter 2

Experimental Methods

2.1 Basic setup

The tank used for experiments discussed throughout was constructed from Perspex with working dimensions 0.5 m × 0.4 m × 0.2 m. It consists of an upper and lower layer separated by a removable solid steel barrier (RB). The tank and barrier are similar to that first used by Linden and Redondo (1991), that consisted of a 1.5 mm aluminium barrier. This was modified by Dalziel et al. (1999) to be replaced by a larger composite barrier, reducing the shear caused by the barrier’s removal at the start of the experiment. Later Davies Wykes and Dalziel (2014) would remove the composite barrier and replace it with a 2 mm stainless steel barrier, the same as is used in this thesis.

The tank is shown filled with fluid, with the lower layer dyed and the RB partially withdrawn in figure 2.1. The two layers of fluid were filled from two 200 L reservoirs of salt solutions of NaNO$_3$ and NaCl. Due to the different rates that the refractive index of each of these solutions changes with concentration, it is possible to have different densities at the same refractive index. As the refractive index of NaNO$_3$ solutions changes more slowly with increasing concentration than for NaCl solutions, for the same refractive index an NaNO$_3$ solution is heavier than a NaCl solution of the same concentration. Thus, NaNO$_3$ solution is used to fill the upper layer.

The two reservoirs are covered with fitted lids and are allowed to rest until they are in approximate thermal equilibrium with the laboratory environment (typically 24 hours). The additional benefit of allowing the reservoirs to rest is that any gas released from dissolving the salts in water is able to escape the solution. This is desirable as bubbles can reduce the quality of images in a number of ways. They frequently attach themselves to the internal front wall of the tank, distorting and partially obstructing the motion that is recorded by the cameras. If the concentration of bubbles is high enough they can make the image appear cloudy, or may be mistaken for buoyant particles. When conducting Particle Image Velocimetry (PIV) this
Experimental Methods

Fig. 2.1 The Perspex tank used in experiments with the stainless steel barrier left partially in obstruction. The lower layer is dyed with fluorescein and food dye to make it opaque. The 3D growth of the RTI instability is clearly seen, as are the initial stages of circulation in the upper layer, with undyed fluid seen to be moving off the edge of the barrier into the dyed mixing region.

can cause errors in the velocity field. The use of these large covered reservoirs throughout a series of experiments ensures that they are conducted at the same Atwood number. The density of each layer was measured at the start of each experiment by taking a sample of fluid and passing it through a density meter (Anton Paar DMA 5000), which has a precision of \( \pm 1 \times 10^{-6} \) g cm\(^{-3}\).

The tank’s removable steel barrier (RB) is 2 mm thick and fits into a machined groove 2.5 mm wide in the centre of the tank. At the start of each experiment the RB is removed by an electric motor which accelerates it rapidly to a constant speed of 0.08 m s\(^{-1}\) in under 0.1 s (i.e. by the time it has moved 4 mm, negligible compared to the full withdrawal width). The barrier fits snugly into the machined groove around the tank. As such there is negligible leakage between the layers before the start of the experiment. At the side of the tank from which the barrier is removed, two neoprene wedges tightly hold the barrier in place. When sufficiently wet these wedges are effective at sealing the tank and there is negligible leakage. The removal of the barrier has a significant impact upon the initial conditions and this will be discussed in section 2.2.

The experiments presented in this thesis regard the effects of an obstruction on the growth of the RTI. In preliminary experiments, the obstruction was created by not fully withdrawing the RB. This was done to acquire qualitative results and test whether the dynamics were interesting enough to warrant further investigation. Creating the obstruction in this way has obvious advantages: It is simple and enables a wide range of obstructions to be tested easily. However, the majority of the experimental techniques available use planar illumination from below. Thus,
2.1 Basic setup

Fig. 2.2 Schematic diagram for the singly-connected domain after the RB has been withdrawn, with the width of the opening parametrised by $\gamma$.

having an opaque barrier in the middle of the domain restricts the view of the upper layer too severely for the partially withdrawn RB to be used effectively in further investigation.

To create a transparent obstruction, a fixed barrier (FB), constructed from a 2 mm polycarbonate sheet, is secured to the tank just above the RB at the start of the experiment. A number of different size FBs were made to allow alterations to the size of the opening. Each FB was secured to within 1 mm of the RB. Plastic tubing was attached to the three sides where the FB made contact with the tank walls and the tight fit held it securely in place. So long as the FB was carefully secured, there was no leakage between the layers and the only exchange of fluid was through the opening. In practice, the small 1 mm gap between the RB and FB traps a small volume of upper layer fluid, such that when the RB is removed this trapped fluid mixes with lower layer fluid beneath the FB. This effect is discussed in section 2.2.5.

2.1.1 Singly connected

Two main scenarios were considered. The first was the singly-connected domain as seen in figure 2.2, in which there is only one opening between the two layers. For this case, the width of the opening is parametrised by $\gamma$, such that, when $\gamma = 1$, the opening spans the length of the tank and we return to the classical unobstructed RT problem. To create the obstruction at the
start of the experiment the FB is secured above the RB and pushed flush against the wall the RB is to be withdrawn through. After allowing the upper layer to become quiescent, the RB is removed beneath the FB and the two layers are able to interact immediately. The effect of removing the barrier on the initial conditions is discussed in section 2.2.

2.1.2 Multiply connected

In the second scenario considered, the obstruction is secured in the centre of the domain, as seen in figure 2.3, such that there are now two potential paths between each layer, the so called multiply-connected domain. The width of the openings are parametrised by $\gamma_1$ and $\gamma_2$ for the left and right opening, respectively. This scenario is discussed in more detail in chapter 7 and was studied as it increases the variety of modes available for mixing. The reflectional symmetry of the singly-connected flow is now broken by the bifurcation of the obstruction. Now the flow attains a rotational symmetry about the obstruction as fluid can pass through either opening. This multiply-connected case more closely resembles scenarios where a RT unstable fluid moves around a solid plate-like object.

To create the obstruction the same polycarbonate sheets used in the singly connected case are used here, except now the plastic tubing which was pressed as a seal against the side walls
has been removed on the side the RB will be withdrawn. The majority of experiments consider the case where $\gamma_1 = \gamma_2$, however, a number of experiments consider the alternate case with $\gamma_1 \neq \gamma_2$, the results of which are discussed in section 7.6.

### 2.2 Effect of the removing the removable barrier (RB)

The impact of removing the removable barrier (RB) is significant. In her thesis, Davies Wykes (2014) calculated the energetics of each of the contributions to the initial conditions resulting from the removal of the RB. Where appropriate, this energetic framework is used here, however, the introduction of the FB alters the picture somewhat. The overall effect of removing the RB is to break the symmetry ideally desired in the initial conditions. The mechanisms by which it does so are discussed in the following subsections.

#### 2.2.1 The dropping of the upper layer

When the RB is removed the upper layer drops down to fill the volume left by the RB (Dalziel et al., 1999). As used by Dalziel et al. (1999), a floating lid sits on top of the tank to ensure that this motion is uniform across the length of the tank. Following Davies Wykes (2014), the largest energetic contribution resulting from this effect is due to reduction in potential energy (PE),

$$\Delta PE = \rho_u \frac{H W L}{2} \times g \times \delta,$$

(2.1)

where $\rho_u$ is the density of the upper layer, $H$ the height, $W$ the width, $L$ the length of the layer, $g$ the gravitational acceleration and $\delta$ the thickness of the removable steel barrier. This change in potential energy is exactly matched by the work from the hydrostatic pressure from the upper layer on the RB as it is removed,

$$EB = \text{hydrostatic pressure} \times \text{area} \times \text{distance removed}$$

(2.2)

$$= \rho_u \frac{H}{2} g \times \delta W \times L$$

(2.3)

$$= \Delta PE.$$  

(2.4)

Note that this is independent of the speed of removal of the RB.
2.2.2 Finite volume removal

As first discussed by Dalziel et al. (1999), when attempting to understand the effect of removing the much larger volume left by the composite barrier, the removal of the RB results in non-hydrostratic pressure fluctuations at the end of the barrier owing to the removal of the volume. This results in a Kutta condition (i.e. that the circulation around a sharp body moving in a fluid will produce a stagnation point at its trailing edge) and a separation region at the trailing edge of the RB, resulting in a jet propagating down the left-hand side wall.

As shown by Dalziel et al. (1999) it is possible to model this condition as an inviscid response, with a stream function

\[ \psi(x, z) = \frac{\psi_0 u_b L \delta}{H} \sum_{n=1}^{N} a_n \sin \left( \frac{n \pi x}{L} \right) \frac{\sinh \left( \frac{n \pi H}{2L} \left( 1 - \frac{2|z|}{l} \right) \right)}{\sinh \left( \frac{n \pi H}{2L} \right)} \],

(2.5)

where \( u_b \) is the constant speed the RB is withdrawn at, \( \psi_0 \) is an \( O(1) \) dimensionless number dependent on the Reynolds number associated with the RB, \( z \) is the vertical distance from the RB and the constants \( a_n \) are determined experimentally. From this it is possible to calculate a kinetic energy,

\[ E_k = \frac{W \pi \rho}{2} \left( \frac{\psi_0 u_b L \delta}{H} \right)^2 \sum_{n=1}^{N} a_n^2 \coth \left( \frac{n \pi H}{2L} \right). \]

(2.6)

Using coefficients calculated by Dalziel et al. (1999) and experimental values appropriate for this thesis (with \( \rho = 1025 \text{ kg m}^{-3} \)), we find \( E_k = 5.25 \times 10^{-7} \text{ J} \). Note this value is \( O(10^6) \) times smaller than the available potential energy at the start of a typical experiment.

2.2.3 Viscous boundary layer

As the RB is removed, viscous boundary layers form above and below it. At the point of removal of the RB from the tank, these boundary layers are peeled off, depositing two strong vortices either side of the line at which the RB exits.

The kinetic energy contribution from these viscous layers can be estimated by assuming that the Rayleigh layers that form above and below through the diffusion of viscosity have a profile

\[ u(z, t) = u_b \text{erf} \left( \frac{|z|}{2 \sqrt{\nu t}} \right), \]

(2.7)
2.2 Effect of the removing the removable barrier (RB)

Fig. 2.4 Adapted from Davies Wykes (2014), the ratio of the barrier kinetic energy against the initial available potential energy, $E_k/E_A$, is plotted against (a) time to remove the barrier, $t_b$, with $A = 5 \times 10^{-3}$ and (b) the Atwood number with $t_b = 5$ s.

where $t$ is the time from when the RB first began moving and $\nu$ is the kinematic viscosity. Ignoring the effects at the ends of the RB, the total kinetic input is

$$E_k = 2\nu \overline{\rho} LWu_b \int_0^{t_1} \frac{\partial u}{\partial z} |_{z=0} dt,$$

$$= \frac{8}{3} \sqrt{\frac{\nu}{\pi}} W \overline{\rho} (u_b L)^{3/2},$$

where $W$ is the RB width (equal to the tank width) and $t_1 = L_b/u_b$ is the time to withdraw the barrier fully. This kinetic energy from the viscous boundary layer exists in both the wake and the vortex stripped from the barrier. Following Davies Wykes (2014), this value is compared to the available potential energy stored in a homogeneous upper layer,

$$E_A = g \int_V z(\rho - \hat{\rho}) dV = \frac{gH^2 LW \Delta \rho}{4},$$

giving the following ratio

$$\frac{E_k}{E_A} = \frac{16}{3} \sqrt{\frac{\nu L_b}{\pi} \frac{u_b^{3/2}}{gH^2 A}}.$$  

Figure 2.4 shows this ratio plotted against variations in the barrier removal time and Atwood number. We can see from figure 2.4a that the viscous boundary layer makes the largest energetic contribution when the barrier removal time is below 4 s. Additionally, we can see from figure 2.4b that the energy ratio is largest for $A < 5 \times 10^{-3}$. Only for very small Atwood numbers would the impact of removing the barrier produce a significant contribution to the energy.
2.2.4 Barrier wake

As the RB is withdrawn, it produces a wake with a preferred wavelength of around 20 mm, essentially creating a regular 2D initial perturbation to the interface (in the $x$, $z$ plane) from which the RTI grows. This is clearly visible in figure 2.1. When a FB is included in the domain the RTI mixing zone in the opening induces laminar flow off the FB into the opening. As this fluid flows into the opening it forms an oscillating interface between the two layers. Whilst there may be a small amount of horizontal shear between the layers the velocity difference is small. This small magnitude of shear is unable to account for the mixing zone width seen in experiments. For typical values used in experiments, the growth of the mixing region by the RTI is an order of magnitude greater than that which could result from Kelvin-Helmholtz instabilities resulting from the shear.

2.2.5 Fixed polycarbonate barrier

The FB is secured within 1 mm of the RB. The volume trapped between the RB and FB represents 0.4 % of the upper layer depth. So if $\gamma = 0.25$, and the obstruction spans 75 % of the domain width, then 0.3 % of the volume of the upper layer is trapped between the FB and RB at the start of the experiment. Once the RB is fully removed this trapped fluid may mix fully with fluid from the lower layer. Assuming this is the case, if the trapped fluid covers an area $w$ and mixes over a depth $d$, due to the RTI, then the new mixed density $\rho_n$ in the volume $V = dw$ will be

$$
\rho_n = \frac{V_L \rho_L + V_U \rho_U}{V_L + V_U},
$$

where $V_U$ is the volume of the upper layer fluid trapped beneath the FB at the start of an experiment, and $V_L$ is the volume of lower layer fluid which mixes with the trapped upper layer fluid. Typical values are $d = 30$ mm (measured from LIF recording), $w = 300$ mm, $\rho_L = 1010$ kgm$^{-3}$ and $\rho_U = 1020$ kgm$^{-3}$. Substituting these values into equation (2.12) gives a density $\rho_n = 1010.25$ kgm$^{-3}$. This small change is assumed to be insignificant to the overall dynamics given that the fluid exchanged through the opening appears to be well mixed.

As the RB is withdrawn to the right-hand side beneath the FB, anticlockwise vorticity is created around the edge of the FB due to the viscous peeling of a boundary layer, now only occurring beneath the FB. This will temporarily limit the growth of the RTI at the edge. However, this effect is quickly forgotten as a circulation is established quickly in each layer, bringing fresh fluid from either side of the barrier, which mixes turbulently at the opposite sidewall. For the multiply connected case, the FB can now be enclosed within a closed contour. By Kelvin’s circulation theorem this induces clockwise vorticity at the edge of the second opening (such that circulation is conserved around the contour of the FB). This, combined with
the initial jet down the left hand wall, establishes a clear preference in direction for the initial exchange between the openings. This effect will be discussed further in chapter 7.

The FB has an effect on the viscous boundary layer, as discussed in section 2.2.3. For the singly-connected domain, when the RB is removed, vorticity is only deposited in one direction beneath the FB. This has little effect on the development of the flow as fluid deposited here must travel the full length of the FB before it can significantly affect the mixing. However, for the multiply connected case, the situation is more complicated. Here, vorticity of both directions is deposited at the exit. The lower clockwise vorticity is stronger than the anti-clockwise vorticity deposited in the upper layer. This is caused by viscous peeling being greater in the lower layer than the upper due to the much longer time the RB has in contact with lower layer fluid, compared with the relatively short contact time with upper layer fluid, when it passes through the second opening.

2.3 Conductivity probe

The density profile of the final state can be measured by traversing a conductivity probe through the fluid once it is quiescent. Dissolving salt in a solution releases ions. Their concentration and mobility both contribute to the conductivity that is measured by the probe. As the fluid is quiescent when it is being measured, the mobility of the ions is determined by the temperature of the solution. In all experiments, the solutions in each layer were premixed and in thermal equilibrium with the laboratory environment, which is itself temperature controlled to 20±1°C (as measured by Davies Wykes (2014)). As the two solutions from each layer mix, there is a heat released from dilution of < 1°C, well within the range of laboratory fluctuations.

The other significant thermal exchange is via evaporative cooling from the upper surface. However, as initially the upper layer is not stratified, and experiments are relatively quick to complete (from beginning filling to measuring the stratification at the end typically takes less than 20 minutes), evaporative cooling is not considered to have a significant impact on the measured stratification. Davies Wykes (2014) found an approximate expression for the density change associated with a change in temperature,

\[
\frac{\delta \rho}{\rho} = \frac{\Delta T}{10^3},
\]

where \(\delta \rho\) is the change in density \(\rho\) caused by a change in temperature \(\Delta T\). Equation (2.13) shows that a temperature change of 1 K equates to 0.1 % error in the density measured by the probe. As a result, the conductivity measured by the probe can be considered, to a good
approximation, only dependent on the concentration of ions. Using these assumptions, the conductivity can be used to measure the final density profile.

The probe is constructed of two concentric cylindrical electrodes which are separated by an insulator. The two electrodes come into contact via fluid siphoned through the centre of the probe at a flow rate of $\sim 0.3 \text{ mms}^{-1}$. The hole in the tip is very narrow, 0.3 mm diameter, and has a very large resistivity such that the conductivity is dominated by fluid passing through the tip. The probe is traversed at a constant speed of $4 \text{ mm s}^{-1}$ by a stepper motor and the conductivity is measured at a sampling frequency of 50 Hz. The probe was encased within a metal sheath and the traverse was attached to a bridge circuit. This ensures the connecting wires are as short as possible, thereby reducing noise in the data captured by the probe. Earthing the bridge circuit to the traverse ensured that interference from the mains frequency was removed.

The probe was calibrated daily against six samples; these data were checked against existing calibration data and, if within an acceptable tolerance, were added to the pre-existing calibration data set. These combined data were then used to recalculate the conductivity-density relationship, shown in figure 2.5. The relationship shown has an coefficient of determination $R^2 = 0.997$. The density of the samples were measured by a density meter (Anton Paar DMA 5000), which has a precision of $\pm 1 \times 10^{-6} \text{ g cm}^{-6}$. The cumulative calibration data in figure 2.5 have a standard deviation of $3 \times 10^{-4} \text{ g cm}^{-4}$, deemed to be sufficiently precise for the purpose of this work. The conductivity-density relation can then be used to calculate the final density profile, from the measured conductivity, to a high level of precision.

2.4 Optical Diagnostics

Optical observations are the primary experimental measurement technique used this thesis. By using a combination of fluorescent dyes and small, neutrally buoyant particles, the density and velocity fields can be measured. These techniques will be discussed in more detail later in this section. Typically these measurements are achieved by illuminating a thin planar light sheet vertically through the tank and recording the motion with a set of cameras. A schematic for the 3D laser traverse system is shown in figure 2.6. The details of this system will be discussed further in section 2.5. The motion is recorded using a Dalsa Falcon 2 8 MP camera recording at 100 fps, and which has a low fixed pattern noise and pixel response non-uniformity.

In this thesis the primary source of light was created using a Litron Nd:YAG double pulse laser, which produces visible light at 532 nm with a maximum frequency of 100 Hz and power 50 mJ. The pulses are combined through the internal optics of the laser to produce a rhombus shaped light beam as shown in figure 2.7. This beam is then passed through a secondary set of
Fig. 2.5 Cumulative conductivity probe calibration, showing all calibrations made.

Fig. 2.6 Schematic of the 3D laser traverse with camera set up.
optics which convert the beam into an hour glass shaped light sheet that is $\sim 5$ mm at its widest part (at the base and top of the tank) and $< 1$ mm at its narrowest (in the centre of the tank).

2.4.1 Light Induced Fluorescence: LIF

The technique of Light Induced Fluorescence (LIF) relies on using a fluorescent dye, a dye that absorbs light at one wavelength and then radiates it, a short time later, at another longer wavelength. Ideally, this radiation wavelength is far from the initial absorption length. The diffusivity of typical fluorescent dyes are comparable to the diffusivity of salt, with Rhodamine 6G (R6G), the dye used in the majority of the experiments, having a diffusivity in water at 25°C of $D_{R6G} = 4 \times 10^{-6}$ cm$^2$s$^{-1}$. By adding the fluorescent dye to one layer and shining a thin light sheet vertically through the tank, the dye can be used as a tracer for the fluid of the dyed layer. As the dyed fluid moves and mixes with the undyed layer, the intensity of the fluoresced light is reduced proportionally; such that the recorded intensity can be used as proxy for the density.

The light source should be chosen with a narrow wavelength band around the absorption wavelength of the dye. The most widely used, and most effective techniques use a laser of a specific frequency as the light source, hence why LIF is more commonly known as Laser Induced Fluorescence. However, it is possible to use other light sources such as an arc lamp Dalziel et al. (1999); Lawrie and Dalziel (2011), which has a large enough peak around the blue end of the visible spectrum to be effective at exciting fluorescein disodium dye.

Density calibration was achieved by mixing known quantities of R6G into the tank and then measuring the intensity change with increased concentration, see figure 2.8. We can see that for all the concentrations used here, the relationship between dye and intensity is linear, with least squares best fit shown (both with $R^2 = 0.99$). These data could be used to determine the density for each experiment, however, such data require several factors to be consistent. Most notably, the intensity of the light source is important. This light intensity is likely to change.
2.4 Optical Diagnostics

Fig. 2.8 Dye calibration plot, with accumulative ml of R6G dye added along the horizontal axis vs the mean intensity of the sample box plotted vertically (crosses), with least squares best fit for each data (solid lines).

with time, and vary based upon how long the light source has been on before an experiment. In each experiment 1 mL of dye at a concentration of $0.2 \text{ gL}^{-1}$ was added to the upper layer. When mixed the concentration of R6G in the upper layer was $10^{-5} \text{ gL}^{-1} \approx 10^{-6} \text{ wt } \%$. This concentration is well within the linear range yet large enough so that the image is as bright as possible without being saturated.

A more reliable calibration method is to utilise the initial linearity of the intensity and conduct a per experiment calibration. This was achieved by thoroughly mixing the two layers at the end of an experiment until the whole tank is homogeneous and then recording the domain when it has become quiescent. This calibration method assumes that the dye is conserved with time and is not lost or damaged throughout the duration of an experiment.

Theoretically, the calibration intensity should be half the initial dyed intensity, and any variations in the intensity of the light sheet will also be captured and removed. This assumes that the dye is conserved with time and is not lost or damaged during an experimental run. This is not always true as will be shown in section 2.6. A further assumption is that there is little to no attenuation of light by the dye itself, which, for the low concentrations of dye used in this
thesis, is true. The final calibrated intensity, $C$, is calculated as

$$C = \frac{I - I_0}{2(I_1 - I_0)}, \tag{2.14}$$

where $I$ is the experimental image intensity, $I_0$ is the background image and $I_1$ is the end calibration image. The background image is removed such that any fixed background noise from the camera is also removed. The processed image should then have the following intensity: $C = 1$ for the unmixed dyed fluid, $C = 1/2$ for any fully mixed fluid and $C = 0$ for undyed unmixed fluid.

2.4.2 Particle imaging

Small 20 µm diameter polyamide particles are seeded into the flow, as shown in figure 2.9. These particles have a density $\rho_p \simeq 1.02 \text{ g cm}^{-3}$, which results in them in being almost neutrally buoyant for the Atwood numbers considered with a settling velocity of $\mathcal{O}(10^{-4}) \text{ m s}^{-1}$. When a light sheet is used to illuminate the tank, the particles scatter light and appear as bright points. The particles are sufficiently small that their inertia is minimal and they follow the flow field accurately. Their shape and constitution ensures they are effective at scattering light, despite
the particles being 100 times smaller than the pixels. As a result of this the particles are easily recorded by a camera and tracked using a computer. For little computational cost, particle streaks can be created. These provide qualitative information on the flow structure and velocity along a particle path. Particle streaks were used in the earliest experiments to visualise the qualitative effects of an obstruction and to provide some insight into the larger scale motions.

A more computationally intensive but much more informative quantitative analysis is provided by using Particle Imaging Velocimetry (PIV). In the simplest form, this technique compares the patterns of particles between a pair of frames; a velocity can be calculated from the displacement of the patterns and the known change in time, $\Delta t$, between frames. Modern algorithms can detect displacements to a sub-pixel level and provide a dynamic range of $\mathcal{O}(10^2)$. Combining the pixel displacement information with a calibrated coordinate system, the real world dimensional velocity can be found.

### 2.4.3 Simultaneous PIV and LIF imaging

The stratified nature of the RTI means that both the density and velocity fields are equally important properties. Therefore, it is desirable to simultaneously record both pieces of information in an experiment. It is necessary to separate the particle information from the dye information, as otherwise bright collections of particles can contribute to the measured LIF intensity and thus the measured density. Similarly, movements in the flow structure of sharp dye boundaries can adversely affect the PIV calculation.
To separate the information two sets of filters need to be used. The PIV particles scatter light from the laser at 532 nm, whilst the R6G fluoresces light at a slightly longer wavelength, with a peak at 560 nm (see figure 2.10). However, a significant proportion of the light is also emitted at much longer wavelengths than the peak, as shown in figure 2.10. To only record fluoresced light, and discard the light scattered from the particles, a long-wave pass filter needs to be used for the LIF camera. A band pass filter would produce inferior (less bright) results as it would filter out the significant proportion of light emitted outside of the peak region by R6G.

For the PIV camera, a short-wave pass filter can be used. However, better results can be achieved if a band pass filter is used for the PIV camera as this filters out all light except for the specific wavelength of light scattered from the laser. This ensures that only the particles illuminated in the laser sheet are recorded, excluding particles or other objects illuminated by other light sources or background infrared radiation.

### 2.5 3D imaging: scanning PIV/LIF

Rayleigh-Taylor instability, and turbulence in general, are known to be highly three-dimensional. As such, the two-dimensionality of LIF and PIV limit the understanding that can be gained experimentally. Techniques such as shadowgraph imagery can only provide an integrated view of the full three-dimensional dynamics.

From these limitations came the desire to design and develop a 3D laser scanning system, of which a simplified schematic is shown in figure 2.6. Here, three cameras were used to capture each experiment. The central camera (Cam C) was used to record the LIF data whilst the two side cameras (Cam A and B) were used for stereo PIV, discussed in section 2.5.2. The standard optics used in 2D laser imaging are now attached to a traverse that, in one sweep, scans the full 0.2 m width of the tank, back to front, in 2.05 s. This is comparable to the timescale of classical RTI to fill the domain \( 1/\sqrt{Ag/H} = 2.25 \) s for the typical parameters used in this thesis). This creates a set of slices of the domain, separated by approximately 1 mm, from which 3D data can be acquired.

Whilst not directly involved in the initial development of this system, undertaken by S.B. Dalziel, it was first tested and used on the experiments presented in this thesis. As such, the data presented in this thesis are some of the first acquired and have been important in developing and improving the system further.
2.5 3D imaging: scanning PIV/LIF

2.5.1 Traverse

The traverse system is an in-house, custom built system, using an Igus traverse with stepper motor. This was carefully chosen such that the motion was smooth, with vibrations kept to an absolute minimum. It is also important that the acceleration and deceleration period are kept as small as possible. This maximises the number of slices through the domain that can be obtained with the same spacing.

The traverse moves continuously back and forth as the laser fires at a regular frequency of 100 Hz. Then, at each time step, a different slice is illuminated from the previous. For the setup used earlier, this produces 205 individual slices of the tank, spaced 0.975 mm apart (excluding the acceleration effects at the ends of the tank which account for 2 frames on each scan). This collection of slices can be used to produce a well-resolved estimate of the density field, however, PIV calculations require at least two images from the same plane, such that there is common particle information that the algorithm can identify.

One possible method to share information is to make the light sheet wider than the stepping distance. Depending on the scan speed, there will be a compromise between the light sheet thickness and the overlap of shared particles between slices. The cameras record a (filtered) 2D projection of the illuminated 3D volume. For anything less than 100% overlap of particles between frames, unwanted noise will be added into the PIV calculation. However, a thick light sheet is undesirable as it limits the spatial resolution of the scanning PIV. There is also a further downside in that by making the light sheet wider, the quality and accuracy of the LIF recording is adversely affected.

The system used in this thesis was designed to maintain the thin light sheet but also to ensure that there are two images recorded on the same plane before the light sheet is stepped to the next location. The stationary light sheet is achieved by translating the position of the beam within the optics producing the light sheet. This then alters the location at which the light sheet is produced at (see figure 2.11 for a schematic). The shift in the light sheet is achieved by using a pair of oscillating mirrors earlier in the beam path. The mirrors used are Thorlabs scanning galvanometers, with a maximum optical scan angle of $40^\circ$, operating at 130 Hz.

In the setup used in this thesis, the mirrors rotate only $\pm 0.2^\circ$ from their resting position, at a frequency of 50 Hz (half the frame rate). The rotation is controlled by a square wave, jumping between the position of the first frame and the position of the second frame. The path of the laser for the second pulse is deflected onto a slightly different path from the first, but results in a laser light sheet in the same location as the first. The extent to which the beam can be deflected is limited by the mirror size, the rate at which it can be rotated, and the optics of the laser sheet. Whilst a larger rotating mirror could in theory support greater deflections, in practice there is an inertial limit on how fast the mirror can be rotated.
To achieve greater accuracy in the PIV measurements, the scanning resolution is reduced by half, with pairs recorded on the same plane, such that two images are recorded on the same plane and then the next pair are recorded at the next step of the traverse. This results in 102 usable slices (each with a pair of images) with a stepping distance of $dz = 1.96$ mm for both the LIF and PIV data. Higher resolution images of the density field can be achieved if simultaneous measurements of the velocity and density are not required.

An alternative method, without the need for the oscillating mirror, would be to step the traverse between discrete locations such that it stopped and started for each slice. However, this would not be practical for high scanning speeds as the inertia of the traverse would prevent the system from accelerating and decelerating onto equally spaced points.

### 2.5.2 Stereo PIV

Stereo PIV uses the same principle as that used by the human eyes. Two images are recorded from slightly different viewing positions and then projected onto a single plane. The perspective error which arises from both of these projections is used to recreate the 3D object. Hinsch and Hinrichs (1996) suggested a classification $(k, l, m)$ where $k = 1, 2, 3$, gives the number of velocity components measured, $l = 0, 1, 2, 3$ gives the number of spatial dimensions being recorded and $m = 0, 1$ indicates whether the measurements were instantaneous or continuous in time, respectively. The system used in this thesis is $(3, 2, 0)$. 

Fig. 2.11 Schematics of (a) oscillating mirrors and deflected beam path and (b) effect of deflected beam path on emitted light sheet.
Fig. 2.12 A schematic showing a simultaneous rotational stereo PIV and LIF imaging system, modified from Hinsch and Hinrichs (1996). The PIV system uses cameras A and B, whilst LIF data is recorded using camera C. The image planes correspond to the planes that the image sensors of the PIV cameras, camera A and B, lie along.

The simplest setup possible is called the translational system (Hinsch and Hinrichs, 1996). In this system, the cameras are placed parallel to one another, such that all three planes, object, lens and image, are parallel i.e. the cameras face directly at the object being recorded. This setup creates uniform magnification across the whole image as well as ensuring uniform spatial resolution across all three images. However, this system comes with severe disadvantages, the first being the restricted common field between the two cameras. The second, more severe, is the strict limit in the off-centre angle between the camera and the object. This is caused by parts of the image being recorded through the extreme edges of the lens. As a typical lens is not designed to be used in this way, recordings made at these edges produce significant errors in the measurements. The limited angle reduces the possible separation distance between the two cameras and thus the accuracy of the in-plane velocity measurements (as the relative perspective error will be reduced).

The other method, called the rotational system by Hinsch and Hinrichs (1996), is that used in this thesis. A schematic is shown in figure 2.12. The cameras are no longer parallel to one
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another. Instead, they are set at an angle from the centre such that their axes intersect the object at approximately the same position. This allows for the off-centre angle to be increased to larger values, resulting in much more accurate out-of-plane velocity measurements. However, the magnification and spatial resolution are no longer uniform over the whole field of view, and this will need to be corrected for. To ensure that all objects are well-focused, the image plane must be separately rotated by the angle $\alpha$ from the lens plane, such that the image, lens and object plane are all collinear (as shown in figure 2.12). This is known as the Schiemflug condition. If there are no refractive index variations, this condition ensures uniform focus but increases the magnification variation across the object.

Fig. 2.13 Particle images used in the PIV system for (a) the left side camera and (b) the right side camera.

The two images produced by the cameras are rhomboids which have been oppositely stretched, see figure 2.13. From these images, two sets of 2D PIV velocity fields can be calculated. At this point, the PIV calculation is undertaken in pixel coordinates and so is unaware of the magnification change across the plane. The velocities calculated, $U_*$, are not accurate representations of real world velocities, $U$. Rather they are the rate at which pixel coordinates appear to change. If $i_s, j_s$ represent the horizontal and vertical locations of a pattern,
respectively, for camera *, then the velocity calculated is

\[ \mathbf{U}^* = \frac{\partial \mathbf{i}^*}{\partial t} + \frac{\partial \mathbf{j}^*}{\partial t} \]  

(2.15)

To calculate real-world velocities it is necessary to find the magnification across the image,

\[ \frac{\partial \mathbf{X}}{\partial i^*} \quad \text{and} \quad \frac{\partial \mathbf{X}}{\partial j^*} \]  

(2.16)

where \( \mathbf{X} = (x, y, z) \) are the 3D real-world coordinates. These magnifications are found by stepping a 3D coordinate grid, throughout the full width of the tank. At each step through the scan a 3D coordinate system that maps the pixel positions to the real-world positions is calculated,

\[ \mathbf{X} = (x, y, z) = f(i_A, j_A, i_B, j_B) \]  

(2.17)

where A, B refer to cameras A, B, respectively. The coefficients of equation (2.17) are found by fitting a least squares solution to the 3D coordinate systems from each step.

Whilst careful attention is made to co-locate the coordinate grid on the same plane as the laser, there may be small differences that can add to errors in the least square fitting. To correct for these potential errors, an additional step is taken to use this preliminary mapping on a sequence of scanned particle images from both cameras. The shared illuminated region is first mapped to the real world for both cameras, this allows a disparity map between the two be calculated. Following a similar algorithm to the PIV calculation, each image has a displacement field calculated for it such that there is a maximum correlation between the images. From this, an optimal shift of the mappings is created to align the coordinate system with the light sheet position. This process is repeated throughout the volume to get a scan-position-dependent coordinate system, with the least squares fitted coefficients used to update equation (2.17).

By combining equations (2.15) and (2.17), we can calculate the 3D real-world velocity

\[ \mathbf{U} = \frac{\partial \mathbf{X}}{\partial t} \]  

(2.18)

which, by applying the chain rule, can be written in terms of pixel displacements as

\[ \mathbf{U} = \frac{\partial \mathbf{X}}{\partial i_A} \frac{\partial i_A}{\partial t} + \frac{\partial \mathbf{X}}{\partial i_B} \frac{\partial i_B}{\partial t} + \frac{\partial \mathbf{X}}{\partial j_A} \frac{\partial j_A}{\partial t} + \frac{\partial \mathbf{X}}{\partial j_B} \frac{\partial j_B}{\partial t} \]  

(2.19)

with \( \mathbf{U} = (u, v, w) \) the 3D velocity field. Equation (2.19) needs to be computed in \( \mathbf{X} \) coordinates (i.e. the two pixel coordinate system) as \( i_A \) and \( i_B \) don’t give the same point for a given \( i_A = i_B \).
As the tank was not custom built for the laser system the captured velocity fields have some inherent errors. The opaque side walls block parts of the light sheet for both cameras at the back of the tank. At the front of the tank the full light sheet is visible. When it has moved 200 mm towards the back of the tank, the visible length has reduced to 370 mm, a reduction of 30 mm. The 3D reconstruction algorithm only calculates the third component of the velocity in the shared region; elsewhere it only uses the 2D velocity calculated from the camera that could see the flow at that location. Thus, this 3D scanning system with oscillating mirrors is able to accurately record 3D velocity which is representative of 95 % of the volume of the tank. A detailed discussion of the errors resulting from this setup are included in appendix B.

2.6 Photobleaching

R6G dye fluoresces when a photon is able to excite its electrons to the first singlet state. This is an unstable state and after a short time, \( \theta \left(10^{-10}\right) \) s, the electrons drop down to their initial energy level by releasing a photon. As the emitted photon cannot have more energy than the absorbed photon (indeed entropy ensures it will be less), the fluoresced photon is at a longer wavelength. When in the singlet state, there is the possibility that another photon can be absorbed by the already excited electron such that it is excited to an even higher energy state: the triplet state. This state is more stable and has a much longer lifetime of \( 10^{-4} \) s. In either of these excited states, R6G can form an irreversible covalent bond with surrounding molecules (\( O_2, H_2O, NaCl, NaN_3 \)). Once bonded, the R6G is no longer able to fluoresce. This effect is called photobleaching (Lichtman and Conchello, 2005). As the triplet state persists for \( 10^6 \) times longer than the singlet state, and in this state the electron is further from its ground state, R6G is significantly more likely to form a covalent bond in the triplet state.

The effect of photobleaching is immediately obvious when the laser is switched on, see figure 2.14. The reduced intensity of the dye, visible as dark arc (shown in red) around the centre of the domain between the two brighter regions (shown in green) is caused by photobleaching. Due to the construction of the optics, the light sheet does not have a uniform thickness over the whole height of the domain. Instead, it has a narrow inflection point near middle of the domain, and expands with distance away from this point. The obvious photobleaching region is the result of the laser being focused into a much smaller volume at the inflection, thereby producing a much greater number of photons per molecule of R6G. As the process is quantum mechanical, the increased number of photons increases the probability that a molecule will be excited to the triplet state and thus increases the probability that it will be bleached. However, photobleaching can occur at any point in the domain. It only requires an additional photon to
2.6 Photobleaching

excite the short-lived singlet state. As such, the rate of bleaching is proportional to the square of the intensity of the light sheet.

Whilst the effect of photobleaching was immediately obvious in the experiment, at the time it was not recognised that the effect was permanent, due to the formation of covalent bonds, and it was expected that the dye would recover some short time later. This permanence was only discovered when the late time calibrated densities were significantly lower than expected. In chapter 5 we present a hierarchy of post-processing methods which attempt to model and correct for the effect of photobleaching.

Fig. 2.14 A calibration image taken at the end of an experiment showing a clear arc of bleaching around the centre of the domain. The other dark shadows are the result of scratches to the base of the tank and the FB. Whilst these are distracting, because their position is fixed, they can easily be accounted for in post-processing.
Chapter 3

Numerical Setup

3.1 Introduction

In addition to the experimental research in this thesis, a number of numerical simulations were conducted to help understand the effect of an obstruction on the growth of the RTI. Due to the large Reynolds numbers present in RT mixing it would be prohibitively expensive to run direct numerical simulations (DNS) down to the smallest scales. As such this thesis makes use of an implicit large eddy simulation (ILES) code, called MOBILE, written for the purpose of solving turbulent buoyancy driven problems by Lawrie (2009). Since its inception, MOBILE has been improved upon and tested in a variety of different scenarios (Lawrie and Dalziel (2011), Davies Wykes (2014), Aslangil et al. (2016)). This chapter will provide a historical background to ILES as well as presenting an overview of the numerical methods used in MOBILE. For a more detailed discussion the reader is referred to Lawrie (2009).

3.1.1 ILES

In turbulent flows with high Reynolds number, such as those present in RTI, the large separation of scales makes Direct Numerical Simulations prohibitively expensive, since it requires the resolution of the smallest to largest scales to be resolved. A method of simulation called Large Eddy Simulation (LES) focuses on resolving the large scales in the flow, using a low-pass filter on the Navier-Stokes equations to remove the small scales. The subgrid scale is usually modelled separately by a semi-empirical model for the viscous dissipation and scalar diffusion. MOBILE uses a variant of LES called Implicit Large Eddy Simulations (ILES) that has no explicit sub-grid model and instead utilises numerical dissipation as a proxy for viscous dissipation. Because of this the ILES technique is controversial, despite a large growing body
of evidence showing that, under the right circumstances, it can be highly successful (Margolin et al., 2006).

The ILES technique was first successfully used in a code called Monotone Integrated Large Eddy Simulation (MILES), used for the study of flows around shocks (Boris et al., 1992). The traditional numerical methods were failing to accurately capture the real physics of the problem, creating unphysical maxima and minima in the density field (Gibbs behaviour). These were the result of Godunov’s theorem: “Linear numerical schemes for solving partial differential equations (PDEs), having the property of not generating new extrema (monotone scheme), can be at most first-order accurate” (Wesseling, 2009). MILES overcame this problem by solving a constrained linear problem with a non-linear method; the constraint being that the solution does not generate new extrema. This algorithm became known as flux corrected transport (FCT) (Boris and Book, 1973).

FCT works by finding both high and low order solutions for the net transportation of flux. These fluxes are combined as a non-linear weighted average. The high order solution is used as much as possible, such that when combined with an updated low order scheme, the weighted average does not create unstable extrema. This non-linear weighting method is known as the “flux-limiter” (Zalesak, 1979).

In the Alpha Group collaboration of Dimonte et al. (2004), a number of different ILES codes were compared against one another to test the accuracy of ILES (using different techniques) in predicting the growth of the RTI. All simulations were run at a resolution of $256 \times 256 \times 512$ and the results showed good agreement and consistency between all methods for the internal mixing structure as well as the overall growth rate of the mixing zone (with values of $\alpha = 0.025 \pm 0.003$). The review of Livescu (2013) found that when initiated with the same ideal initial conditions DNS, LES and ILES all show growth rates of $\alpha \sim 0.02 - 0.03$.

Youngs (2013) tested the effect of resolution on the growth of the RTI by running ILES up to resolutions of $1000 \times 1000 \times 2000$. The increased resolution had very little effect on the value of $\alpha$ found by Dimonte et al. (2004). A direct comparison between TURMOIL ILES (a well tested code upon which MOBILE is heavily based) and DNS was performed by Youngs (2017) for a range of RTI applications from single-mode to RT mixing on an angle, with both codes run at resolution of $1000 \times 1000 \times 1550$. For self-similar mixing at a plane boundary both the ILES and DNS gave growth rates of $\alpha = 0.03$. ILES displayed much more fine-scale structure than the DNS, however, the molecular mixing was very similar for both codes.

One limiting factor of ILES worth mentioning is the fixed effective Kolmogorov length scale imposed by the grid resolution. As the flow in viscous fluid decays, the energy dissipation rate drops, which increases the Kolmogorov length scale. However, this is not possible for ILES, where instead the effective viscosity decreases. This results in small-scale structure being
removed from the viscous fluids, whilst for ILES, high wave number velocity gradients persist (Aspden et al., 2009). This can result in small scale motion, such as internal gravity waves, existing at late times where viscosity would have remove these features. For the simulations used in this thesis, the lack of viscosity in MOBILE will result in KE decaying more slowly at later times and, potentially, will result in greater mixing when compared to experimental data. 

The acceleration of flows acts to prevent back-scatter from the finite resolution of ILES becoming significant at the dominant (integral) lengthscales (Aspden et al., 2009). However, the scenarios considered in this thesis are interested in significant times where the flow is decelerating and thus the finite resolution of the ILES may affect some of the results. Despite this, MOBILE has been used successfully in other comparable cases where the flow is decelerating (Davies Wykes, 2014; Lawrie, 2009).

### 3.2 Numerical methods

In this section we provide a brief summary of some of the numerical methods used by MOBILE. A thorough discussion of the code, methods and extensive validation is presented in Lawrie (2009).

MOBILE simulates incompressible variable density fluid flows with the following governing equations

$$\frac{\partial c_k}{\partial t} + \frac{\partial (c_k u_j)}{\partial x_j} = 0,$$

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \rho g_i,$$

$$\rho \frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i} = \frac{\partial^2 p}{\partial x_i^2},$$

where $c_k$ is the volume fraction of the $k$’th advected tracer with density $\rho_k$. The density of each cell is calculated by

$$\rho = \sum (c_k \rho_k),$$

with

$$\sum c_k = 1.$$

The Boussinesq approximation is applied and incompressibility is accounted for by implicitly adjusting the pressure field to conserve volume. A 2D representation of the cell structure is shown in figure 3.1. Here we see that the scalar information is stored on the $(i, j)$ grid at the centre of the cells, whilst the velocity (and flux) data are stored at the centre of each cell’s boundary (face).
Fig. 3.1 A 2D cell diagram for upwinded momentum, from Lawrie (2009). The arrow enclosed by the circle is the point being updated. The solid line grid indicates the scalar cell boundary, with scalar information stored at the centre of each cell. The dashed lines indicate the boundaries of the offset momentum data. The black dots and smaller arrows indicate the data that is needed when \( u > 0 \) and \( v > 0 \).

Equations (3.1) are solved by separating the equations into their hyperbolic and elliptical terms using a fractional step approach. The hyperbolic terms conserve mass and momentum but not volume. Volume is conserved through calculation of the elliptical terms via a pressure correction step.

The hyperbolic component of the fractional step solves the tracer advection and momentum equations. A weakened conservation law is enforced locally at individual cells in the grid such that

\[
\iiint \frac{\partial \phi}{\partial t} dV + \iiint \phi \mathbf{u} \cdot \mathbf{n} dS = 0, \tag{3.4}
\]

where \( \phi \) is a conserved variable, stored at the centre of a grid cell (where the grid cell has volume \( V \), surface \( S \) and unit normal \( \mathbf{n} \)) and the velocity \( \mathbf{u} \) is stored on the grid cell face. For a finite volume, Stoke's theorem ensures equation (3.4) is conserved globally across the total volume.

The conserved variables, tracers and momentum, are then advected via an upwind scheme evaluated at the cell boundaries (a schematic is shown in figure 3.1). In figure 3.1 the \( \mathbf{u} \) momentum point to be updated by the upwind scheme is indicated by the arrow enclosed in the circle, located at \( \left( i - \frac{1}{2}, j \right) \). The black dots represent the scalar values and the small arrows...
represent the velocity data. The large arrows show the momentum fluxes with the small triangle indicating how data is mapped from cell boundary to the cell centre.

The accumulated contributions of the flux from all neighbouring cells are combined in a volume weighted average (calculated from the volume transferred by the flux from each neighbouring cell) for each conserved variable over the volume of the cell that is being updated. This scheme remains stable as long as the total volume advected in a time step does not exceed the volume of the cell.

By making use of the fractional step method, MOBILE breaks down a multidimensional problem into a series of 1D update instructions. The fractional step method breaks the transition from one timestep to the next into a series of intermediate steps whose solutions are not required to satisfy the consistency and stability conditions of the original equations at each fractional step (Janenko, 1971). Here, the most up-to-date values of variables are used to update the next set of values in the sequence. This consists of a series of one-dimensional update instructions in the directions X-Y-Z-Z-Y-X. This particular sequence is chosen as it has been shown by Strang (1968) to limit the growth of accumulated error and is known as Strang splitting. To implement Strang splitting as originally proposed would require each dimensional split to occur at each half timestep. MOBILE instead uses the Strang splitting over two timesteps. While this is only formally first order accurate (with original Strang splitting second order accurate) it has been empirically found to have slower error accumulation (Lawrie, 2009).

The conserved variables, $\phi$, are stored at the cell centre, represented in figure 3.1 by the black dots. However, the flux $F$ is calculated on the cell faces, where the velocity information is stored (shown as arrows in figure 3.1). This requires that a value of $\phi$ must be found for the cell edge. The simplest first-order approximation uses the value in the upwind cell. The use of higher-order approximations in linear combinations results in unstable oscillations in the regions with sharp boundaries (Gibbs phenomena). To make use of more accurate higher-order approximations, but prevent such oscillations, MOBILE includes flux-limiters to conserve monotonicity. The flux, $F$, is calculated on a set of modified states derived from the MUSCL extrapolation method (Van Leer, 1997). This method uses higher-order approximations on smooth parts of the flow and reverts to lower order approximations in regions with large gradients. The low order approximations result in more numerical dissipation, however, regions with large gradients typically result in greater physical dissipation. Thus the error from the low order approximation can be used as a proxy for the actual dissipation in the system.

The final result of the hyperbolic step of the calculation is to produce a velocity field, $U^*$, which conserves mass and momentum but may not conserve volume. Volume conservation is then achieved by mapping $U^*$ onto a divergence free field. This constitutes the elliptical part of the ILES scheme. There is no unique projection of $U^*$ onto the divergence free field and, by
Numerical Setup

definition, none can conserve linear momentum. However, we can achieve angular momentum conservation by using a Helmholtz decomposition, \( \mathbf{U}^* = \mathbf{U}_{\text{no curl}} + \mathbf{U}_{\text{no div}} \). From here it is possible to form a Poisson equation,

\[
\nabla \cdot \mathbf{U}^* = \nabla^2 \Phi,
\]

where \( \Phi \) is the velocity potential such that \( \nabla \phi = \mathbf{U}_{\text{no curl}} \). To solve equation (3.5) numerically, a system of equations is produced that is discrete in space. In MOBILE this system is solved via Successive Over Relaxation (SOR), and this constitutes the most time expensive part of the calculation.

Boundaries are created in MOBILE by using three rows of “ghost cells” located outside the domain (see figure 3.2). To create free-slip boundary conditions (the ones used in the simulations of this thesis), zero velocity is imposed on the outward face of the boundary cell (a so called Dirichlet condition). In the row of ghost cells immediately outside the domain a pressure exactly equal to internal pressure is prescribed, enforcing a von Neumann condition. During the pressure correction calculation the boundaries act as though they have infinite mass (during the volume weighted averaging) such that the boundary is unaffected by fluxes but neighbouring cells in the interior are. The imposition of a more realistic no-slip boundary condition is achieved by imposing an equal and opposite wall-parallel velocity in the ghost cell to velocity just inside the boundary, resulting in a net velocity of zero at the boundary. However, the transverse gradients created at such a boundary would not activate the flux limiters, which is where the dissipation is calculated. As a result there is no additional dissipation caused by no-slip boundary when there is no explicit viscosity. Hence, for ILES there is no significant difference between free-slip and no-slip boundaries.

The majority of the simulations presented in this thesis were run with an additional solid obstruction (or boundary) imposed in the centre of the domain. Inside the domain it is not appropriate to use ghost cells. Instead an internal obstruction is created by preventing information from being passed between neighbouring cells across the obstruction. MOBILE uses a Message Passing Interface (MPI) protocol to distribute a single problem over multiple processors. This separates the domain (consisting of all internal cells) into several large cuboidal blocks (a schematic is shown in figure 3.2). In MOBILE all processes are aware of the existence, location and size of every block that fills the domain. Information is usually freely transmitted between block boundaries. However, it is possible to stop information from being passed between neighbouring blocks at the location of the central imposed obstruction. This forces the governing equations to be solved as if cells around the obstruction were isolated from one another across the obstruction but still able to interact with the rest of the domain. This allows us to create an infinitely thin obstruction, but only at limited locations and geometries.
Fig. 3.2 Domain diagram showing that the simulation domain (shown in blue) is composed of smaller processing blocks (green). Each block is filled with cells (shown as grey boxes), in which the tracer and velocity data are stored (at the centre and face of each cell respectively). Ghost cells are stored outside of the domain and are used in the calculation of the boundary.

This solid boundary in the centre of the domain will be free-slip, resulting in a difference between the numerical and experimental obstructions. This will likely result in a more uniform, slightly faster stream flowing off the end of the obstruction, potentially creating a more symmetric RTI mixing zone than that of the experimental data. The increased velocity from the end of the barrier may reduce the total growth of the RTI mixing zone, as the fluid spends less time in the opening before it interacts with the side wall. However, this impact is likely small compared to the different aspect ratios of the experiments and numerics of $H/L = 1.2$ and $H/L = 2$ respectively.

The simulations were initialised with two layers at density $1010 \text{ kgm}^{-3}$ and $1000 \text{ kgm}^{-3}$ for the upper and lower layer respectively, corresponding to an Atwood number of $A = 5 \times 10^{-3}$. This low Atwood number ensures that the flows are Boussinesq. MOBILE uses the standard RTI initial conditions, where the initial perturbation applied to the interface of the two layers is random with small amplitude and small wavelength (Dimonte et al., 2004). The amplitude, $a$, scales as $a \sim k^4$ between a minimum wave-number and $k_a$, the wave-number with the greatest amplitude. The amplitude of any wave-number greater than $k_a$ scales as $a \sim k^{-5/3}$ up to a maximum wavelength.

A number of validations tests were performed by Lawrie in his thesis (Lawrie, 2009). He tested single-mode RTI, high aspect RTI, Kelvin-Helmholtz instability and lock-exchange gravity currents against experimental and theoretical data. MOBILE performed well in all tests, comparing favourably to the available (experimental and theoretical) data, and displaying
good grid convergence. Further discussion of the effect of resolution, initial conditions and numerical errors can be found in appendix A.
Chapter 4

First Impressions

4.1 Introduction

This chapter discusses the qualitative dynamics of the singly connected domain, where there is only a single opening on one side of the domain between the two layers, as shown in figure 1.1. This chapter is crucially important for understanding the new dynamics that are caused by the inclusion of an obstruction. The base scenario for comparison will be the case where there is no obstruction. The size of the opening is parametrised by $\gamma$, such that the classical case with no obstruction has a value of $\gamma = 1$, whilst the half open case has $\gamma = 0.50$. The $\gamma = 0.50$ case is discussed alongside the classical unobstructed RTI base scenario. This case was chosen due to its simplicity and symmetry.

This chapter will first present the LIF data as a time series for classical RTI in an unobstructed domain. Comparable LIF images will then be presented for the same times in the $\gamma = 0.50$ singly connected domain. Comparisons between the two flows will be made, including a discussion of the different dynamic regimes responsible for the mixing of the two layers. In addition to the LIF data, a time series of PIV data will be presented and discussed, which will be used to reinforce the deductions made from the LIF data.

4.2 LIF data

The two cases presented in this chapter were conducted at the same Atwood number, $A = 6.8 \times 10^{-3}$, with the same concentration of dye included in both, $3 \times 10^{-4}$ g of R6G dissolved into 40 L of water at a concentration of $7.5 \ \mu g L^{-1}$. Each layer was filled from a separate covered reservoir that was well mixed and allowed to come to thermal equilibrium with the laboratory. Dye was added to the lower layer for the classical unobstructed case and the upper
layer for the singly connected case. This does not impede the visibility of the dynamics. The difference is only because the classical unobstructed case was one of the first experiments done to test the system and dye concentration. The only significant difference in the setup between the two sets of experiments is the inclusion of the 200 mm long polycarbonate barrier at the start of the experiment for the singly connected case.

Each of the figures presented in this chapter uses raw images from the experiment that have not been modified or corrected in any way. As a result, the quality of the images suffers in a number of ways. Scratches in the base plate cast shadows throughout the whole domain and the spatial variation of the light sheet intensity alters the brightness of the image, with the brightest region being the centre bottom where the light sheet is thickest (in the $y$ direction) and first enters the tank (such that $\int C I dy$ is maximal where $I$ is the light sheet intensity and $C$ the concentration of dye). Despite these limitations, it is still possible to gather significant insight into the dynamics of the flow. These problems will provide motivation for the work in Chapter 5, in which a number of post-processing methods are developed and presented. These significantly improve the quality of the experimental images, which in turn increases the accuracy of the quantitative analysis.

### 4.2.1 Classical RTI

Figure 4.1 shows a time series of LIF images of a classical RTI experiment; one in which there is no permanent obstruction between both of the layers. The layering is RT unstable with the upper layer consisting of NaNO$_3$ solution, which is more dense than the refractive index matched NaCl solution in the lower layer. A removable steel barrier (RB) initially separates the two layers. At the start of the experiment the RB is withdrawn through the right-hand side wall.

In the first image, figure 4.1a, the barrier is only partially withdrawn. The effect of the removal of the RB on the initial conditions is clearly visible, with the wake from the barrier withdrawal seen as a regular 2D wavelike perturbation to the interface. This perturbation can be seen to grow due to the RTI with time since the RB was opened, such that the perturbation appears to be most developed on the left-hand side. The RTI first appears as small perturbations to the surface at the end of the RB. These perturbations have grown to form the distinctive ‘mushroom’ structure of RTI near the centre of the domain before transitioning to turbulence on the far left side. The right-hand side of the lower layer appears much brighter than the left-hand side due to the laser reflecting back into the lower layer from beneath the partially withdrawn RB.

As discussed in section 2.2.1 an initial jet of upper layer fluid propagates down the left-hand side of the tank, entraining lower layer fluid as it moves, a process clearly visible on the left-hand side in figure 4.1b. The downward vertical extension of the jet is seen to be more
than twice the height of the mixing region at the interface. Disturbances at the interface have now transitioned from the 2D wake to turbulence for the whole horizontal extent of the domain. Despite this transition to turbulence, memory of the initial perturbation remains. The height of the mixing region is seen to decrease from left to right (the direction the barrier was opened). There is a regular wavelength visible amongst the bubbles of turbulence, with smaller structures superimposed on top. Also evident in this figure is the 3D nature of the turbulence generated from the RTI, with bubbles appearing in the lower layer that are completely detached in the current plane from the mixing region above.

The range of scales present in the flow continues to grow as the mixing region spreads further into either layer, see figure 4.1c. The large scale motion is dominated by three large bubbles extending into much of each layer. At this scale the dynamics still display memory of the initial perturbation, with a clear left-right divide in the height of the bubbles. Amongst these bubbles are smaller scale RT and KH instabilities, growing from the bubbles and mixing them further with each of the layers.

At the bottom of the domain in figure 4.1c, the initial jet can be seen to propagate from left to right as a gravity current. It entrains significant amounts of (unmixed) lower layer fluid as it moves, made visible by the intrusion of small structures into its interior. This gravity current then collides with the right-hand side wall, overturning and mixing with fluid remaining in the lower layer, as is visible by the mixed fluid now present at the very bottom of the domain in figure 4.1d. The three-dimensionality of the overturning motion is illustrated by this figure. A large wedge of heavy fluid that has moved into the plane is particularly visible on the right-hand side of the domain. This heavy fluid begins mixing with lighter fluid trapped in the bottom right-hand corner. The interface between these two fluids grows diagonally as the RTI grows on top of a moving interface.

Continuing to look at figure 4.1d, the motion in the upper layer is now highly turbulent, with large velocities from the conversion of available potential energy. The range in scales remains large, with the biggest scale now comparable to the size of the domain. Whilst fine-scale structure can be seen on the dye contours, these sharp density differences are reduced as the layer continues to be mixed. In figure 4.1e and figure 4.1f the domain is almost fully mixed. The large density differences from the start of the experiment are now greatly reduced, as is made evident by the near homogeneous intensity of the full domain. At this stage the smallest scales in the upper layer begin to feel the effects of viscosity and no longer grow as rapidly. The dark shadow cast in an arc across the centreline is the result of photobleaching from the laser, as discussed in section 2.6. A hierarchy of post-processing methods will be presented in chapter 5 that attempt to remove the effect of this photobleaching.
Fig. 4.1 LIF images from the $\gamma = 1.0$ experiment at $A = 6.8 \times 10^{-3}$ with rhodamine dye added to the lower layer, at times (a) $\tau = 1.1$ ($t = 3$ s), (b) $\tau = 2.6$ ($t = 7$ s), (c) $\tau = 4.0$ ($t = 11$ s), (d) $\tau = 5.8$ ($t = 16$ s), (e) $\tau = 7.3$ ($t = 20$ s), (f) $\tau = 8.8$ ($t = 24$ s). The colourbar indicating intensity for all images is shown.
Fig. 4.2 LIF images from the $\gamma = 0.50$ experiment at $A = 6.8 \times 10^{-3}$ with rhodamine dye added to the lower layer, at times (a) $\tau = 1.1$ ($t = 3$ s), (b) $\tau = 2.6$ ($t = 7$ s), (c) $\tau = 4.0$ ($t = 11$ s), (d) $\tau = 5.8$ ($t = 16$ s), (e) $\tau = 7.3$ ($t = 20$ s), (f) $\tau = 8.8$ ($t = 24$ s), (g) $\tau = 10.3$ ($t = 28$ s), (h) $\tau = 11.8$ ($t = 32$ s), (i) $\tau = 13.2$ ($t = 36$ s). The colourbar indicating intensity is shown in figure 4.1.
4.2.2 Singly-connected domain

We now introduce an obstruction to the classical RTI problem such that $\gamma = 0.50$. This obstruction is created by securing a 200 mm fixed polycarbonate barrier (FB) along the interface of the two layers, secured against the right-hand side wall as shown in figure 1.1. Apart from the dye being added to the upper layer and the introduction of the FB, the experimental setup is identical to that in section 4.2.1. A comparable time series of the evolving obstructed flow is shown in figure 4.2. This time series will be described and the differences between the classical and obstructed case will be discussed.

Figure 4.3a shows the streamlines of the singly-connected domain, calculated from the PIV data in figure 4.4e (to be discussed in section 4.3), whilst figure 4.3b makes clear the different dynamical regions present in each layer. Looking close to the left-hand side wall in figure 4.3a, the streamlines can be seen to split between each layer as mixed fluid from the RT mixing zone is transported vertically via two wall plumes to the upper and lower layers. The fluid is then deflected along the horizontal boundary and propagates as a gravity current before interacting with the side-wall, overturning and returning to the fixed barrier as a fountain. Observe in figure 4.3a that the streamlines moving onto the opening (in the middle of the domain) are largely horizontal (and parallel) exemplifying that the flow is laminar (moving in the same direction) off the barrier.

Looking first at figure 4.2a, the removable barrier can be seen to be removed left to right, with dye now in the upper layer. The effect of the opaque steel barrier is to cast a dark shadow into the right-hand side of the upper layer. As the RB is removed it leaves a wake, as seen in the classical case, but in this case, only in the open region. From this perturbation to the open interface, the RTI grows almost identically to the early-time growth of the classical instability seen in figure 4.1a. Again, as for the classical case, the removal of the RB results in a jet of upper layer fluid being forced into the lower layer, the start of which can be seen beginning to descend into the lower layer on the left-hand side in figures 4.1a and 4.1b. At this stage in its development, the RT mixing zone appears unaffected by the obstacle, with the height of the mixing zone being comparable to the classical case. The structure of the RTI mixing region displays the characteristic mushroom-like structure, transitioning to turbulence left to right across the opening. Whilst the mushroom structures appear more stretched than in the classical case, the mean height of the mixing region is the same, with the stretched appearance caused by the unpredictable 3D growth of random perturbations in the out of plane ($y$) direction.

Continuing with figure 4.1b, as the mixing region grows in the opening, the two layers begin to mix together, resulting in a horizontal density gradient between the mixed fluid in the opening and the ‘fresh’ unmixed fluid either side of the barrier. Note that this does not exist in the classical case, up until now the two flows have been indistinguishable. The horizontal density
4.2 LIF data

Fig. 4.3 Streamlines of the singly connected flow at $t = 20$ s are shown behind a PIV velocity field in (a) (the scale for the vectors is shown in figure 4.4). A cartoon identifying the different dynamical regimes present in each layer is shown in (b).

Gradient establishes a baroclinic torque either side of the barrier such that fresh, unmixed fluid is forced off the edge of the barrier into the open region. Looking at the edge of the barrier in the centre of figure 4.2b, we can see that fresh unmixed fluid has moved off the edge of the barrier where it can be seen by the flatter interface to occupy the half of the opening nearest to the end of the FB. The unstable interface created by this motion develops a RTI mixing zone which grows as the two streams flow off the FB. These two streams are at the initial densities, with the upper layer stream being more dense than the lower. The RTI grows on the moving interface of these two streams as is seen to start at the left of the FB’s edge in figure 4.2b (more clearly developed at later times in figure 4.2c).

Looking at the left-hand side of figure 4.2b, the large volume of mixed turbulent fluid is the turbulent stage of the initial RTI mixing zone first seen in figure 4.2a. We can see that the streams of fresh fluid have forced this mixing zone towards the left-hand side wall. The displacement of the initial mixing region has a retarding effect on the extent of the initial jet that penetrates into the lower layer. After $\tau = \sqrt{Ag/Ht} = 2.6$, the jet in the classical case had extended the full depth of the lower layer, see figure 4.1b. However, for the obstructed case it only extends some 75% of the depth, see figure 4.2b. Interestingly, the initial mixed region in the upper layer also extends 75% of the domain height. Conservation of volume requires
that a volume of fluid equal to that carried by the initial jet in the lower layer be returned to
the upper layer. This forms a bulge of lower layer fluid penetrating into the upper layer; this is
seen as the large bubble growing into the upper layer for the classical case on the left-hand side
of figure 4.1b. For the obstructed case, this large bulge is squeezed into a narrow area by the
left-hand wall and stretched vertically such that it now occupies a greater height than was seen
for the classical case.

As the motion develops, the symmetry between the two layers is improved as memory of
the asymmetric initial condition is lost through turbulent motion on the side wall. Looking at
figure 4.2c, we can see that, as fresh fluid flows off the edge of the barrier, it begins to mix and
develop a RT mixing zone. The growth of this mixing zone is directly comparable to that of the
work by Ramaprabhu and Andrews (2004) who looked at the spatial development of RT mixing
in a channel with two RT-unstable streams flowing off a splitter plate. Ramaprabhu found that
the height of the mixing region grew with the square of the distance from the splitter, with a
small offset to account for the effect of the stream moving off the end of the splitter plate. In
figure 4.2c we can see that the height of the mixing region grows with distance from the edge of
the barrier; the rate of growth of this will be discussed in chapter 6. At this time, the interface
remains approximately flat for 25% of the opening, while to the left small perturbations on the
interface between the layers grow rapidly before transitioning to larger scales that are expected
to grow quadratically with time as found by Ramaprabhu and Andrews (2004).

As the mixing region grows, more fluid is drawn from above and below the barrier, which
forces the mixing region into the left side wall (see the left-hand side of figures 4.2b and 4.2c).
At this point the fluid is stretched rapidly vertically up the side walls, forming two well-mixed
wall plumes. When these wall plumes interact with the top and bottom of the tank they form
gravity currents that propagate along the horizontal boundary. This results in a circulation cell
being established in each of the layers, with fluid constantly circulated onto the opening and
then being carried away from the opening via wall plumes into each layer.

The gravity currents that form as a result of the circulation are large and blunt nosed with
a height roughly half the layer depth. This significant height is due to the large amount of
unmixed fluid the wall plumes have entrained, reducing the density difference between the
gravity current and the ambient fluid. The subsequent motion down the side wall and deflection
along the horizontal boundary results in the gravity current being composed of highly turbulent
fluid, which when combined with the small density difference results in a large amount of
entrainment and subsequent increase in the height of the gravity current as it moves.

The sharper nose (compared to that seen at earlier times) of the gravity current in the lower
layer is due to the initial jet of upper layer unmixed fluid being rapidly forced into the lower
layer. The front of the gravity current is comparable to that seen for the classical case in
figure 4.1c. However, behind the nose, the gravity current is much taller and comparable to that in the upper layer. Interestingly, despite the disparities at $\tau = 2.6$, the progression of the front of the gravity current in the lower layer is similar to that in the classical case. However, the gravity currents are slight more progressed in the singly-connected case. This increased progression of the gravity current is likely caused by the circulation established in each layer helping to advect the gravity current further around the layer.

Comparing figures 4.1c and 4.2c, we can see already that an obstruction results in dramatically different mixing dynamics. Where for the classical case the RTI grows from the interface between the two fluids and spreads rapidly throughout the whole domain, in the singly connected case the growth of the RT mixing region is restricted to a maximum of about 25% of the layer height. As new fluid is drawn onto the opening from the right, it forces the RT mixing region to be swept constantly into the left-hand side wall, limiting the time the RTI has to grow between the two layers. This results in much larger tranches of unmixed fluid in each layer than in the classical case at $\tau = 4.0$. However, the fluid that does move into each layer in the singly connected case is typically well mixed, having passed through two highly efficient mixing processes.

The large reservoirs of unmixed fluid in each layer in the $\gamma = 0.50$ case continue to feed fresh fluid into the opening. This results in a RTI mixing region that remains quasi-stable for a significant period of time. This is demonstrated by there being little difference in the internal structure and height of the RTI mixing region when comparing figures 4.2c and 4.2d.

The continuous influx of mixed fluid into either layer adds to the volume of each gravity current. The gravity currents propagate around each layer until they interact with the right-hand side wall. As each gravity current interacts with the side wall, it would be expected that they would experience a large amount of overturning and subsequent mixing with surrounding fluid as they form a negatively buoyant wall plume or fountain (Rottman et al., 1985). This mixed fluid would then be expected to settle to a neutral buoyancy height between the original fluid and the horizontal boundary of the layer. However, the layer-wide circulation draws these fountains further from their neutral height towards the barrier, see figures 4.2d and 4.2e.

As the circulation advects the mixed fluid from the gravity current further around each layer, it forces the remaining unmixed fluid into the regions on either side of the opening, as seen on the left-hand side of figure 4.2e. The circulation draws more mixed turbulent fluid from the gravity current up to the barrier. This results in mixed turbulent fluid flowing leftward onto the open interface from either layer. The two streams, from the upper and lower sides of the FB, still have a density difference between them, though now at reduced Atwood number. From this density difference the RTI continues to grow on the interface between the two streams.
The combination of these two factors, trapped unmixed fluid either side of the opening and turbulent mixed fluid coming onto the opening, result in the interface losing its quasi-stability (compare the size of the mixing region in the opening of figures 4.2e and 4.2f). The trapped unmixed fluid in the lower layer is now much more buoyant than the fluid moving onto the opening and mixing there, with the reverse being true for the upper layer. The relative buoyancy of the trapped fluid now forces the trapped fluid against the circulatory flow and into the opening. There, the two regions of unmixed fluid mix via RTI. At the same time the stream of mixed fluid continues to flow into the opening from above and below the barrier, forcing the RTI mixing region leftward into the side wall. The large volumes of negatively and positively buoyant fluid result in a turbulent mixing region comparable to that seen for classical RTI (compare the opening in figure 4.2f to figure 4.1c). Clear bubbles and spikes, which are indicative of RT mixing, are visible in figure 4.2f, despite the counterflow occurring in the opening.

The circulation continues to bring fluid onto the interface even with the reduced density difference, visible in the growing interface at the end of the barrier in figure 4.2f and the continued growth of the RT mixing zone in figure 4.2g. The deflection of the RTI mixing zone into the lower layer in figure 4.2g is the result of the departure from symmetry in the system, symmetry that existed when fluid moving onto the interface was laminar and homogeneous. The two streams now moving onto the interface are more turbulent, no longer homogeneous and not necessarily at opposing densities as is evident by the contorted density interface in the opening and seen more clearly in the movies. This can result in planes of the domain displaying temporary departures of the interface from the centre line. However, conservation of volume requires that the depth averaged exchange be bidirectional and provide no net volume flux into either layer, as is seen from the switch in centre-line offset from figures 4.2g to 4.2i.

Continuing to look at figures 4.2g to 4.2i, we can see that the domain-wide motion continues quasi-steadily for the remainder of the experiment. Fluid is mixed across the interface and transferred into each layer by wall plumes. These plumes interact with the horizontal boundaries and propagate as blunt gravity currents entraining large amounts of fluid as they move. Once these gravity currents interact with the side wall there is a large amount of overturning and visible mixing within each layer. The motion then begins again, the same physical process which began the circulation repeats, albeit at a much smaller Atwood number.

### 4.3 PIV data

A time series of PIV data from a $\gamma = 0.50$ experiment at $A = 5 \times 10^{-3}$ is shown in figure 4.4. Here the velocity field (arrows) is superimposed onto the vorticity field (colour). It is worth noting that the timescale of evolution of the RTI is much longer than that of individual vortical
4.3 PIV data

structures. In figure 4.4a, the wake from the barrier is clearly visible, whilst the rest of the fluid in both layers is at rest.

In figure 4.4b, the initial jet discussed in section 2.2 can be seen to propagate down the left-hand side wall. We can also see the growth of the initial perturbation in the opening via the RTI. The vortical structures seen in the PIV images are indicative of highly turbulent regions where mixing is likely to occur. The RTI mixing region generates a horizontal buoyancy gradient that can be seen to begin drawing fresh fluid from either side of the barrier into opening.

The isolated vortical structure seen beneath the barrier on the right-hand-side of figure 4.4b is the deposition of vorticity left as the RB is withdrawn through the side wall, as discussed in section 2.2. This structure can be seen to be advected beneath the FB and gradually dissipate with time as seen in figures 4.4c to 4.4e.

By 11 s from the barrier being opened, shown in figure 4.4c, the initial mixing region is seen to have been forced into the left-hand side wall and carried vertically away from the interface by two wall plumes, one in each layer. These can be seen transporting turbulent fluid towards the horizontal boundaries in each of the layers. At this point we can clearly see the establishment of a circulation cell in each layer with fluid rapidly transported in a narrow vertical band along the left-hand side wall. This then interacts with the horizontal boundaries where it is deflected horizontally. In the opening we see that the stream coming off the FB is mostly laminar and horizontal. Once in the opening the stream is seen to acquire vorticity as the RTI grows on the interface and the two streams begin to mix.

In figure 4.4d, the circulation is well established and continues to transport fluid from the interface around each layer despite the large amount of vorticity now visible in each layer. The gravity current that was propagating along the horizontal boundary can be seen being deflected by the right-hand wall of both layers in figure 4.4d. In figure 4.4e the overall motion is notably similar. The RTI mixing region has remained in the same location unmoved for a long time, continuing to transport turbulent fluid via two quasi-stable wall plumes. We can see, in figure 4.4e, that the overturning region is carried by the circulation in each layer towards the FB, where it is then deflected horizontally along the FB.

We can see in figure 4.4f that fluid with a large amount of vorticity (i.e. more turbulent) now moves onto the opening. This more turbulent fluid can be seen to deflect the interface in the opening vertically upwards, temporarily breaking the symmetry (stability) in the system seen until this point. However, outside of this region, the circulation continues unimpeded. Indeed, looking at figure 4.4g, we can see that the deflection of the interface has not disrupted the circulation significantly. We can still see that two streams continue to flow off the FB into the opening almost completely horizontally. At the left-hand side of the opening, this stream is then split, almost equally, between the upward and downward wall plumes.
Fig. 4.4 PIV for the $\gamma = 0.50$ experiment at $A = 5 \times 10^{-3}$, with the barrier superimposed as a black line on all images. The velocity field is shown with the vorticity field in the background, at times (a) $\tau = 1.1$ ($t = 3$ s), (b) $\tau = 2.6$ ($t = 7$ s), (c) $\tau = 4.0$ ($t = 11$ s), (d) $\tau = 5.8$ ($t = 16$ s), (e) $\tau = 7.3$ ($t = 20$ s), (f) $\tau = 8.8$ ($t = 24$ s), (g) $\tau = 10.3$ ($t = 28$ s), (h) $\tau = 11.8$ ($t = 32$ s).
In the latest time shown, figure 4.4h, the density difference between each of the layers has decreased and the motion can be visibly seen to slow, as shown by the reduced arrow lengths in figure 4.4h. Despite this reduced motion, layer wide circulation is still clearly visible by the clockwise and anticlockwise motion along the boundaries in the upper and lower layers respectively. Fluid is seen to continue to flow largely horizontally either side of the FB onto the interface, where the circulation continues. Whilst not shown here, motion comparable to that shown in figure 4.4h continues for a long time, with the largest velocities seen along the boundaries. The residual circulation continues to mix the remaining density differences between each of the layers by recirculating fluid back through the RTI mixing process in the opening.
Chapter 5

Improved Diagnostics

5.1 Photobleaching

As discussed in section 2.6, photobleaching damages the fluorescent dye in an experiment thereby modifying the intensity of the measured. Photobleaching is a quantum-mechanical process whereby a molecule of dye is doubly excited to a triplet state. The probability of photobleaching occurring is proportional the square of the intensity of the light sheet, which is approximately inversely proportional to the thickness of the light sheet. The process of photobleaching can be expressed mathematically by separating the total dye concentration $C$ into its different energetic states, with the concentration of dye in the base state (the unexcited energy state) represented by $C_0$. The concentration of dye in the singlet (first excited energy) state is $C_1$. If there is no photobleaching, then these concentrations change as follows

\[
\frac{dC_0}{dt} = -\gamma_{01}IC_0 + \Gamma_1C_1 \\
\frac{dC_1}{dt} = \gamma_{01}IC_0 - \Gamma_1C_1,
\]

where $\gamma_{01}$ is the probability a dye particle is excited to the first energy state, $\Gamma_1$ is the probability that a dye molecule will drop down from the singlet to base state and is proportional to the inverse lifetime of the singlet state (such that $\Gamma_1$ is very large) and $I$ is the intensity of the light sheet (inversely proportional to the thickness of the light sheet). Excitation from base state to singlet state, depends on the intensity, but fluorescence depends only on the number of excited molecules, $C_1$.

We now include the triplet state concentration, $C_2$, into our excited concentration model. We assume that excitation to the triplet state is only possible from the singlet state with a
probability of $\gamma_{12}$ and that the dye is able to return from this triplet state directly to the base state with a probability $\Gamma_2$. Note that the triplet energy state has a much longer lifetime than the singlet state such that $\Gamma_2 \ll \Gamma_1$. This results in the following updated set of equations

$$\frac{dC_0}{dt} = -\gamma_{01}I^2C_0 + \Gamma_1C_1 + \Gamma_2C_2$$  \quad (5.3)

$$\frac{dC_1}{dt} = \gamma_{01}IC_0 - \gamma_{12}IC_1 - \Gamma_1C_1$$  \quad (5.4)

$$\frac{dC_2}{dt} = \gamma_{12}IC_1 - \Gamma_2C_2.$$  \quad (5.5)

The source for the triplet state, $\gamma_{12}IC_1$, can be approximated by $\gamma_{01}I^2C_0$ (i.e. the probability that a base state molecule is excited by two molecules almost immediately), given the very short time that the dye remains in singlet state.

Whilst the effect of photobleaching was immediately obvious in the experiment, at the time the images were captured it was not known that the effect was permanent and cumulative as it was expected that the dye would recover some short time later. It was discovered that this was not the case when the late-time calibrated densities were significantly lower than expected. This modifies the above concentration model equations by including two sink terms for the singlet and triplet states,

$$\frac{dC_0}{dt} = -\gamma_{01}I^2C_0 + \Gamma_1C_1 + \Gamma_2C_2$$  \quad (5.6)

$$\frac{dC_1}{dt} = \gamma_{01}IC_0 - \gamma_{12}IC_1 - \Gamma_1C_1 - f_1(C_1)$$
$$= \gamma_{01}IC_0 (1 - I) - \Gamma_1C_1 - f_1(C_1)$$  \quad (5.7)

$$\frac{dC_2}{dt} = \gamma_{12}IC_1 - \Gamma_2C_2 - f_2(C_2)$$
$$= \gamma_{01}I^2C_0 - \Gamma_2C_2 - f_2(C_2),$$  \quad (5.8)

where the sink terms of $f_1$ and $f_2$ represent the amount of excited dye that form covalent bonds with the surrounding molecules and are permanently bleached.
5.2 Exponential correction

As the reaction is a quantum mechanical process, the number of dye molecules able to fluoresce is expected to decay exponentially with time. To test this, at the end of an experiment the two layers are stirred together such that they are well mixed. When the fluid is quiescent, a number of scans are recorded. From this movie, a time average of each scan is taken and the mean intensity of each scan is plotted in figure 5.1a. From these data, a least squares fit to an exponential decay is fitted. This is shown in figure 5.1a and has a correlation coefficient of $R^2 = 0.96$. As there is no mixing, with the dye being evenly distributed and conserved with time, we can see that the damage caused by photobleaching results in an exponential decay of the intensity of R6G with time. The simplest correction for this is to divide the whole image by the fitted intensity at that time. The mean of those corrected images is shown in figure 5.1b, from which we can see that there is very little change with time especially when compared to figure 5.1a (note the change of scale in the intensity axis).

An uncorrected experiment image is shown in figure 5.2a with the exponential correction applied in figure 5.2b. Comparing figures 5.2a and 5.2b we can see that overall the correction is quite effective with the unmixed fluid in the upper and lower layer being almost uniform with $C = 1$ and 0 respectively. The fluid that is mixed in the opening has an intensity of $C = 0.5$, showing that on average it is well mixed. The bright region above the opening in the upper layer in figure 5.2b is inaccurately displaying an intensity of $C = 1.2$. This implies that the region is more dense than the rest of the unmixed fluid in the upper layer, which clearly is un-physical. Thus, this correction is too simple. By amplifying the whole image we have implicitly assumed that the bleached dye is uniformly distributed through the tank. However, this assumption clearly is not true with some regions, particularly those near the opening appearing much brighter and hence more dense than they are in reality after correcting.

It is necessary to correct only the bleached dye, which requires knowing where the bleached dye is distributed at any given time. This can be estimated by advecting two tracers (one each for the bleached and unbleached dye) using the stereo PIV that was recorded simultaneously with the LIF images. The hierarchy of models used to achieve this are discussed in the following sections.

5.3 Advection model

The simplest model is to advect two tracers about the domain. The first tracer, $C$, will be used to track the concentration of dye in both layers and the second, $F$, will be used to track the bleached dye. By also modelling the extent to which $F$ has been bleached, the LIF images can
Fig. 5.1 Mean intensity of each frame of a time averaged calibration movie shown in (a) with no correction and a least squares best fit (red), and (b) the same movie with the fitted exponential applied as a correction.
Fig. 5.2 The effect of the exponential correction at $t = 5 \text{ s}$, applied to a time series of one slice of LIF data. The uncorrected raw experimental image is shown in (a) the applied exponential correction in (b) and the corresponding colourbar for intensity in (c).
be corrected by
\[
Im_{\text{cor}} = Im_0 \frac{C}{F}
\] (5.9)
such that the original image is multiplied by the fraction \(C/F\).

In the previous section we deduced that the rate of bleaching was inversely proportional to the square of the thickness of the light sheet, which was itself an hourglass shape. Thus, to model the continuous bleaching effect of the laser we let \(I\) represent the inverse thickness of the light sheet. This inverse thickness, \(I\), has a maximum of 1 at the inflection point and decreases as a function of the estimated light sheet distance such that it has minimum at the top and bottom of the tank where the light sheet is thickest. Note that as the thickness of the light sheet is reduced, the volume illuminated is also reduced. Hence,

\[
\int_y IC \, dy = \text{const},
\] (5.10)
while
\[
\int_y I^2C \, dy
\] (5.11)
increases as \(I\) increases.

With this we can construct a set of governing equations for the tracers
\[
\frac{DC}{Dt} = 0,
\] (5.12)
\[
\frac{DF}{Dt} = -\beta I^2F,
\] (5.13)
where \(\beta\) is a constant that is determined from fitting to the exponential decay of the LIF images. Due to computational and experimental limitations, it was decided to only use the mean scan-averaged 2D velocity field rather than the full 3D field. This was justified as the dominant dynamics are 2D and the 3D scanning system sweeps the entire volume in one scan such that not all the motion in the tank is captured. Attempting to calculate the advection fully in three dimensions would slow the correction process greatly and would not necessarily produce significantly more accurate results than using the 2D field alone.

The system used to advect the tracers is a first order backwards Euler method, which was chosen for its simplicity, stability and speed. The initial setup was idealised, with the tracers set to 1 in the upper layer and 0 in the lower layer. No perturbation was applied to the interface as this is already captured in the PIV data.

Using each PIV slice from a scan is unlikely to accurately transport the tracer when used in combination. Each PIV slice represents a different plane, which can lead to large discontinuities...
between slices. To correct for this we use the time averaged velocity field,

$$\bar{u}(t) = \frac{1}{T} \int_{t'}^{t'+T} u \, dt'$$

(5.14)

with $T$ being the time taken for one scan to advect the tracer for $T$ s.

Whilst the PIV data captures the motion of the flow well, it does not necessarily guarantee a conservative field (i.e. the velocity field is not necessarily divergence free). The reason for this is that the time averaged velocity field is used instead of the instantaneous velocity. Additionally, there is experimental noise in the data. However, we can create a divergence free velocity field by solving the discrete Poisson equation for the streamfunction $\psi$,

$$\nabla^2 \psi = -\nabla \times u$$

(5.15)

$$u^* = \frac{\partial \psi}{\partial y}$$

(5.16)

$$v^* = -\frac{\partial \psi}{\partial x}$$

(5.17)

where $U^* = (u^*, v^*)$ represents the estimated divergence free velocity field. By solving equation (5.15) such that the left and right hand side match to within a tolerance of $10^{-10}$ we find that

$$\nabla \cdot U^* < 10^{-5}$$

(5.18)

with $U^*$ accurately representing $U$.

If the domain is discretised into $n \times m$ gridpoints, then the interior cells of the tracer are defined by $C[1 : n-1, 1 : m-1]$, similarly for $F$. To ensure that the tracer is conserved at the boundaries such that,

$$\frac{\partial C}{\partial n} = 0$$

(5.19)

where $n$ is the unit vector perpendicular to the boundary, the interior cells (i.e. the cells not on the boundary) are advected first before applying the update to the boundary. The solid boundaries are modelled by setting the exterior cells (i.e. the cells that do not contain dye information) equal to the mean of the neighbouring cells

$$C^{i+1}[0, :] = \frac{C^i[0, :] + C^{i+1}[1, :]}{2}$$

(5.20)

$$C^{i+1}[n, :] = \frac{C^{i+1}[n - 1, :] + C^i[n, :]}{2}$$

(5.21)
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\[ C^{i+1}[i,0] = \frac{C^i[i,0] + C^{i+1}[i,1]}{2}, \]  
\[ C^{i+1}[i,m] = \frac{C^{i+1}[i,m-1] + C^i[i,m]}{2}, \]

where the superscript refers to the time step. The interior boundary cells (i.e. the cells adjacent to the boundary, still within the domain) are set equal to the exterior boundary cells such that

\[ C[1,:] = C[0,:], \]  
\[ C[n-1,:] = C[n,:], \]  
\[ C[:1] = C[:0], \]  
\[ C[:m-1] = C[:m]. \]

With the above corrections, the tracer is conserved for the duration of advection.

A time series of the advected tracer is shown in figure 5.3. The tracer is initiated with a flat interface and advected using the appropriate time-averaged PIV velocity field \( U^* \). By comparing the time series of the LIF data to that of the tracer we will assess the qualitative success of each advection scheme (the details of the dynamics are discussed in chapter 4). Looking at the opening in figure 5.3a we can see that some mixing is occurring, however, it is limited to an unrealistically narrow strip. The small amount of vertical spreading near to the side wall is the result of the large vertical velocities (shown in figure 4.4). These vertical velocities rapidly carry the fluid in narrow strips along the boundaries. The entrainment and spreading of the tracer does not appear to be captured even as the tracer moves along the horizontal boundary. At the later time in figure 5.3b the interface remains narrow, with a periodic exchange shown to be caused by large fingers of tracer. This is not how the exchange occurs in experiments, where there is a large amount of mixing at the opening and an equal exchange of well mixed fluid into both layers. Looking at the right hand side of figure 5.3b we can see that the tracer is overturning as it is forced down the side wall. Parts of the tracer are carried either side of the barrier toward the opening.

At the much later time in figure 5.3c, the motion as discussed for figure 5.3b continues. The tracer has spread further through the layer, though still predominantly in narrow bands. Large regions of both layers are unchanged from their initial concentration with very little mixing of
the tracer occurring on the opening. The final image is not representative of the LIF images at a similar time. The layers are poorly mixed and only some of the features of the flow are captured by this advection model.

5.3.1 Including an initial perturbation

To assess the impact of including an initial perturbation we consider the case where a sinusoidal perturbation (comparable to that seen left by the RB in experimental) is applied to initial interface in the opening, a time series is shown in figure 5.4. The initial perturbation is a simple sine function with a wavelength comparable to that of the wake from the removal of the RB. The amplitude decreases quadratically with distance across the opening as a simple model of the growth from the RTI. A more complicated initial perturbation could be introduced. However, this is unlikely to have an effect on the evolution of the tracer as there is little difference between this case and that where no perturbation was applied (compare figures 5.3a and 5.4b). Comparing these images we can see that the interface is once again flat, with little mixing occurring there, and the transportation of the tracer is restricted to narrow fingers along the edges of the layers. At later times, figures 5.4c and 5.4d, there is little difference in the dispersion of the tracer throughout the layers when compared to the flat interface case. The most notable difference appears to be the change in the phase of the exchange across the opening.

5.3.2 Summary

While the advection model fails to accurately capture the physics of the mixing, it does provide some useful information that is not immediately obvious from looking at the PIV data. Looking at the regions either side of the barrier in figures 5.3b and 5.3c, we can see that the fluid that is fed back into the opening is carried in a narrow band from the opposite side of the tank. Interestingly, this narrow band appears to sit a small distance from the FB.

5.4 Advection turbulent diffusion

The advection-only model failed to capture the mixing of the fluid as it moved around the layer. It also struggled with the turbulent mixing and subsequent exchange of fluid across the opening. This is caused by only using the time-averaged velocity field. Such a field loses the turbulent motion responsible for large amounts of mixing. To attempt to capture these effects we use a
Fig. 5.3 Time series of tracer C for advection only scheme, with the appropriate colourbar for the intensity is shown in (d).
Fig. 5.4 Time series of tracer C for advection only scheme with an initial perturbation applied as shown in (a).
Reynolds decomposition, splitting the velocity as follows:

\[ \mathbf{u} = \mathbf{\bar{u}} + \mathbf{u}', \]  

where \( \mathbf{u}' = \mathbf{u}'(t) \) is the fluctuating velocity. From this we can calculate the turbulent intensity,

\[ \overline{u'^2} = \frac{1}{T} \int_0^T (u - \bar{u})^2 \, dt. \]  

Following Taylor (1921), we can introduce a turbulent diffusivity term in the advection equations, equations (5.12) and (5.13), such that

\[ \frac{DC}{Dt} = \kappa_T \nabla^2 C, \]  
\[ \frac{DF}{Dt} = \kappa_T \nabla^2 F - \beta \overline{t^2 F}, \]

where \( \kappa_T = \bar{u}L_T \) is the eddy diffusivity and \( L_T \) the integral length scale. The choice of \( L_T \) is taken to be the resolution of the PIV, such that \( L_T = 6 \) mm. This is the smallest scale captured by the PIV.

A time series is shown in figure 5.5. Again a flat interface was chosen to initiate the tracer. Starting with the opening in figure 5.5a, the interface extends much further from the centre, with significantly more mixing occurring than in the advection-only system. However, it should be noted that this interface still appears significantly smaller and less mixed than that seen in experiments. This mixing continues along the boundaries, with the tracer clearly entraining more as it is advected. In particular, looking at the movement of the lower boundary, the tracer displays the distinctive overturning of the frontal nose of a gravity current.

Looking at the overturning region on the right hand side of figure 5.5b, the extent of overturning is similar to that seen in figure 5.3b, however, now the overturning has interacted much more with the surrounding tracer. The transportation of the tracer onto the interface is no longer limited to a narrow band and now encompasses a mixed mass filling a third of each layer either side of the barrier. Only a small part of this mixed tracer moves onto the opening, with a large proportion being entrained by the motion up the side walls.

Looking at the late-time structure in figure 5.5c, the tracer has mixed moderately through both layers, though unrealistically large regions of unmixed tracer remain in both layers. While the addition of the turbulent diffusion term has mixed the narrow streaks seen in the advection-only model, neither layer is as well mixed as it should be at this late time. This appears to be caused by the flux across the opening being too small and the tracer being poorly mixed in the opening.
5.5 Advection, turbulent diffusion and RT mixing region

From experiments, we observe that there is a bidirectional exchange of mixed fluid through the opening that the advection-diffusion system above is unable to capture accurately. The problem appears to be that a large proportion of the mixing and exchange are occurring on a scale that is smaller than the PIV system, as set up here, is able to record. Thus we must develop a suitable subgrid-scale model for the mixing in the opening to account for the large scale motion that is observable.

The inclusion of turbulent diffusion generated significantly more mixing than the advection-only model. However, it still fails to account for the turbulent transfer of fluid across the opening, which is clearly observable in the LIF images. The problem appears to be that the highly turbulent nature of the transport in the opening is occurring on a length scale lower than the resolution of the PIV velocity field. Because there are no clear velocities connecting the two layers being captured in the mixing region, tracers from each layer are not being advected across the interface. This results in the large-scale motion (i.e. growth of the mixing region) being captured but not the process by which fluid is transferred across the opening from one layer to the other.

To account for the motions that are not being captured we need to develop a subgrid scale model for the RT transport across the opening. To do this we follow a method similar to Ramaprabhu and Andrews (2004), allowing the r.m.s. vertical velocity, \( v_{rms} \), to be related to the width of the self-similar RT mixing zone \( h \) by

\[
v_{rms} = \frac{dh}{dt} = 2\alpha Agt. \tag{5.32}
\]

As the velocity moving off the FB is approximately laminar (i.e. flowing in a parallel plane to the FB), we can use the relation derived by Ramaprabhu and Andrews (2004) for the width of the RTI mixing region for two streams of fluid moving off a splitting plate,

\[
h = \alpha Ag \left[ \frac{x - x_0}{U_b} \right]^2. \tag{5.33}
\]

Here \( x_0 \) is a virtual origin accounting for the effect of the FB and \( U_b \) is the upstream horizontal velocity off the FB. By using appropriate values from the experimental data, with \( U_b \) being
Fig. 5.5 Time series of tracer $C$ for advection and turbulent diffusion scheme.
calculated as the mean of the horizontal velocity from both sides of the FB we can write \( v_{rms} \) as

\[
v_{rms} = 2\alpha Ag \frac{x - x_0}{U_b}.
\]

(5.34)

Using dimensional analysis we can write an r.m.s vorticity, \( \omega_{rms} \), as

\[
\omega_{rms} \approx \frac{v_{rms}}{\lambda},
\]

(5.35)

where \( \lambda \) is the horizontal integral length scale taken to be the regular wavelength visible in the LIF images. Finally, to account for the movement of the stream we multiply \( \omega_{rms} \) by a time varying component giving the vorticity perturbation in the opening,

\[
\omega = 2\alpha Ag \frac{x - x_0}{\lambda U_b} \sin (kx + \Omega t),
\]

(5.36)

where \( k = 2\pi/\lambda, \ \Omega = 2\pi/T \) and \( T = (\gamma L)/U_b \) is the time period for a parcel of fluid to traverse the opening. Then \( \omega \) is added to the vorticity field of the PIV along the centre-line of the opening such that the Poisson equation in equations 5.15 is updated to be

\[
\nabla^2 \psi = -\nabla \times \overrightarrow{u} - \omega \delta(z).
\]

(5.37)

When solved this produces a divergence free velocity field that is then used to advect the tracers.

The time evolution of this model is shown in figure 5.6. Starting first with the opening in figure 5.6a, the interface is now significantly broader and resembles much more closely what is seen in experiments. As we move from the edge of the FB to the side wall, the tracer from either layer progressively mixes until it is well mixed at the side wall. The mixed fluid then forms comparable wall plumes up both side walls, which are seen to entrain as they move. The overturning region is significantly larger than in the previous model, which is the result of the larger flux of better mixed tracer through the opening.

Looking at the later time in figure 5.6b, both layers appear much more substantially mixed than the latest time of the advection-diffusion model in figure 5.5c. This is again evidence of the greater exchange of tracer between the layer more accurately representing the physics of the problem. At late times the width of the mixing region grows quadratically with distance from the end of the FB with the region next to the wall becoming well mixed.

By the latest time (see figure 5.6c), the layers appear substantially more mixed than in any of the previous models, evidence that the model applied at the interface is working more effectively to transport the tracer between the layers. This also demonstrates that the turbulent intensity is more accurately capturing the mixing generated by turbulence in either layer. Interestingly, the
narrow unmixed region located either side of the FB has remained constant throughout all of
the models. The final result shows that there is still significant available potential energy left in
the system which could be used for mixing.

5.5.1 Summary

The effect of the advection, turbulent diffusion and RT mixing region model on experimental
LIF imagery is shown for an early and late time in figure 5.7. Looking at the early time (see
figure 5.7a), the photobleaching arc identified in the introduction to section 5.1 is still visible,
though much reduced when compared to the early correction. However, at later times when
more of the dye has been distributed about the layer, the photobleaching arc is not as visible
(see figure 5.7b). Indeed looking at subsequent late time images (not shown here) the model
described in section 5.5 works for the remaining duration of the experiment. This is despite a
clear photobleached arc appearing throughout all the uncorrected experimental images.

5.6 Quenching and combined model

The advection-diffusion correction captures the mid to late time decay of dye well, neither
over or under correcting. However, it fails to capture the early time bleaching of the dye. This
implies that there is a disparity between the early and late time photobleaching. The most
obvious difference between early and late times is the chemical composition of the layers. At
early times the upper layer is primarily a NaNO$_3$ solution and the lower layer is primarily NaCl.
At later times the layers are much more mixed. Experiments conducted by the author suggest
that R6G is unaffected by long term exposure to both NaNO$_3$ and NaCl solutions. However,
the NaNO$_3$ solution produced noticeably brighter images than the NaCl solution despite the
same concentration of rhodamine being used. The reason for this difference is believed to
be caused by a process called quenching, which is where NaCl ions aggressively capture the
electrons from fluorescent dyes, thereby preventing them from fluorescing (Lakowicz, 2006).

It appears as though the photobleaching decay is greater in the predominantly NaNO$_3$
solution where the excited R6G molecules can only form permanent covalent bonds with
NaNO$_3$. However, in the presence of NaCl the excited R6G molecule can lose its electron to
an NaCl ion via quenching. The process of quenching prevents a photon from being fluoresced
and so appears identical to photobleaching, however, unlike photobleaching the process is not
permanent. The captured electron can be returned to a quenched R6G molecule enabling it
fluoresce again. This modifies our earlier expression for the base, singlet and triplet states in
Fig. 5.6 Time series of tracer $C$ for advection, turbulent diffusion and model RT growth scheme.
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Fig. 5.7 Corrected LIF image using the advection-diffusion model shown at an early time, \( t = 7 \) s, in (a) and late time, \( t = 38 \) s, in (b), with the appropriate colourbar for the intensity shown in (c).

Equations (5.6) to (5.8) to be

\[
\frac{dC_0}{dt} = -\gamma_0 I C_0 + \Gamma_1 C_1 + \Gamma_2 C_2 + g_1 \left( C_1, [Cl] \right) + g_2 \left( C_2, [Cl] \right) \tag{5.38}
\]

\[
\frac{dC_1}{dt} = \gamma_0 I C_0 - g_1 \left( C_1, [Cl] \right) - f_1 \left( C_1 \right) - g_1 \left( C_1, [Cl] \right) \tag{5.39}
\]

\[
\frac{dC_2}{dt} = \gamma_1 I C_1 - f_2 (C_2) - g_2 \left( C_1, [Cl] \right) \tag{5.40}
\]

where \( g_1 \) and \( g_2 \) represent the proportion of dye that is lost to quenching when excited to the singlet and triplet states respectively.

To accurately capture this additional process in our advection model we must now include the expected concentration of NaCl ions, \( (1 - C) \). We present a combined model of photo-bleaching decay plus a quenching growth model, for which a cartoon is shown in figure 5.8. This figure demonstrates the assumptions of this model. As the photobleaching arc was visible
in early times of figure 5.7a we assume a faster photobleaching than was previously used in section 5.5. The effect of quenching is not significant at early times as there is little to no NaCl interacting with R6G. As the two layers mix, and the quantity of NaCl in contact with R6G increases, so too does the effect of the quenching term. The decay of the combined model decreases and approaches the (accurate) late time decay of the original advection-diffusion photobleaching model, as demonstrated by figure 5.8.

The effect of the combined correction applied to experimental data is again shown for early and late times in figure 5.9. At early times the effect of the photobleached arc is no longer visible (see figure 5.9a). Indeed this improved decay correction continues to work well for the full duration of the experiment, as shown by the late time image in figure 5.9b.

A more quantitative comparison is shown in figure 5.10. Here we plot the mean intensity of the full tank for each full scan for: uncorrected, photobleaching only and combined photobleaching and quenching effects. In a perfect scenario, the mean intensity of the full tank would be expected to be 0.5 for all time. However, it is expected that experimental data would have some variation from this, there being a time delay between scanning the front and rear of the tank, while mixing continues. Looking at figure 5.10, we see that without correcting the data the mean intensity data decreases by more than 10% over the course of an experiment. As seen in the previous sections, by including a photobleaching correction, initially the mean intensity is very close to 0.5. However, at later times the photobleaching correction is insufficient and results in a mean intensity significantly beneath 0.5. The combined correction system produces a near constant value for the full duration of the experiment, decreasing by only 2%.
Fig. 5.9 Corrected LIF image using the full quenched advection-diffusion model at early times, $t = 7$ s, in (a) and late time, $t = 38$ s, in (b), with the appropriate colourbar for the intensity is shown in figure 5.7c.

Fig. 5.10 Mean intensity of $\gamma = 0.50$ LIF data, comparing the different correction regimes against no correction.
5.7 **Summary and application to LIF images**

This chapter has shown that the previously unrecognised effects of photobleaching and quenching can both dramatically reduce the recorded intensity of an LIF image and thus distort the density field in an physical manner. These effects must be accounted for correctly in the analysis of LIF data. We present an innovative post-processing technique that uses PIV data to advect a tracer. This allows us to track the location and condition of the dye. Where the velocity field from the PIV data was insufficiently resolved, well-developed theory was used to supplement the velocity field such that the tracer was advected in a physically accurate way.

The combined photobleaching and quenching correction procedure derived in this chapter will be used to correct all LIF data calculated throughout the remainder of this thesis, unless otherwise stated. This correction forms a crucial cornerstone for the analysis of 3D LIF density analysis in this thesis. Without this correction it is likely that the quality of the data, its subsequent discussion and the conclusions drawn from it would suffer significantly.

It is expected, as the cost of lasers decrease, and as researchers within the field of experimental fluid dynamics continue to seek to increase the accuracy, precision and quality of their data, that more laboratories will begin to use lasers as their primary source of fluorescent dye illumination. Previously, it may have been assumed that the fluorescent intensity of laser illuminated dye is conserved. We have shown here that this assumption can be incorrect. If, as is seen in this thesis, the dye’s fluorescence is not conserved, great care must be taken to correct the data to ensure that the dye’s fluorescence, and therefore density, is conserved for all time. It is hoped that the novel techniques and ideas of this chapter could be applied to or adapted for use in a wide range of experimental scenarios.
Chapter 6

Singly Connected Domain

6.1 Introduction

This chapter discusses the case where there is a single opening connecting the two layers, which we call the ‘singly connected’ case. The obstruction is created by securing a thin fixed barrier constructed of polycarbonate on the right hand side of the tank, the side through which the removable (steel) barrier is withdrawn as described in chapter 2. The introduction of the obstruction results in dramatically different dynamics from classical RT problems. To understand this process, experimental data and numerical ILES data will be used in unison, with, where appropriate, the numerical data used to supplement and provide further insight from the experimental data.

6.1.1 Setup

The three-dimensional data that will be presented in this chapter were collected by the laser scanning system discussed in section 2.5. The LIF data is then post processed using the techniques presented in chapter 5 to ensure the results are as accurate as possible. Where a $y$ depth average is used, one scan from the back to front (or front to back) is taken as a single time step of 2.05 s, the time taken for the laser to complete one scan front to back. The dimensions and parameters for the domain are shown in figure 1.1.

6.2 Mean concentration profile

A commonly used method to visualise the width of the mixing region uses the plane averaged concentration field $\overline{C}(z,t)$, where $C = (\rho - \rho_L)/\Delta \rho$ is the concentration and the overbar represents an averaging over the horizontal plane. This is plotted against time in figure 6.1 for
Fig. 6.1 Development of the mean concentration density profile for the classical RTI MOBILE simulation at resolution $256 \times 256 \times 512$. The superimposed coloured curves represent the quadratic growth of the similarity law with $\alpha = 0.025, 0.03$ and $0.05$ in red, green and black respectively.

the classical unobstructed case from a MOBILE simulation. Unfortunately the 3D scanned experimental data was corrupted at the point of the recording and this was not seen until the data was more thoroughly analysed later. As such there is no experimental data for the classical unobstructed domain and simulation data will be used instead. The colour scheme varies from turquoise for $\bar{C} = 0$, the initial concentration for lower layer at $t = 0$, to yellow for $\bar{C} = 1$, the initial concentration for the upper layer. The colour scheme tends towards black when the mean concentration of a layer is well mixed such that $\bar{C} = 0.5$.

The mixing zone of the classical RTI is known to grow quadratically with time, as found by Youngs (1984), such that $h = \alpha A t^2$. This model is superimposed on the mean concentration field with values of $\alpha = 0.025, 0.03$ and $0.05$ in red, green and black respectively. This range of values was chosen because high resolution simulations by Dimonte et al. (2004) found $\alpha = 0.025$ to be most accurate, whilst Lawrie (2009) used $0.03$. For experimental data with non-idealised initial conditions larger values such as $0.05$ were seen to be more appropriate (Dalziel et al., 1999).

Looking at figure 6.1, we can see that quadratic growth with $\alpha = 0.025$ best captures the growth of the RT mixing zone for a simulation initialised with ideal initial conditions. Looking at the dye profile in figure 6.1, we can see that at early times, $\tau = 3$, that there has been a large displacement of the initial fluid from the central region, $|z/H| < 0.05$, such that equal quantities of upper and lower layer fluid now exist at this height. We saw in chapter 4 that the motion in the central region was highly turbulent, such that it can be reasonably assumed that regions with $\bar{C} \approx 0.5$ are areas in which fluid is well mixed. Returning to figure 6.1 we observe
that the first well mixed fluid is seen along the $z = 0$ line and that this spreads vertically out towards $z/H = \pm 0.5$

### 6.2.1 Obstructed data

Figures 6.2 and 6.3 show the mean concentration profiles calculated from 3D scanned experimental LIF data and MOBILE simulation data respectively for openings with $\gamma = 0.75$, 0.50 and 0.25. The experimental profiles have been post-processed using the combined photobleaching-quenching method described in section 5.6. The time, $\tau$, shown in figure 6.2 is the non-dimensional time measured from where the RB is first opened. The removal of the RB is initiated manually and so human reaction time slightly modifies the position within a scan at which the RB was opened. However, this only limits the number of slices available for analysis in the first scan. The time, $\tau$, shown in figure 6.3 is the non-dimensional time from the start of the simulation.

As for the classical unobstructed ILES concentration shown in figure 6.1, the quadratic growth with time is superimposed here for all openings presented in figures 6.2 and 6.3. Looking at figures 6.3a to 6.3c we can see that, as for the classical case, the $\alpha = 0.025$ envelope most accurately captures the growth of the mixing region. However, for figures 6.2a to 6.2c, we can see that both $\alpha = 0.025$ and 0.03 underestimate the growth of the initial mixing and that $\alpha = 0.05$ more accurately fits the envelope for the growth of the mixing region. Similar results were seen by Dalziel et al. (1999) and appear to be caused by differences in the large scale initial conditions generated by the barrier versus the typical idealised small random perturbations used in numerical simulations. This effect is investigated further in appendix A.

We first discuss the case with the largest opening, $\gamma = 0.75$, (see figures 6.2a and 6.3a). The FB prevents all of the fluid along $z = 0$ from being mixed (as was seen in the classical case, where $\bar{C} = 0.5$ along $z = 0$ in figure 6.1). For the obstructed case some fluid is trapped by the FB, preventing it from mixing and resulting in the sharp divide in $\bar{C}$ across $z = 0$. The circulation induced by the FB causes mixed fluid from $z = 0$ to be transported along the side walls to $z/H = \pm 0.5$, visible by $\bar{C} = 0.5$ at $\tau = 5$ and 6 for figures 6.2a and 6.3a respectively. The fluid that was transported away from $z = 0$ is replaced by unmixed fluid trapped by the FB from the rest of the layer. Thus the first (fully) mixed region is seen along $z/H = \pm 0.5$, the opposite of the classical unobstructed case in figure 6.1 where $z/H = \pm 0.5$ was the last region to change and the mixing region spread vertically from $z = 0$.

The mixed fluid that is transported to $z/H = \pm 0.5$ forms a locally stable stratification above the unmixed fluid in the upper layer and beneath it in the lower layer. It is only the result of the circulation in the rest of the layer that these regions overturn and are advected towards $z = 0$. 
Fig. 6.2 Development of mean concentration profile for the singly connected domain taken from 3D scanned LIF data, with openings of (a) $\gamma = 0.75$, (b) $\gamma = 0.50$ and (c) $\gamma = 0.25$. The colourbar for the mean concentration $\bar{C}$ is shown in (d). The superimposed coloured curves represent the quadratic growth of Youngs (1984) similarity law with $\alpha = 0.025$, 0.03 and 0.05 in red, green and black respectively.
Fig. 6.3 Development of the mean concentration profile for the singly connected domain taken from MOBILE simulations at resolution $256 \times 256 \times 512$, with openings of (a) $\gamma = 0.75$, (b) $\gamma = 0.50$ and (c) $\gamma = 0.25$. The colourbar for the mean concentration $\bar{C}$ is shown in (d). The superimposed coloured curves represent the quadratic growth of the similarity law with $\alpha = 0.025$, 0.03 and 0.05 in red, green and black respectively.
This is observed in the mean concentration profiles of figures 6.2a and 6.3a by $C = 0.5$ being observed first at $z/H = \pm 0.5$ before spreading towards $z = 0$ as time progresses.

No more experimental data is presented for $\gamma = 0.75$ beyond $\tau = 8$ as the LIF image by this time is almost identical to the well mixed final calibration image. As processing the LIF image requires division by the end calibration image, small variations caused by noise or flickers in the light sheet dominate and give inaccurate changes in the concentration. An example of this can be seen at $\tau = 8, z/H = -0.5$ in figure 6.2a where the concentration is much larger than would be expected when compared to the similar profile in figure 6.3a and demonstrated later in a conductivity probe measurement, see figure 6.6. Looking at the later times ($\tau > 8$) in figure 6.3a we can see that the circulation continues to mix fluid with the mean concentration profile, steadily approaching $C = 0.5$ at $\tau = 25$.

Next, we discuss the $\gamma = 0.50$ profiles (see figures 6.2b and 6.3b), which at early times ($\tau \leq 4$ and 5 respectively) appear quite similar to early time growth of the $\gamma = 0.75$ profiles. However, the larger FB prevents more fluid from mixing along $z = 0$, resulting in a decrease in the rate of change of $C$ in the interfacial region. Observe that compared to the $\gamma = 0.75$ case there is a larger region of fluid closer to the initial concentration at $\tau = 4 - 5$ and 5 - 6 for figures 6.2b and 6.3b respectively.

As for the $\gamma = 0.75$ case, the fastest change in concentration occurs at $z/H = \pm 0.5$ as fluid from each layer is transported across $z = 0$ up the side walls to the horizontal boundaries along $z/H = \pm 0.5$ where it mixes with the ambient. However, the change along $z/H = \pm 0.5$ at $\tau = 5$ and 6 in figures 6.2b and 6.3b is greatly reduced from what was seen in figures 6.2a and 6.3a. The smaller opening reduces the size of the mixing region which in turn reduces the volume flux between the two layers.

Despite the smaller fluxes through the opening, we can see that the mixed fluid along $z/H = \pm 0.5$ is recirculated back onto $z = 0$ at $\tau = 7$ and 8 for figures 6.2b and 6.3b respectively, the same time as was seen for figures 6.2a and 6.3a. However, the smaller flux does reduce the rate of change in concentration along $z = 0$. These smaller fluxes also reduce the rate of mixing as after $\tau = 8$ there is a larger density difference between the two layers for both experimental and numerical data.

The density difference between the two layers again drives continued circulation in each layer, though due to the larger density difference preserved between the two layers with the larger obstruction of $\gamma = 0.50$, the circulation persists for much longer. Looking at figures 6.2b and 6.3b, we can see the continued recirculation resulting in concentration change towards $C = 0.5$ along $z/H = 0.5$ leads the change in the rest of the layer from $\tau = 10$ and 11 respectively. The mean concentration of each layer can be seen to tend towards $C = 0.5$ with the concentration near $z = 0$ lagging behind the rest of the layer.
Mean concentration profiles for smallest opening, $\gamma = 0.25$, are shown in figures 6.2c and 6.3c. As expected, the much smaller opening reduces the rate of change of $C$ for both experimental and numerical data when compared to the $\gamma = 0.50$ and 0.75 profiles. The concentration change along $z/H = \pm 0.5$ still occurs at a similar time to the other opening sizes but, due to the reduced flux through the opening, the rate of change in $C$ is significantly reduced.

Despite the larger obstruction, a circulation is still established in each layer such that the density change along $z/H = \pm 0.5$ still leads the concentration changes in the rest of the layer. The larger obstruction now traps more fluid, resulting in a greater volume of relatively unmixed fluid in the interfacial region in figures 6.2c and 6.3c. However, despite this smaller opening, fluid is still recirculated around each layer from $z/H = \pm 0.5$ back onto $z = 0$ at $\tau = 8$ and 9 for experimental and numerical data respectively. Note that this is slightly later than for the same recirculation in the $\gamma = 0.75$ and 0.50 cases.

At later times of $\tau > 10$, the experimental and numerical profiles appear very similar, with the visible effect of a circulation having been established for long times indicated by the mean concentration profile along $z/H = \pm 0.5$ leading the change in each layer in figures 6.2c and 6.3c. The circulation is maintained by the consistent density difference between the layers visible until late times in both figures 6.2c and 6.3c.

The numerical data in figure 6.3 appears much smoother than the experimental data in figure 6.2 as a result of the different methods for producing a 3D concentration field. MOBILE prints a full 3D field snapshot every time step, whereas experimental mean concentration calculation is spread out over a full scan. Thus, the changes caused by the mixing of the two layers appear more abrupt in the experimental concentration profiles.

As a result of the increased time resolution of the numerical data, we can observe more fine scale structure in the development of the mean concentration profiles. In particular looking at $z = 0$ for $\tau = 5 - 10$ in figures 6.3b and 6.3c, we can see distinctive periodic curves extending from $z = 0$ to $z/H = \pm 0.5$. These curves appear alternately in each layer, suggesting that there are temporary disruptions in the bidirectional exchange of fluid between each layer, with large bursts of lower layer fluid being exchanged into the upper layer and then vice versa.

As these effects are only seen after $\tau = 5$, it can be assumed that the disruption in bidirectional exchange is due to turbulent fluid from the layer-wide circulation moving onto the opening. As the stream flowing off the barrier is no longer composed of just the initial density fluid, instead it is composed of mixed fluid, the flow is neither laminar nor are the buoyancy and kinetic energy of either stream necessarily equal. This can result in one stream dominating over the other in the opening.
This motion appears most commonly in figure 6.3c, becoming less obvious in figure 6.3a, suggesting that in a large opening, where the RTI is able to grow for longer, and become more turbulent, there is ultimately a reduction in these differences. Instead, for smaller openings, the two streams are kept apart for longer and the RTI has less time to develop into turbulence, resulting in the differences in buoyancy and energy having a greater impact on the exchange between the two layers. These periodic curves were not captured in the experimental data. They may exist, but due to recording frequency it is unlikely that they would be captured in the data.

Despite the difference in dynamics, there are also similarities to the classical case. The most notable is that the timescale for fluid to be first transported from \( z = 0 \) to \( z/H = \pm 0.5 \) is the same for the numerical simulations of the classical and obstructed data. This timescale is slightly longer than in the experiments, which found that the mixing region reached the horizontal boundaries at \( \tau = 3 \). This difference is expected due to the differences in initial conditions between experiment and numerics.

The rate at which fluid is transported from \( z = 0 \) is nearly the same for all cases, as made clear by the red and black superimposed lines, which provide a near perfect envelope for the change in density from the initial value for numerical and experimental data respectively. This is caused by the initial perturbation to the interface growing under the RTI and spreading into each layer. Thus the initial rate that fluid can be transferred between the two layers is enveloped by the growth of the RTI. This is a surprising result, as the initial exchange between the two layers can be considered similar to a starting plume, whose maximum height is expected to grow as \( z \sim t^{3/4} \) (Ai et al., 2006). This is significantly slower than the \( t^2 \) growth of the RTI, showing that the growth of the starting plumes is accelerated by the mixing of the RTI on the open interface.

### 6.3 Vertical density profiles

Vertical profiles of the horizontal-mean density for the unobstructed classical MOBILE data are plotted in figure 6.4 and for three singly connected cases with \( \gamma = 0.75, 0.50 \) and 0.25 in figure 6.5 for experimental and numerical data. The mean density of the horizontal plane is plotted as series of lines for different times. The initial profile for all the figures was \( \hat{\rho} = -0.5 \) for \(-0.5 < z/H < 0\) and \( \hat{\rho} = 0.5 \) for \(0 < z/H < 0.5\). The change in time is represented by the changing colour of lines with the relevant colourbar attached to each figure. It is worth noting that each figure has a different time scale, with respective changes in the colourbar axes. This accounts for the different times for mixing for each of the opening sizes. Plotted on each figure, as a dashed black line, is a perfectly mixed profile, \( \hat{\rho} = 0 \) for all \( z \).
Looking first at the classical density profile evolution in figure 6.4, the profile can be seen to change first along $z = 0$ as the RTI grows on the interface between the two layers. The anticipated quadratic growth of the height of the RTI mixing as it fills the domain is represented here by the curved density profiles for $\tau = 0 - 4$. After $\tau = 4$ the mixing zone has spread the full height of the domain. The large spacing between the lines for $\tau = 4 - 8$ indicates rapid mixing across the full height of the domain.

The overturning nature of the classical RTI is seen by the increased curvature of the profiles for $\tau = 6 - 8$. The density along $z/H = \pm 0.5$ is much closer to $\hat{\rho} = 0$ (the perfectly mixed density) than the density between $0.25 < |z/H| = < 0.4$. The length scale of the RTI mixing zone continues to grow until it is comparable to the size of the domain. This results in relatively unmixed fluid at the edge of the mixing region from one layer being transported to the horizontal boundary of the other layer before it has been perfectly mixed. This is why the density at $z/H = \pm 0.5$ can be seen to change before the rest of the layer.

As the domain continues to mix from $\tau = 8$ onwards, the density of each layer becomes more homogeneous, as indicated by the significant increase in the gradient of the profiles. However, the domain is not perfectly mixed and significant amounts of overturning can be seen in each layer. This is made evident in the upper layer by the large concentration of lines to
Singly Connected Domain

the left of $\dot{\rho} = 0$ for $z/H = 0 - 0.25$ and, similarly, in the lower layer for $z/H = -0.1$ to $-0.4$ (though it is less clear in this layer). This motion results in a near stable stratification at around $\tau = 10$. The subsequent change in density profiles is now much slower than at the early times, as the vertical density variation, the driving force for mixing, is now greatly reduced. The density profile is changed very slightly and slowly as the remaining motion gradually mixes the two layers.

The final stratification, indicated by the solid black line, is almost perfectly mixed when compared to the initial stratification. However, compared to the uniform stratification shown by the dashed black line there is a clear final stable stratification.

6.3.1 Obstructed data

In this section, comparisons between the singly connected and classical density profiles will be made for both experimental and numerical data. The first case considered will be that with $\gamma = 0.75$, the smallest obstruction, and, as such, the case that is most similar to the classical case. After that, the two cases with larger obstructions, $\gamma = 0.50$ and 0.25, will be discussed.

Figure 6.5 presents the vertical profile of the horizontal-mean density for openings with $\gamma = 0.75$, 0.50 and 0.25 for both the 3D scanned and numerical simulation data. Note that non-dimensional time is shown indicated by the colourbar on the right of each plot, the values of which vary for each plot.

We first consider the case with the largest opening, $\gamma = 0.75$, see figures 6.5a and 6.5b. For $\tau < 3$ and 5 for experimental and numerical data respectively, the growth of the initial perturbation is made visible by the change in profiles occurring first along $z = 0$ before spreading towards $z/H = \pm 0.5$, similar to early changes seen for the classical data in figure 6.4. However, after this time there is a stark change in the evolution of the density profiles. In the classical case, at early times, the density changed most rapidly at the interface, $z = 0$. However, looking at figures 6.5a and 6.5b, at $\tau \approx 4.5$ and 6 respectively, we can see that the density in the region with $|z/H| < 0.25$ has not changed significantly from its initial value. Indeed it is approximately constant in each layer with $|\dot{\rho} \approx 0.35|$. Instead the largest change in density, at early times, occurs along $z/H = \pm 0.5$, the opposite to what was observed in the classical case.

The density profiles adopt a hook like shape whereby the density along $z/H = \pm 0.5$ leads the change in the rest of the layer, with the density along $z = 0$ lagging behind. Interestingly, in both figures 6.5a and 6.5b, at $\tau \approx 5.5$ and 20 respectively, the density profile along $z/H = \pm 0.5$ crosses to the opposite sign in density than for the rest of the layer. This is evidence of an overturning process, where fluid from one layer is transported to the horizontal boundary of the other. As was seen in figure 6.4, overturning regions produce stable stratifications that are difficult to mix. However, the inclusion of an obstruction along $z = 0$ enforces a density
6.3 Vertical density profiles

![Fig. 6.5](image)

**Fig. 6.5** Vertical profiles of the horizontal-mean density for the singly connected domain, with openings of (a,b) $\gamma = 0.75$, (c,d) $\gamma = 0.50$ and (e,f) $\gamma = 0.25$, for experimental LIF and numerical data respectively i.e. in the left and right hand columns. The experimental profiles have a time separation of: (a) $\delta \tau = 0.74$, (c) $\delta \tau = 0.74$ and (d) $\delta \tau = 0.96$, while for the numerical data in (b,d,f) the time separation is $\delta \tau = 0.31$. 

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difference across the interface. This continues to support circulatory motion in each layer such that fluid along \( z/H = \pm 0.5 \) is transported back into the layer and mixed.

Both layers continue to mix via this circulatory motion. At \( \tau = 4.5 \) the density difference between \( z/H = \pm 0.5 \) and \( z = 0 \) is \( |\Delta \hat{\rho}| \approx 0.5 \) and 0.3 for the upper and lower layer respectively. By \( \tau = 8 \), this density difference has reduced to zero, \( |\Delta \hat{\rho}| \approx 0 \), in both layers (see figure 6.5a). Asymmetries between the upper and lower layer are likely due to variations in the intensity of the light sheet between the experimental movie and final calibration at late times.

The numerical data indicates similar mixing behaviour to the experimental data (see figure 6.5b), resulting in nearly homogeneous layers from \( \tau = 18 \) onwards. As the density difference between the two layers is reduced, so too is the mixing rate and the separation between subsequent density profiles decreases. The increased run time of the numerical data allows us to see that the circulation in each layer continues to quasi-stably mix the layers until the final stratification almost reaches \( \hat{\rho} = 0 \) (perfectly mixed) for the full depth. It is interesting that there is a significant difference between the final profile of figure 6.5b and that of figure 6.4. This shows that the introduction of a obstruction has resulted in a much more uniformly mixed final state than the classical case, itself renowned for its efficiency at mixing layers of fluid.

If we now consider the \( \gamma = 0.50 \) profiles (figures 6.5c and 6.5d) we can see that initial, early-time profiles (for \( \tau < 3 \) and 5 respectively) are similar to the density changes seen for \( \gamma = 0.75 \) in figures 6.5a and 6.5b. The smaller opening size can be observed to reduce the difference in density between \( z/H = \pm 0.5 \) and \( z = 0 \) at \( \tau = 4.5 \) from \( |\Delta \hat{\rho}| \approx 0.5 \) and 0.3 for the upper and lower layer of figure 6.5a to \( |\Delta \hat{\rho}| \approx 0.1 \) and 0.15 for the upper and lower layer of figure 6.5c. We see similar results for the upper and lower layer numerical data, where \( |\Delta \hat{\rho}| \approx 0.3 \) (for both layers) at \( \tau = 7 \) in figure 6.5b and \( |\Delta \hat{\rho}| \approx 0.15 \) at \( \tau = 7 \) in figure 6.5d. This reduction in density difference is due to the smaller opening, \( \gamma = 0.50 \), limiting the rate that fluid can be transferred from each layer to the horizontal boundaries.

The decreased flux has the other notable effect of making the layers significantly more homogeneous with depth, observed by comparing figures 6.5a and 6.5c for \( \tau > 7 \) and, similarly, figures 6.5b and 6.5d for \( \tau > 10 \). After these times the density change in each of the layers is observed to slow significantly. However, the density difference across the interface is sufficient to maintain the circulation in each layer such that each layer is steadily mixed towards \( \hat{\rho} = 0 \). Note, though, that because of the circulation of fluid around the full layer, the density change along \( z/H = \pm 0.5 \) leads the change in the rest of the layer.

The simulation ends before a stable final density is reached. The reason for this early termination is that the evolution at this time was extremely slow. It was decided that the extra information was not worth the computational cost. Comparing the evolution of the density profiles for \( \gamma = 0.50 \) to \( \gamma = 0.75 \), it is expected that the final stratification for \( \gamma = 0.50 \) would
be closer to $\hat{\rho} = 0$ than in the $\gamma = 0.75$ case, which itself was almost indistinguishable from $\hat{\rho} = 0$.

The smallest opening case considered, $\gamma = 0.25$, is shown in figures 6.5e and 6.5f for experimental and numerical data respectively. As a result of the much smaller opening, the size of the initial mixing region is reduced. This in turn decreases the change in density along $z/H = \pm 0.5$ at early times for both experimental and numerical data, with $|\hat{\rho} = 0.4|$ along $z/H = \pm 0.5$ at $\tau = 3$ in figure 6.5e compared to $|\hat{\rho} = 0.25|$ and $|\hat{\rho} = 0.3|$ for figures 6.5a and 6.5c respectively. Similar values are seen for the numerical data in figure 6.5f where $|\hat{\rho} = 0.45|$ along $z/H = \pm 0.5$ at $\tau = 5$ compared to $|\hat{\rho} = 0.25|$ and $|\hat{\rho} = 0.35|$ for figures 6.5b and 6.5d respectively.

As for the other obstructed cases, the density change along $z/H = \pm 0.5$ leads the change in the rest of the layer. However, due to the smaller opening, this change is slower than the other larger openings considered for both experimental and numerical data, indicated by the reduced separation of density profiles in figures 6.5e and 6.5f.

The larger obstruction is able to trap a greater volume of fluid, resulting in the density near $z = 0$ lagging significantly further behind the change in the rest of the layer compared to figures 6.5c and 6.5e for $\tau > 7$ and figures 6.5d and 6.5f for $\tau > 10$. This results in the density profiles for $\gamma = 0.25$ having a distinctly different shape from those for the other obstructions. For $\gamma = 0.75$ and 0.50 the density profile of each layer was observed to be almost homogeneous for the full depth for all times. In contrast, for the $\gamma = 0.25$ case a large density difference is maintained between $z/H = \pm 0.5$ and $z = 0$ such that the profile for both experimental and numerical data appears like a backwards ‘s’.

Despite this difference in the shape of the vertical density profile, the circulation in each of the layers is able to continuously mix fluid in each layer. By bringing fluid from $z/H = \pm 0.5$ back onto $z = 0$ to be remixed, the density profiles in figures 6.5e and 6.5f are observed to gradually progress towards $\hat{\rho} = 0$. The separation between density profiles is also observed (as for the other obstructed cases) to decrease with time while maintaining the backward ‘s’ profile.

It is interesting to note that there are distinctive groupings of density profiles, clearly visible for $z > 0$ at times $\tau = 25, 30, 40$ and 50. These groupings are separated by relatively large gaps, where the layer mixes rapidly and transitions to the next grouping. These bands are visible in figure 6.3c as spine-like structures in the mean concentration, followed by a rapid decrease in the mean concentration as these temporary structures are mixed.
Fig. 6.6 Final non-dimensionalised density profiles measured with the conductivity probe for various opening sizes at $A = 5 \times 10^{-3}$. The initial profile is shown by the orange dashed line in (a) and figure (b) shows close ups of the final profiles.
6.4 Final density profile

The classical unobstructed RTI is very efficient at mixing two layers of fluid, as was seen in chapter 1. In this section we present measurements from traversing the conductivity probe through the final stratification for experiments with various opening sizes $0.125 < \gamma < 0.95$. The final stratification is that which occurs at the end of mixing when fluid in the the domain has reached a quiescent state. The smallest opening was $\gamma = 0.125$ and the largest, with an obstruction present, was $\gamma = 0.95$, with the classical unobstructed case having $\gamma = 1$. For this work, unlike the visualisation experiments, the various opening sizes were created by partially withdrawing the RB at the start of the experiment. All of the experiments presented were initiated at the same initial Atwood number, $A = 5 \times 10^{-3}$. The technical specifications and further experimental setup regarding the conductivity probe can be found in section 2.3.

Figure 6.6a shows the final non-dimensionalised density profiles for the range of openings considered. In addition, the stratification at the start of the experiment is indicated by the dashed orange line. We can see from figure 6.6a that, for all opening sizes, the RTI can quite effectively mix the two layers. The most striking difference is a clear distinction in final profiles between the obstructed cases $\gamma < 1$ and the unobstructed case with $\gamma = 1$.

A close-up of these final stratifications is shown in figure 6.6b. This figure shows, even more clearly, the divide between obstructed and unobstructed mixing. The most surprising result is that the size of the obstruction, where one is present, has little effect on the final stratification. The smallest obstruction considered, $\gamma = 0.95$, obstructed just 5% of the domain width (i.e. 20 mm). However, the final stratification of the $\gamma = 0.95$ case is near identical to all other obstructed cases, especially when contrasted with the $\gamma = 1$ profile. From the data, it does appear that the smaller openings with $\gamma \leq 0.25$ result in a slightly more stable final stratification than when the opening is larger, but nowhere near as stable as the $\gamma = 1$ case with no obstruction. Ultimately we observe that the obstructed cases finish more well mixed than the unobstructed data.

6.4.1 Mixing efficiency

In figure 6.7 we plot the mixing efficiency, $\eta$, as defined in section 1.3, for the final density profiles shown in figure 6.6, as well as an additional set of experiments that were conducted at the same Atwood number. The source of the errors shown in figure 6.7 are discussed in appendix B.2.1.

Looking at figure 6.7a there is a distinct difference between the obstructed cases ($\gamma < 1$) and the unobstructed case ($\gamma = 1$), as was seen in figure 6.6. The value of $\eta \approx 0.4$ for $\gamma = 1$ is comparable to what others have found for similar setups, with $\eta = 0.35$ found by Linden...
et al. (1994), and $\eta = 0.4$ by Holford et al. (2003). Note that the theoretical maximum mixing efficiency of the two-layer stratification used at the start of these experiments is $\eta = 0.5$ (Dalziel et al., 2008).

A close-up of the obstructed cases is shown in figure 6.7b. From this we can see that the lowest mixing efficiency occurs when the opening is smallest. This correlates with the more stable final stratification for openings with $\gamma < 0.25$, seen in figure 6.6b. The overall trend in figure 6.7b is a weak positive correlation with increased opening size, decreasing slightly when $\gamma = 0.95$, though still significantly larger than the values for $\gamma = 1$. 

Fig. 6.7 Mixing efficiencies calculated from initial and final profile conductivity probe measurements for various opening sizes at $A = 5 \times 10^{-3}$ including obstructed and unobstructed cases in (a) and only obstructed cases in (b).
6.5 Model for mixing rate

The previous sections have discussed the change in density of each layer in detail. One particularly striking result from the singly-connected domain is the homogeneity of the mean horizontal density with height in each layer (see section 6.3). This effect, combined with the near perfect symmetry in mixing dynamics between the two layers, suggests that the mean density of each layer, here denoted by $\bar{\rho}_{U,L}$, can be used as a meaningful parameter for mixing where the subscript refers to the upper and lower layer respectively.

Figure 6.8 shows the mean density profiles of the lower layer for experimental and numerical data. These data are plotted against the standard non-dimensional time $\tau$ in figures 6.8a and 6.8c. Looking at figures 6.8a and 6.8c we see that there is quite a large spread amongst the data for the different opening sizes. We observe that the evolution time is approximately proportional to the opening size. It is with this in mind that a new time-scale, $\tau_\gamma = \gamma \sqrt{A_0 g / H} \tau = \gamma \tau$, is proposed. In figures 6.8b and 6.8d we plot the lower layer mean density against $\tau_\gamma$ and observe that the obstructed data for both experimental and numerical data now collapse onto a similar curve. Figure 6.8d indicates that the mean density profiles for the classical unobstructed domain with $\gamma = 1$ are distinct from the obstructed data.

To understand how the mean density, $\bar{\rho}_{U,L}(t)$, of the upper and lower layer changes with time we will make use of our knowledge of the mixing dynamics to develop a hierarchy of models to describe the mean density change in each layer. These models will be fitted against the obstructed data in figure 6.8, replotted as an ensemble against $\tau_\gamma$ in figure 6.9.

6.5.1 Constant flux model

It takes a short time (typically $\tau < 5$) for the initial perturbation to grow large enough for a circulation to be established in each layer. This circulation brings fluid from each layer into the opening, where it mixes with fluid from the opposite layer before being transported away from the interface by two well mixed wall plumes at the other end of the opening. Thus, the fluid that flows onto the opening forces an equal exchange of well mixed fluid into each layer at the other end of the opening. We begin by assuming that a volume flux, $Q$, of perfectly mixed fluid, with density $\rho = \rho_U(t = 0) + \rho_L(t = 0)$,

$$\bar{\rho} = \frac{\rho_U(t = 0) + \rho_L(t = 0)}{2}, \quad (6.1)$$

leaves the interface and moves into each layer. By continuity, an equal volume of fluid with density $\rho_{U,L}$ leaves each layer such that mean density of each layer varies according to

$$\frac{d\rho_{U,L}}{d\tau} = -\frac{Q}{V} (\rho_{U,L} - \bar{\rho}), \quad (6.2)$$
Fig. 6.8 Mean density of the lower layer for various openings, plotted against two different non-dimensionless times: $\tau = \sqrt{A_{0}g/\dot{H}} t$ in (a,c) and, $\tau_{\gamma} = \gamma \sqrt{A_{0}g/\dot{H}} t$, in (b,d). Figures (a,b) are a combination of 3D scanned LIF data (seen earlier) and point measurements from multiple experiments. Figures (c,d) are MOBILE simulation data for various opening sizes shown in the key, at resolutions of: $128 \times 128 \times 256$ and $256 \times 256 \times 512$, indicated by solid and dashed lines, respectively.
where \( V = L \times W \times H \) is the volume of the domain. Assuming that the flux, \( Q = Q_c \), is constant, or varies on a much longer time scale than the mean density change in each layer, equation (6.2) has solution

\[
\rho_{U,L} = \bar{\rho} \pm \frac{\Delta \rho}{2} \exp \left( -\frac{Q_c}{V} \tau \right).
\]  

(6.3)

A least squares fit is plotted against experimental and numerical data in figures 6.10a and 6.10b, respectively. Looking first at the experimental data in figure 6.10a, we can see that an exponential model fits the experimental data well, with a coefficient of determination \( R^2 = 0.90 \). The data at early times (\( \tau < 5 \)) has very little variance, yet equation (6.3) overestimates the change slightly.

Looking at the simulation data in figure 6.10b, we can again see that at early times, \( \tau < 5 \), equation (6.3) overestimates the change in density. The overestimate is more significant here. Then, at slightly later times \( 5 < \tau < 20 \), equation (6.3) slightly underestimates the ensemble mean density change of the layer. The overall fit of equation (6.3) to MOBILE simulation data has \( R^2 = 0.96 \).

This model is incredibly simple and captures some of the basic density change in each layer. However, it fails to capture the early time growth for the numerical data seen in figure 6.10b. The problem is due to our assumptions; of a constant flux and that the layer of fluid interacting with the interface is well mixed. In the next section we will present a time varying flux model.
Fig. 6.10 Constant flux model least squares fit shown for ensemble of obstructed cases for (a) experimental data and (b) MOBILE simulation data.
6.5.2 Time varying flux model

Our model can be improved by constructing a time varying volume flux, \( Q(t) \), which is equal to an average exchange velocity, \( u_E (\Delta \rho(t), \gamma L, H) \), multiplied by the area of the opening \( A = \gamma LW \),

\[
Q = \gamma LWu_E. \tag{6.4}
\]

Assuming an instantaneous balance, which has been shown to work well in other RTI contexts (Dalziel et al., 1999; Davies Wykes and Dalziel, 2014; Lawrie and Dalziel, 2011), and using dimensional analysis across the exchange, we can write the velocity as

\[
u_E = \kappa_1 \left( \frac{gH \rho_U(t) - \rho_L(t)}{2\bar{\rho}} \right)^{1/2}, \tag{6.5}\]

where \( \kappa_1 \) is a dimensionless constant. The volume flux is then

\[
Q = \kappa_1 \gamma LW \left( \frac{gH \rho_U(t) - \rho_L(t)}{2\bar{\rho}} \right)^{1/2}. \tag{6.6}\]

When written in terms of non-dimensional time \( \tau = t \sqrt{gA_0/H} \), this becomes

\[
Q_\tau = \kappa_1 \gamma LWH \left( \frac{A(\tau)}{A_0} \right)^{1/2}, \tag{6.7}\]

where

\[
A(\tau) = \frac{(\rho_U(\tau) - \rho_L(\tau))}{(\rho_U(\tau) + \rho_L(\tau))} \tag{6.8}\]

is the instantaneous Atwood number and

\[
A_0(\tau = 0) = \frac{(\rho_U(\tau = 0) - \rho_L(\tau = 0))}{(\rho_U(\tau = 0) + \rho_L(\tau = 0))} \tag{6.9}\]

is the initial Atwood number. Bringing these together, equation (6.2) becomes

\[
\frac{d\rho_{U,L}}{d\tau} = -\kappa_1 \gamma \left( \frac{A(\tau)}{A_0} \right)^{1/2} (\rho_{U,L} - \bar{\rho}). \tag{6.10}\]

As we have seen in previous sections, it takes some time for mixed fluid from the opening to be transported around the full layer and return to the opening. In section 6.2 we saw that this occurred at \( \tau_1 = 6.0 \pm 0.5 \) for both the experimental and numerical data. We introduce \( \rho_{U,L}^*(\tau) \) to represent the density immediately above and below the barrier. Up until this time (\( \tau_1 \)) the
fluid that flows onto the opening is unmixed and has a density equal to the initial density of each layer $\rho_{U,L}(\tau) = \rho_{U,L}(\tau = 0)$, such that $A(\tau) = A_0$ for $\tau < \tau_1$ and equation (6.7) simplifies to

$$Q_{\tau_1} = \kappa_1 \gamma V,$$

(6.11)
a constant value. Substituting this into equation (6.2) we find

$$\frac{d\rho_{U,L}}{d\tau} = -\kappa_1 \gamma (\rho_{U,L}(\tau = 0) - \bar{\rho}).$$

(6.12)

From this expression we propose a new timescale

$$\tau_\gamma = \gamma \tau = \gamma \sqrt{\frac{A_0 g}{H}},$$

(6.13)

responsible for the collapse of the obstructed density profiles in figures 6.8b and 6.8d. Note that the unobstructed case does not collapse onto the $\gamma < 1$ cases. Using $\tau_\gamma$ in equation (6.12) we find the solution

$$\rho_{U,L} = \rho_{U,L}(\tau_\gamma = 0) \pm \frac{\kappa_1}{2} \Delta \rho_0 \tau_\gamma,$$

(6.14)

where $\mp$ refer to the upper and lower layer, respectively, and $\Delta \rho_0 = \rho_U - \rho_L$ is the difference between the initial unmixed density of the upper and lower layer. Least squares fits for equation (6.14) for experimental and numerical data are shown in figures 6.11a and 6.11b for early times. Data at late times is included to show the eventual departure from equation (6.14).

Looking first at the experimental data in figure 6.11a, we can see that for $\tau_\gamma < 3.2$ there is little variance, equation (6.14) fitting the data well with $R^2 = 0.95$. The same is true for the numerical data in figure 6.11b with $R^2 = 0.95$. After $\tau = 3.2$ we see the mean density begins to spread, changing faster than equation (6.14) predicts. This departure from equation (6.14) was expected and is the result of mixed fluid moving onto the interface after being circulated around the full layer, decreasing the density contrast across the barrier. The next section will present a model that captures the density change caused by this recirculation.

### 6.5.2.1 Late time model

After the circulation has transported mixed fluid around the full layer, at approximately $\tau_\gamma = 3.2$, the assumption that $\rho_{U,L}^\gamma(\tau = 0)$ is invalid. Returning to equation (6.10), we find the following solution

$$\rho_{U,L} = \bar{\rho} \pm \frac{\Delta \rho (\tau_1)}{2 + \frac{\kappa_1}{2} (\tau - \tau_1) - \gamma \Delta \rho_0 \tau_1},$$

(6.15)
Fig. 6.11 Early time linear model least squares fit shown for (a) experimental data and (b) MOBILE simulation data.
Fig. 6.12 Late time rational model least squares fit shown for (a) experimental data and (b) MOBILE simulation data.
6.5 Model for mixing rate

where $k_2$ is a non-dimensional constant to be found and $\Delta \rho (\tau_1)$ is the difference between the mean density of the upper and lower density at $\tau_1 = 3.2$.

The least squares best fit for equation (6.15) is shown for experimental data in figure 6.12a. Here we see that there is quite a large amount of variance in the data for $\tau_\gamma > 3.2$ and that the least squares fits the change seen fairly well with $R^2 = 0.61$. This $R^2$ value is significantly lower than the other values we have seen previously, caused by the significant variation in experimental data for the range of times equation (6.15) is applied to. If a median filter is applied to the data the coefficient of determination becomes $R^2 = 0.90$.

The combination of the early time linear model of equation (6.14) in figure 6.11 and the late time variable flux model of equation (6.15) in figure 6.12 fit the density changes in each layer well for all times, far better than the constant flux model of equation (6.3) in figure 6.10, especially at earlier times.

However, equation (6.15) is not perfect and over-predicts the rate of change for $\tau_\gamma = 3.2 - 8$ (see figure 6.12, in particular the numerical data in figure 6.12b). We can attempt to improve this late time model by introducing a $K - \varepsilon$ model, similar to Launder and Spalding (1974), which does not rely on an instantaneous balance between buoyancy and inertia as was used previously.

### 6.5.3 Non-instantaneous balance model

The assumption that the flux responds instantaneously to density changes in each layer is inaccurate. We can improve the accuracy of our model by taking into account the non-instantaneous balance between inertia and buoyancy. The $K - \varepsilon$ model of Launder and Spalding (1974) is a two equation model that links the turbulent kinetic energy, $K$, to turbulent dissipation, $\varepsilon$, using two transport equations in an attempt to describe turbulence in general. We take inspiration from this approach to adapt equation (6.2) to form our own pair of linked equations for the mean density change in each layer, $\rho_{U,L}$ and the exchange kinetic energy, $U^2$. We have

$$\frac{d \rho_{U,L}}{d \tau_\gamma} = -\frac{Q}{V} (\rho_{U,L} - \bar{\rho}),$$

which can be written as

$$\frac{d \rho_{U,L}}{d \tau_\gamma} = -\frac{\kappa_3}{H} U (\rho_{U,L} - \bar{\rho}),$$

(6.17)
Fig. 6.13 $K - \varepsilon$ model least squares fit shown for experimental data of density, $\rho$, in (a) and the velocity, $U$, in (b). The same result for the MOBILE simulation data for $\rho$ and $U$ are shown in (c) and (d), respectively.
where $U$ is the characteristic exchange velocity and $\kappa_3$ is a non-dimensional constant, and an equation for the kinetic energy, given by

$$\frac{dU^2}{dt} = \left(\frac{U_0}{L}\right) \left[\left(\frac{\Delta \rho U L}{2 \rho g H}\right) - U^2\right], \quad (6.18)$$

where $U_0$ is the initial exchange velocity at the end of the linear mixing period. The first term inside the square parenthesis of equation (6.18) represents the buoyancy forcing, the second represents the dissipation of energy. These two equations are solved numerically, with $\kappa_3$ fitted via a least squares algorithm. The fitted results of equation (6.17) are shown with the appropriate experimental and numerical data in figure 6.13. The early time change in density, from $\tau_\gamma = 3.2 - 10$, is captured well by equations (6.17) and (6.18), fitting through the middle of the ensemble for the density data. The agreement is a significant improvement over equation (6.15), particularly when comparing MOBILE simulation data in figures 6.12b and 6.13c. Indeed, even at later times, $\tau_\gamma = 10 - 20$, equations (6.17) and (6.18) fit the ensemble change for both experimental and MOBILE data better when compared to figures 6.12b and 6.13c.

These improved fits result in higher coefficients of determination, $R^2 = 0.94$ and 0.98, for the experimental and numerical data respectively. The exchange velocities predicted by the model in figures 6.13b and 6.13d are comparable to values seen for the openings in PIV and MOBILE data. The qualitative difference between figures 6.13b and 6.13d is likely caused by the reduced ensemble size of the experimental data compared to MOBILE, especially when comparing the profiles at late times.

### 6.6 Energetics

To understand the different mixing processes that occur as a result of the inclusion of an obstruction we have so far only considered various measures derived from the density changes in the domain. Further information can be gained from considering the different energy changes resulting from mixing of the two layers. The total potential energy (PE), kinetic energy (KE), available potential energy (APE), background potential energy (BPE) and total energy ($TE = PE + KE$) are shown for the classical unobstructed case in figure 6.14 and the obstructed cases with $\gamma = 0.75, 0.50$ and 0.25 in figures 6.15a to 6.15c and figures 6.16a to 6.16c from experimental and numerical data respectively.

First we look at the classical unobstructed energetics presented in figure 6.14. The APE is, by definition, the difference between the PE and the BPE. The process of mixing reduces the APE as the stratification tends towards stability. The energy lost from APE is transferred into...
increasing KE and BPE. We define the solution to be perfectly mixed when the BPE is zero. Thus, the closer to zero the final BPE, the more mixed the final state.

Looking at figure 6.14 for $\tau = 0 - 3$, we can see that PE is converted primarily into BPE, with very little growth in KE as the small initial perturbation for all openings grows uninterrupted in the first stage of the RTI. After $\tau = 3$ there is rapid change in APE. APE is converted into BPE and KE. The peak in KE occurs at $\tau = 6$, just after the mixing region has spread to $z/H = \pm 0.5$ at $\tau = 5$. Note that the peak in KE is substantially less than the maximum value of the potential energies. After the peak, KE decreases monotonically (through viscous dissipation). The PE converges towards BPE as KE tends towards zero.

### 6.6.1 Obstructed cases

We now consider the evolution of energy for the obstructed experimental and numerical data, presented in figures 6.15 and 6.16 respectively. It is worth noting that, due to the shadow cast by the removable barrier, early information for KE for the experimental data is not available in the upper layer. As such the earliest data shown are taken from the first full scan. The time shown for experimental data is still measured from when the barrier was first opened.

We begin with the largest opening, $\gamma = 0.75$, shown in figures 6.15a and 6.16a for experimental and numerical data respectively. For the numerical data, from $\tau = 0 - 3$, the change in energy is comparable to the classical data in figure 6.14, as the initial perturbation grows uninterrupted by the obstruction in the first stage of the RTI. After $\tau = 3$ there is a rapid conversion of PE for both experimental and numerical data, similar to what was seen for the classical unobstructed case. This rapid conversion of PE results in a peak in the KE with
Fig. 6.15 Energetics for experimental scanned 3D data with openings: (a) $\gamma = 0.75$, (b) $\gamma = 0.50$, and (c) $\gamma = 0.25$. Note that the early times are not included as the RB blocks the view of the upper layer until is fully withdrawn.
Fig. 6.16 Energetics for MOBILE simulations with openings: (a) $\gamma = 0.75$, (b) $\gamma = 0.50$, and (c) $\gamma = 0.25$. 

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$KE/PE_0 = 0.45$ and $0.35$ for the experimental and numerical data respectively at $\tau = 6$. This corresponds to a time when the gravity currents have propagated fully along the horizontal boundaries at $z/H = \pm 0.5$ and begin to overturn down the side wall. Once they begin to overturn, the KE is converted into more mixing and increases the BPE.

The KE peak is comparable to a similar peak observed in the classical data, though the obstructed peak is significantly sharper. This increased sharpness appears to be the result of the PE plateauping for both experimental and numerical data at $\tau = 6$, most clearly observable in figure 6.16a. Due to the lower time resolution and spread in data due to the scanning procedure, such a plateau is not as clearly visible in the experimental data, however, the change in PE is uncharacteristically small compared with the rest of profile.

After $\tau = 6$ the PE is observed to continue to decrease, though less rapidly, for both the experimental and numerical data, while the KE remains relatively constant and the BPE continues to increase rapidly. The PE of the experimental data is observed to reach approximately zero at $\tau = 9$ in figure 6.15a. The change for numerical data is slower and better resolved at later times with a secondary peak in the KE observed at $\tau = 13$ with $KE/PE_0 = 0.2$ in figure 6.16a. Again this peak corresponds to a plateau in the potential energies. The PE then slowly decreases to zero, increasing the KE and BPE with a final peak in the KE observable at $\tau = 21$. After this time there is little PE left in the system and the subsequent increases in the BPE (mixing) are driven by residual KE changes.

Next we discuss the $\gamma = 0.50$ opening, see figures 6.15b and 6.16b for experimental and numerical data respectively. We observe that the smaller opening slows the conversion of energy in both sets of data. However, in the numerical data (see figure 6.16b) the early time change, for $\tau = 0 - 3$, is comparable to what was observed for $\gamma = 0.75$. For both experimental and numerical data, a peak in the KE is observed at $\tau = 6$, the same time as for $\gamma = 0.75$. However, the height of this peak is much reduced, with $KE/PE_0 = 0.2$ and $0.12$ for the experimental and numerical data respectively. This is almost a factor of two smaller than the peak for $\gamma = 0.75$. Note also that the peaks are not as pronounced in this case as the smaller opening limits the rate at which PE can be released. We do, however, observe similar plateaus in the potential energies around these peaks in KE. For both experimental and numerical data, the potential energies at all times are observed to change more slowly in figures 6.15b and 6.16b than for the $\gamma = 0.75$ data. Later peaks in the KE at $\tau = 12$ for experimental and $\tau = 9, 17$ and 27 for numerical data also have corresponding plateaus in the potential energy.

Finally we discuss the smallest opening case presented here with, $\gamma = 0.25$, shown in figures 6.15c and 6.16c for experimental and numerical data respectively. Again, for $\tau = 0 - 3$, the initial perturbation results in a similar energetic profile in figure 6.16c when compared to the classical data. However, after this time the impact of the much smaller opening has a significant
effect, dramatically reducing the rate of change in the energy profiles for both experimental and numerical data when compared to larger openings. The peaks in KE are not visible in the experimental data of figure 6.15c with KE appearing very small but approximately constant for most of the duration of the experiment. Peaks in KE are visible in the numerical data (see figure 6.16c), however, they are much less prominent than for cases with larger openings. Where there are peaks, such as at $\tau = 6, 15$ and 20, the potential energy plateaus in a manner similar to what was seen for figure 6.16b.

The early time behaviour is similar for both experimental and numerical data, when the motion is dominated by the growth of the initial perturbation. However, the similarities are less clear at later times when the effect of the obstruction begins to dominate the resulting dynamics. By plotting the same energy profiles against the opening scaled time of $\tau_\gamma = \gamma \tau$ in figure 6.17 we see that the energetic profiles now appear much more similar. This is particularly true for the numerical data in figure 6.17b. Such a collapse provides further support for $\tau_\gamma$ being the most suitable time-scaling for the mixing dynamics of the singly-connected domain.

The PE for the $\gamma = 0.75$ experimental data decreases faster than for the other two openings sizes, resulting in a much larger KE at later times. A similar effect is seen in the numerical data. The total energy is observed to decrease at a similar rate for both sets of data. A clear difference between profiles, not captured by the $\tau_\gamma$ timescale, is the position of the plateau points. We see that the $\gamma = 0.25$ MOBILE profile (see figure 6.17b) has more frequent plateau points than the $\gamma = 0.50$ and 0.75 cases. We also note that the peaks in KE for both sets of data do not coincide when plotting over this obstructed timescale, $\tau_\gamma$.

It is interesting to note that for all the obstructed MOBILE cases, the KE grows faster than the BPE for early times (compare figures 6.16a to 6.16c to that of figure 6.14). However, this cannot be said to be true for the experimental data where the BPE outgrew the KE at almost all times (see figures 6.15a to 6.15c). As this effect was only seen for early times, this difference is likely caused by differences in the initial conditions. However, the difference between the KE and BPE is much larger for the unobstructed domain than the obstructed domain for both experimental and numerical data. This suggests that at early times the PE is primarily used for mixing in the classical case, whereas for the obstructed cases a larger proportion of PE is used in establishing the circulation about each layer. Subsequent mixing (increases in BPE) are then dependent on energy stored within this circulation.

Another significant difference caused by the introduction of the barrier is a variation in the smoothness of the different energy profiles plotted in figure 6.16. For $\gamma = 1$, the energy profiles are smooth (see figure 6.14). However, for the obstructed cases the energy profiles display clear plateau points. These differences are a result of the barrier limiting the release of PE in system. For $\gamma = 1$, most of the PE in the system is released very rapidly such that
Fig. 6.17 Energetic profiles for all opening sizes are shown for experimental data in (a) and numerical data in (b), plotted against $\tau_\gamma$ with openings: $\gamma = 0.75$, $\gamma = 0.50$ and $\gamma = 0.25$ shown as solid, dashed and dotted lines respectively.
there is a single, continuous large release of energy from the growth of the RTI. However, the inclusion of the obstruction prevents all of this energy from being used in the initial mixing event. This trapped energy is then released at later times through secondary RT instabilities that are able to grow, be swept into the opening, and regrow on the open interface such that there are secondary releases of PE. These discontinuities are responsible for the plateau points that are characteristic of the obstructed domain. The cause of these is discussed further in the following section.

6.6.2 Plateauing energy

The plateauing of the PE and BPE, as seen in figures 6.15b, 6.15c and 6.16a to 6.16c, is a new effect resulting from obstructing the RTI. What these plateau, or saddle points, in the BPE indicate are pauses or reductions in the mixing of the two layers that are unstable to RTI, usually renowned for the speed and efficiency of mixing. The fact that they occur for vastly different opening sizes and at regular intervals is evidence that they are not just one-off events but a distinctive feature of the mixing dynamics arising via the introduction of an obstacle.

A blow-up of a number of saddle points in the BPE for $\gamma = 0.75$ is shown in figure 6.18. Visible in this figure are saddle points at $\tau = 6, 9.5, 14$ and $20$. A time series of the isosurfaces of density for $\gamma = 0.75$ is presented, around the time of the $\tau = 9.5$ saddle point, in figure 6.19.

In figure 6.19a we can see that there is an equal vertical exchange of fluid occurring in the plane with $x = 1$. We also see that along the surface of $z = 0.5$ there is a large amount of mixing and motion from $x = 1$ to 0, as expected. The stream flowing off the barrier is expected to flow along $z = 0$, but here, in the $y = 0$ plane, we can see that it is deflected below $z = 0$ by a large volume of relatively unmixed upper layer fluid pushing it into the lower layer.
Fig. 6.19 A time series of the density rendered in 3D for $\gamma = 0.75$ at times: (a) $\tau = 7.8$, (b) $\tau = 8.4$, (c) $\tau = 9.4$ and (d) $\tau = 10.3$. The obstruction is located on the right hand side of the image between $x = 0 - 0.25$ and spans the full length of the domain in the $y$ direction.
A short time later, in figure 6.19b, the stream flowing off the edge of the barrier at \( x = 0.25 \) has corrected itself and now flows along \( z = 0 \). However, the deflected stream and a volume of unmixed upper-layer fluid now flow in a confined plume down the \((x, y) = (1, 0)\) corner. This displaces an equal volume of lower-layer fluid, allowing it to flow up into the upper layer in the opposite corner, \((x, y) = (1, 1)\), creating a two-way exchange of fluid between the layers without significant mixing occurring (see \( x = 1 \) in figure 6.19c). This can be thought of like a funicular where an equal mass is exchanged between two different heights without changing the PE of the whole system. The counter exchange of an equal and opposite mass between the two layers results in no change of the PE and the lack of mixing in the exchange results in the BPE remaining unchanged. This two-way exchange of unmixed fluid is the cause of the saddle points for both the PE and BPE.

The two-way exchange of different density fluids is inherently unstable and at \( \tau = 10.3 \) the two streams can be seen in figure 6.19d to have become well mixed as they interact with the horizontal boundaries and mix with the ambient fluid. This mixing increases the BPE. The stream along \( z = 0 \) can be seen to continue to mix fluid via the RTI and transfer the mixed fluid between the two layers which reduces the PE in the system. Although not presented here similar exchanges are visible at all the plateaus seen in figures 6.16a to 6.16c.

It might be expected that this two-way exchange would become more prevalent as \( \gamma \) decreases (or as the tank becomes wider in the y direction). Indeed, as this becomes more prevalent, it may be expected that the mixing efficiency would decrease. This type of motion, where the direction reverses, is suggestive of there being unsteady periodic orbits (UPO) of the different exchange characteristics. However, the discovery of such UPO’s is beyond the scope of this thesis.

### 6.7 Different aspect ratios

Currently, only two aspect ratios have been considered, \( H/L = 1.25 \) and 2.0, for experimental and numerical data respectively. We have seen that the obstruction forces fluid from each layer to be exchanged via a spatially developing RT mixing zone in the opening. At the side wall of the opening, the fluid is transported vertically to \( z/H = \pm 0.5 \) via two wall plumes. The fluid that is transported to this height at early times is stably stratified compared to the ambient density and is only moved from this height by a circulation that is established in each layer. Typical vortical structures have an aspect ratio of one. In all cases currently considered, the width and height of each layer have been comparable such that a vortical structure encompassing the whole layer could stably be formed. However, for other aspect ratios the vortical size may be restricted by the geometry and fail to span the full layer.
In this section we will consider two extreme cases: the first, with high aspect ratio, will have a domain height eight times the horizontal width. The second, a low aspect ratio case, will consider a domain where the height is a quarter of the domain width. Currently, only numerical simulations have been used to investigate the these geometries, and those are presented here. This section will build on earlier work presenting the time series of the density field with a description of the different dynamics. The horizontally averaged density profile will be presented and discussed alongside the energetics for each case.

6.7.1 High aspect ratio

Dalziel et al. (2008) looked at RT mixing in very high aspect ratio tubes, $H/L = 40$. They found that the dynamics were very different to other cases where the aspect ratio was closer to one. The mixing was transported through the layer by a stack of small vortical structures that were limited in size by the very narrow tube width. Another striking result was that reducing the tank width increased the mixing efficiency. Whilst the aspect ratio considered in this section is only $H/L = 8$, the large separation between the horizontal and vertical scales could be expected to change some of the mixing dynamics seen earlier and introduce a new mixing regime.

Figure 6.20 presents a time series of the density field rendered in 3D for $\gamma = 0.50$ with an aspect ratio of $H/L = 8$ at Atwood number $A = 5 \times 10^{-3}$. The resolution used in the simulation was $64 \times 64 \times 512$, comparable to that used by Lawrie and Dalziel (2011). The non-dimensional time used is $\tau = \sqrt{Ag/Hz}$, where $H$ is the height of the domain (here four times larger than the previously considered height).

Looking at figure 6.20a, we can see that the initial mixing zone has been carried into the side wall as the spatially-developing RT mixing zone continues to grow on the open interface, as was seen previously. Once again, the fluid that is swept away forms two equal wall plumes that propagate vertically up (down) the side wall at $x = 0$. At this time, $\tau = 3.1$, each plume has travelled a vertical distance of $|z/L| = 1$ ($|z/H| = 1/8$) from the interface. This is the distance that the plume would interact with the horizontal boundary in the $H/L = 2$ cases previously considered. In figure 6.20a we can see that the wall plumes continue to grow vertically, but there has been significant entrainment and overturning whilst travelling this distance such that parts of the plumes now have a width equal to half the horizontal width of the domain.

The horizontal spreading of the wall plumes is seen more clearly in figure 6.20b. The plumes have spread almost throughout the full horizontal width in both of the layers. Despite this, the plumes continue to grow vertically as more fluid is drawn onto the open interface and mixed via the RTI before being forced into the side wall. The stream flowing from the end of barrier requires fluid to replace it, which draws fluid from the centre of each layer towards the
Fig. 6.20 Time series of a high aspect ratio $H/L = 8$ MOBILE simulation at resolution $64 \times 64 \times 512$ of the density field rendered in 3D with $\gamma = 0.50$ at times: (a) $\tau = 3.1$, (b) $\tau = 5.3$, (c) $\tau = 7.5$, (d) $\tau = 10.6$, (e) $\tau = 15.0$, (f) $\tau = 32.9$. 

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interface. This process, around the interface at \( z = 0 \), is the same as that seen in the previous cases considered.

In figure 6.20c the wall plumes can be seen to have extended to the horizontal boundaries where they collide and overturn in the same way as was seen earlier. At the interface, the motion remains the same with fresh fluid being drawn from either side of the barrier and into the opening. A significant amount of mixing can be seen to have occurred between \( 0.5 < |z/L| < 4 \) \((1/16 < |z/H| < 1/2)\) in both layers. For \( |z/L| < 2 \) \((|z/H| < 1/4)\), this mixing cannot have occurred from gravity currents propagating along the horizontal boundary and overturning as at \( \tau = 7.5 \) the plumes have only just reached the horizontal boundaries and the overturning region has not had enough time to spread through the full depth. The mixing at these lower depths is instead caused by horizontal spreading of the wall plumes as they propagate vertically. We see also that the flow is not as two-dimensional as for previous cases, with distinct differences in density in the \( y \) direction in figure 6.20c.

The spreading of the wall plumes is a new effect of the increased height in the mixing dynamics. The increased height results in the wall plumes having longer to entrain and spread laterally, this introduces a new mechanism allowing fluid to be remixed on the interface. The recirculation of fluid parcels is no longer solely driven by gravity currents propagating along the horizontal boundary. Now parts of the wall plumes can detach at lower heights and be recirculated through the opening, as is visible at \( |z/L| = 1 \) \((|z/H| = 1/8)\) in figures 6.20d and 6.20e.

In figure 6.20d, motion is visible along the \( x = 0 \) side wall, away from \( z = 0 \) to \( |z/L| = 4 \) \((|z/H| = 1/2)\), and then along the other side wall at \( x = 1 \) towards \( z = 0 \). Thus we have two counter-flowing plumes that both mix with one another and, at the same time, drive one another. Despite the vastly different horizontal and vertical scales, a layer wide circulation is established in both layers. In figures 6.20e and 6.20f we can see that this circulation brings fluid from \( z = \pm 4 \) all the way to \( z = 0 \).

Figure 6.21 presents a time series of the \( y \)-averaged density field with a variable colour bar, changing according to the maximum of \( |\hat{\rho}| \). These figures differ from those in figure 6.20, providing further information about the in-depth motion and including views of the late time dynamics (as in figure 6.21h).

In figure 6.21b, we can see fluid flowing off the obstruction with the circulation caused by this entraining fluid from the buoyant wall plumes, drawing it towards \( z = 0 \). In figure 6.21c, the plumes can be seen to reach \( |z/L| = 4 \) \((|z/H| = 1/2)\) and begin overturning. However, just as was seen in figure 6.20c, significant mixing has occurred outside the overturning region as the wall plumes have been entrained laterally. The circulation can be seen to draw fluid from
Fig. 6.21 Time series of a high aspect ratio $H/L = 8$ MOBILE simulation at resolution $64 \times 64 \times 512$ with the depth (y) averaged density field for $\gamma = 0.50$ at times: (a) $\tau = 3.1$, (b) $\tau = 5.3$, (c) $\tau = 7.5$, (d) $\tau = 10.6$, (e) $\tau = 15.0$, (f) $\tau = 32.9$, (g) $\tau = 122.4$, (h) $\tau = 215.2$. 

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6.7 Different aspect ratios

|z/L| = 4 (|z/H| = 1/2) down towards z = 0 in figure 6.21d. After this, mixed fluid exists throughout the whole depth, but the circulation continues quasi-steadily.

The steadiness of this mixing regime in a high aspect ratio is exemplified by the strong similarity between figures 6.21e to 6.21h despite the time changing from \( \tau = 15.0 \) to \( \tau = 215.2 \) and the maximum density reducing by more than a factor of 20. In these late time figures we can see that each layer is almost homogeneous for the full depth. The least mixed fluid is trapped on either side of the obstruction and continues to drive the circulation in each of the layers. The fluid flowing off the obstruction mixes through the RTI and forms two well mixed wall plumes that extend the full height of the domain, before overturning and recirculating.

### 6.7.1.1 Density profile

The horizontally averaged density profile for the high aspect ratio scenario discussed above is presented in figure 6.22. A density profile is plotted for each time step, \( \Delta \tau = 0.16 \), which, when combined with the large domain, requiring much longer simulation run time, results in many more lines drawn than seen in previous cases (e.g. figure 6.5).

The first observation from figure 6.22 is that it is very similar in structure to what was seen in previous obstructed cases, as discussed in section 6.3.1. However, the density profiles here are much more uniform than in the other obstructed cases with the difference between the interface at \( z = 0 \) and the horizontal boundaries at \( z/H = \pm 0.5 \) significantly less than was seen previously. This is a surprising result if we expected that the dynamics for mixing were the same as for the \( H/L = 2 \) domain, where a parcel of fluid is circulated from the opening around...
the full layer before it returns to the opening again. However, as we have seen in figures 6.20 and 6.21, the wall plume that transports mixed fluid from the interface becomes unstable as part of it is entrained by the counter-current on the other wall. This mixes fluid at much shallower depths in each layer resulting in a more homogeneous layer.

As the density difference between the two layer reduces, the rate of mixing decreases significantly, as made visible by the reduced separation between the density profiles for $\tau = 25$ onwards. The mixing continues very slowly but consistently, as was seen for the other obstructed cases in section 6.3.1, however, here, the much greater height reduces the rate of mixing substantially.

**6.7.1.2 Energetics**

Figure 6.23 shows profiles of the energetics for the high aspect ratio domain. The energy profiles in figure 6.23 appear remarkably similar to the earlier $\gamma = 0.50$ case seen in figure 6.16b. The PE is initially flat as the initial perturbation grows on the interface. After this the PE decreases rapidly while KE and BPE increase. However, the change in magnitude of KE is significantly less than was seen in the smaller aspect ratio energetic profile (see figures 6.15b and 6.16b). This difference is due to the increased height of the domain, such that the initial PE is significantly greater for the high aspect ratio case. In absolute terms, the maximum KE of the high aspect ratio domain is $4 - 5$ times greater than that of the smaller aspect ratios cases previously considered.
6.7 Different aspect ratios

Peaks in KE are again seen to occur repeatedly in figure 6.23, followed by plateaus in the PE. Thus the new plateauing phenomena, caused by the impact of the obstruction and discussed in section 6.6.2, is again seen here for the tall domain. Though not shown here, the same exchanges across the opening, as were seen in figure 6.19, are visible in this case. This is to be expected given that the motion across the opening was seen to be unaffected by the greater layer height with the RTI still able to grow on a constant stream of fluid flowing off the obstruction.

6.7.2 Low aspect ratio

So far we have looked at scenarios where the opening is smaller than the full domain height. In these cases a circulation is established in each layer and fluid is transported from the interface via two wall plumes that flow up the side wall connected to the opening. In this section we will look at a domain where the domain has dimensions \( x \times y \times z = 4L \times L \times L \), with \( \gamma = 0.5 \), such that the opening is twice as large as the vertical height. A time series is shown in figure 6.24. The left-hand column shows the density field rendered in 3D and the right-hand column shows the \( y \) averaged density field at the same time.

In figures 6.24a and 6.24b the region in the opening can be seen to mix via the RTI with a growing mixing region extending towards the horizontal boundaries at \( |z/L| = 1/8 \ (|z/H| = 1/2) \). The density difference between the mixing region and the unmixed fluid trapped by the barrier establishes a horizontal buoyancy gradient creating a baroclinic torque between the layers. By the same process as has been seen in all other cases considered, this torque draws unmixed fluid trapped either side of the barrier into the opening, made visible by the flat interface and deflected mixing region along \( z = 0 \) around \( x = 2 \) in figures 6.24a and 6.24b.

The initial mixing region can be seen to spread to \( |z/L| = 1/8 \ (|z/H| = 1/2) \) in figures 6.24c and 6.24d. However, looking at figure 6.24c the mixing region does not appear as well mixed as in other cases. We also see that there is a significant volume of lower-layer fluid at \( z/L = 1/8 \ (z/H = 0.5) \). The smaller domain height, compared to the width, restricts the extent that the RTI can develop into turbulence such that large amounts of fluid simply get overturned rather than mixed.

The fluid that was transported to \( |z/L| = 1/8 \ (|z/H| = 1/2) \), and was not well mixed, can be seen to propagate rightward as a broad gravity current from \( x = 2 - 4 \) in figures 6.24c and 6.24d. As the gravity current moves rightward, the stream flowing off the barrier continues to extend further into the opening. This is made visible by the flat interface spreading from \( x = 2 \) to \( x = 1.5 \) in figures 6.24c and 6.24d. Between \( x = 0 \) and \( x = 1.5 \) the initial perturbation continues to mix through the final stages of the RTI.
In figures 6.24e and 6.24f the initial mixing region has now been further reduced in length, lying between \( x = 0 \) and \( x = 1 \) as the stream continues to flow off the obstruction. At \( x = 1 \) the stream becomes unstable and, instead of mixing fluid on the interface, it displaces large volumes of relatively unmixed fluid, causing them to be exchanged between each layer. This can be seen in figure 6.24e at \((1, 0.5, 0.5)\), made apparent by the large volume of lower-layer fluid. The cause of the instability in the stream appears to be a combination of entrainment by the gravity current flowing rightward and the large, relatively unmixed, block of low density fluid between \( x = 0 \) and \( x = 1 \). The fluid in this region is trapped by the side walls and has a relatively stable stratification. Thus, when the stream flows into this region, the relative buoyancy between the two deflects the stream vertically towards \( z = 0.5 \), indicated by the large volume of relatively unmixed lower layer fluid deflected towards \( z = 0.5 \) in figure 6.24e.

The deflected unmixed fluid is split between spreading laterally towards \( x = 0 \) and joining the gravity current flowing to the right. The fluid that joins the gravity current further increases the density difference between the core of the gravity current and the ambient fluid. This reduces the height of the gravity current and accelerates it rapidly (compare figures 6.24c and 6.24d to figures 6.24e and 6.24f). The gravity current, propagating rightward rapidly along \(|z/L| = 1/16 \ (|z/H| = 1/4)\), and the stream flowing leftward off of the obstruction combine to create a strong counter current with little separation. Indeed, the sharp density and velocity difference along \( z = \pm 0.25 \) results in Kelvin-Helmholtz billows developing on the interface, two of which can be seen very clearly in figure 6.24e between \( x = 3 \) – 3.5.

The Kelvin-Helmholtz billows can be seen to continue to grow on the sharp density interface between the rightward flowing gravity current and the leftward off-obstruction stream in figure 6.24g. The gravity currents can be seen to overturn in figures 6.24g and 6.24h. This overturning results in two bores propagating back on themselves on either side of the obstruction. A thin band of initial density fluid is trapped between the returning gravity current and the obstruction.

The motion in the opening in figures 6.24g and 6.24h remains similar to what was seen at the earlier times in figures 6.24e and 6.24f. Fluid continues to flow as a horizontal stream off the end of the obstruction, but becomes unstable at \( x = 1 \) and deflects large volumes of relatively unmixed fluid to \(|z/L| = 1/8 \ (|z/H| = 1/2)\). This deflected unmixed fluid is split between the rightward flowing gravity current and that spreading laterally leftwards towards \( x = 0 \). Though not visible here, we have observed from looking at other images that the fluid which spreads leftward overturns around \( x = 0 \) and begins to connect with the gravity current flowing along \( z = -0.5 \). Evidence of this can be seen by the reduced density in the lower layer around \( x = 0 \) when comparing figures 6.24g and 6.24h to figures 6.24i and 6.24j.
The overturned fluid connects with the gravity current along $z/L = -1/8 \ (z/H = -1/2)$ creating a strong rightward flow. This flow entrains the stream moving off the obstruction into the opening, forcing the stream down towards $z/L = -1/8 \ (z/H = -1/2)$; see the large volume of upper layer fluid descending towards $z/L = -1/8 \ (z/H = -1/2)$ in figures 6.24i and 6.24j. As seen for the upper layer (not shown here), some of this large dense volume of fluid spreads both to the left and right. The fluid that spreads left collides with the side wall at $x = 0$ and reverses the circulation there such that there is now a concentrated current of fluid flowing to the right along $z = 0.5$.

For the rest of the mixing process, a sloshing motion is established as the density difference of fluid trapped on either side of the obstruction causes a periodic exchange between the upper and lower layer. An example of this occurring at late time is shown in figure 6.24l. Looking at both figures 6.24k and 6.24l we can see that a stable stratification is established for the whole domain, much stronger than has been seen for any other aspect ratio considered.

### 6.7.2.1 Density profile

Figure 6.25 presents the vertical profile of the horizontally averaged density profile for the low aspect ratio case, with $H/L = 0.25$. Initially, the density profiles appear similar to the larger opening cases, with $0.5 < \gamma < 1$, as discussed in section 6.3. The RTI can be seen to grow from the initial perturbation in the opening, with the density change progressing from $z = 0$ towards $z/H = \pm 0.5$. However, the change in density at $z/H = \pm 0.5$ is now much more rapid and pronounced than was seen for any of the other cases, including the unobstructed case.

The reduced layer height halts the growth of the RTI mixing zone resulting in fluid at the horizontal boundaries being poorly mixed. As was seen earlier, this fluid forms rapidly flowing gravity currents that are fed by more unmixed fluid from the unstable stream on the interface. These gravity currents rapidly displace the fluid that was originally at this height. This is seen in figure 6.25 by the density profiles at $\tau = 10$ being far to the left of $\hat{\rho} = 0$ in the upper layer in figure 6.25 (vice versa in the lower layer).

The effect of counter current flow off the obstruction can be seen by the cluster of density profiles around $\hat{\rho} = \pm 0.25$ around $\tau = 10$, as initial density fluid from both layers is forced towards $z = 0$. This cluster is broken up and rapidly converges towards $\hat{\rho} = 0$ when the gravity currents flowing along $z = \pm 0.5$ overturn at $\tau = 15$ and begin flowing back along $z = 0$ towards the opening. The small band of fluid that was seen to be trapped between the returning gravity current and the obstruction in figure 6.24j is seen in figure 6.25 by a stretching of the density profile away from $\hat{\rho} = 0$ for $0.05 < z < 0.05$.

Looking at later times, $\tau > 15$, we can see that the density around $z = \pm 0.5$ is little changed from the stable stratification established at $\tau = 10$. The fluid trapped by the barrier in
Fig. 6.24 Time series of a low aspect ratio $H/L = 0.2$ MOBILE simulation at resolution $512 \times 128 \times 128$ with the density field rendered in 3D for the left column and the $y$ averaged density field in the right column at times: (a,b) $\tau = 3.5$, (c,d) $\tau = 6.2$, (e,f) $\tau = 10.6$, (g,h) $\tau = 13.7$, (i,j) $\tau = 19.4$, (k,l) $\tau = 74.7$. 

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Singly Connected Domain

\[
\hat{\rho} = \frac{\rho - \bar{\rho}}{\Delta \rho}
\]

$0.05 < z < 0.05$ is gradually mixed. Interestingly, the density at $z = 0$ is not $\hat{\rho} = 0$ and instead approaches $\hat{\rho} = 0.05$, this is further evidence of the significant overturning occurring in the mixing process here.

The density profile presented here is vastly different from the other obstructed cases. The lack of a strong, layer-wide circulation enables a stable stratification to be established at early times and this persists for the whole mixing process.

6.7.2.2 Energetics

The energy profiles for KE, PE, BPE and APE for the low aspect ratio domain with $H/L = 0.25$ and an obstruction of $\gamma = 0.50$ are shown in figure 6.26. The early time energy profiles have the same structure as that seen for all other cases during the time when the initial perturbation is growing through each layer until it interacts with the horizontal boundary at $\tau = 5$. There is then a rapid decrease in the PE from $\tau = 5 - 8$, causing increases in both BPE and KE, with local maximums at $\tau = 8$. The rate of change of both BPE and KE decreases after this point. The fluid in the opening has been mixed with the remaining unmixed fluid (and PE) trapped by the obstruction, limiting its release. At $\tau = 20$, the remaining PE in the system is trapped by the barrier and not so readily accessible. This reduces the the rate of change of PE significantly such that PE is almost flat in figure 6.26.
6.8 Summary

The KE peaks at $\tau = 14$, the point at which the overturned gravity currents have travelled the full length of the domain. Now there is a significant amount of energy stored as KE compared to PE. After this the KE decreases rapidly, resulting in significant increases in BPE until $\tau = 20$. This time corresponds to the point when the stream of relatively unmixed fluid that had been flowing through the opening is mixed. After this time the majority of available energy has been used in the system. For very late times, the fluid trapped by the large obstruction is gradually released into each layer resulting in the small PE and BPE changes seen for $\tau > 30$ in figure 6.26.

6.8 Summary

The inclusion of a simple 2D obstruction into a confined unstably stratified domain results in significantly different mixing dynamics compared to the unobstructed domain. Without an obstruction the initial perturbation to the interface between the two layers grows via the RTI. This mixing region spreads from the interface to fill the two layers. With the inclusion of an obstruction the growth from the initial perturbation is limited as fluid trapped either side of the obstruction is drawn by a horizontal buoyancy gradient into the opening. This influx of fluid sweeps the mixing region horizontally onto the opening towards the vertical side wall where it is then transported vertically towards the horizontal boundaries by two well-mixed wall plumes, one in each layer. We call this motion a bidirectional exchange.

The circulation is seen to continue quasi-steadily for long periods of time, with unstable density differences between each layer being maintained for the whole duration of mixing,
albeit reducing with time. The time taken to fully mix each layer can be $2 - 5$ times as long as the classical unobstructed case, depending on the opening size, with smaller openings taking the longest. This is due to the more restricted RT growth in the smaller opening compared with a larger opening where the streams of fluid moving onto the opening have more time (space) to grow. The smaller RTI mixing region reduces the amount of mixing that can occur and, thus, the amount of PE that is released.

A surprising effect of introducing an obstruction to the classical RTI was to significantly increase the final mixing efficiency, compared to the already high value in the classical RTI. Significant increases to the mixing efficiency were observed when the obstruction occupied as little as 5% of the total domain width. The reason for this increased mixing arises from the continuous layer-wide circulation that is observed to occur for long times.

For the classical RTI the mixing region was observed to grow from the interface and spread through each of the layers until it reached the horizontal boundaries at which point the majority of the PE is released and any additional mixing is caused by residual KE. However, the KE is insufficient to ensure that the remaining fluid becomes well mixed in all locations, in particular along the horizontal boundaries, resulting in a weakly stable final stratification.

With the introduction of an obstruction, mixed fluid is transported directly from the interface to the horizontal boundaries. Once here it is transported via a gravity current, entraining ambient fluid as it moves before overturning and interacting with the obstruction. Once alongside the obstruction, the fluid is carried by the circulation onto the opening where it mixes with its counterpart, fluid from the other layer, and is recirculated again about each layer. This continuous recirculation of fluid around each layer, which is then mixed via the bidirectional exchange on the opening, ensures that there are very few locations where fluid is not continuously being mixed. This motion continues quasi-steadily for as long as a density difference exists across the obstruction, resulting in a well mixed final state even for small obstructions.

The PE and BPE profiles for all obstructions considered, for both experimental and numerical data, displayed clear steps or plateau points that occurred frequently throughout the mixing. These were shown to be caused by sudden two way vertical exchanges through the opening. These two-way exchanges resulted in significant volumes of fluid from each layer being transported to the opposite layer without significant mixing occurring, thus allowing the PE and BPE to remain unchanged. However, this exchange is unstable and the system returns to the bidirectional exchange process. Such motion is suggestive of there being an unsteady periodic orbits caused by the obstruction.

It was observed through 3D experimental and numerical data that each layer was very close to being homogeneous, apart from a narrow band along the horizontal boundaries. As a result
of this uniformity of density in the layers, the mean density of each layer was taken to be a
meaningful parameter for the overall density change of the domain. From this it was observed
that the mean density from a range of opening sizes collapse onto a single curve when plotted
against the opening-scaled time of $\tau_\gamma = \gamma \sqrt{Ag/\bar{H}t}$. Other aspects of the mixing dynamics,
such as the energetics, showed similar dependency on this time scale $\tau_\gamma$. However, the classical
unobstructed case with $\gamma = 1$ remained clearly distinct from any grouping, further suggesting
that the obstructed domain’s dynamics are fundamentally different from the unobstructed
domain.

A hierarchy of analytical models were developed for the singly-connected domain. Begin-
ning with simple assumptions, the complexity of each of the models was gradually increased,
improving the accuracy at which the models predicted the density change in each of the layers.
From developing these models two clear mixing regimes were identified. In the first regime,
fluid moving onto and mixing on the interface was at the initial density, such that $\rho^{*}_{U,L} = \rho_{U_0,L_0}$
(where $\rho^{*}_{U,L}$ is the density of fluid either side of obstruction). This resulted in a linear change
of mean density with time in each layer. After some time (observed to be $\tau_\gamma \approx 3.4$) mixed
fluid had been recirculated around the full layer and now moved onto the opening such that
$\rho^{*}_{U,L} \neq \rho_{U_0,L_0}$. In this regime an instantaneous model was proposed that captured the density
change fairly accurately. However, this was improved upon by developing a non-instantaneous
model inspired by the $K - \varepsilon$ model of Launder and Spalding (1974).

A number of numerical simulations were run as a preliminary investigation into the effect
of the aspect ratio on the obstructed domain’s dynamics. For the high aspect ratio domain, with
$H/L = 8$, the dynamics appeared similar to the $H/L = 2$ cases seen earlier. A bidirectional
exchange exists on the opening, transporting fluid away from the interface towards the horizontal
boundaries by two wall plumes. However, these plumes spread horizontally as they entrain
more fluid until their width is comparable to the domain width. This effectively results in
several co-rotational circulation cells filling and transporting fluid about each layer rather than
the solitary circulation cell seen for the $H/L = 2$ case (where the height of each layer was equal
to its width). The increased number of circulation cells appeared to result in more homogeneous
layers at the end of the simulation than the similar $\gamma = 0.5$, $H/L = 2$ case.

For the low aspect ratio domain of $H/L = 0.25$ the mixing dynamics began similarly to
the other cases seen, with a horizontal buoyancy gradient between the RTI mixing region and
the fluid on either side of the barrier drawing this unmixed fluid into the opening. However,
due to reduced layer height, the RTI mixing region is able to grow to the full height of the
domain before the stream flowing off the obstruction forces it into the side wall. This results in
a bifurcation of the opening. On the (left-hand) side furthest from the obstruction, the fluid is
now fairly well mixed via the unhindered growth of the RTI. However, on the (right-hand) side
closest to the obstruction, fluid continues to flow from above and below the obstruction and into the opening.

The significant buoyancy difference between the two sides of the opening in the low aspect ratio domain results in fluid flowing into the opening being deflected to the horizontal boundary without mixing significantly. The fluid spreads horizontally along the upper and lower boundaries, resulting in a more stable stratification on the left hand side of the opening, flowing as a gravity current towards the right. This fluid travels through the whole layer before returning to the opening. The circulation is too weak to establish a bidirectional exchange in the opening and instead the interface is seen to oscillate between the upper and lower boundary. This results in a significantly more stable stratification than was seen for any other aspect ratio including the unobstructed domain.
Chapter 7

Multiply-connected domain

7.1 Introduction

The work presented in the previous chapter concentrated on cases where an obstruction was firmly fixed to one edge of the domain, thus there was a single connection between each layer. A schematic of the singly-connected setup is shown in figure 1.1. The horizontal asymmetry at the interface results in a bidirectional exchange flow driven by two circulation cells, one in each of the layers. These circulation cells carry fluid from each of the layers onto the interface where they interact and mix via the Rayleigh-Taylor Instability (RTI). The subsequent Rayleigh-Taylor (RT) mixing region is carried along the interface to the end wall. The mixed fluid then flows vertically along the end wall, forming well mixed wall plumes. Once at the horizontal boundaries the fluid continues as a gravity current before interacting with the opposite end wall and forming an overturning fountain extending from $|z/H| = 0.5$ to $z = 0$ for both layers. These dynamics exist for a wide range of obstructions, $0.125 < \gamma < 0.8$ and continue quasi-steadily until both layers are well mixed. The singly-connected domain can take up to 3 - 5 times longer to become quiescent compared to classical unobstructed cases.

An extension to this work is to consider multiply-connected cases where the obstruction is disconnected from the side walls, as indicated by the schematic in figure 2.3. The opening sizes are parametrised by $0 < \gamma_1, \gamma_2 < 1$. For the symmetric case, the openings are equally sized with $\gamma_1 = \gamma_2$, while for asymmetric cases $\gamma_1 \neq \gamma_2$. We will define $\gamma = \gamma_1 + \gamma_2$ representing the total opening size.

The dynamics for the multiply-connected domain can be predicted to consist of one of two physically realisable mixing regimes. In the first of these possibilities, the dynamics are expected to be similar to the singly-connected domain, with two circulations cells established in each of the layers, remaining quasi-steady for the duration of the mixing. In the second
regime, an equal but opposite unidirectional flow passes through each opening as the layers 
overturn. As we shall demonstrate, an unexpected combination of both regimes is seen.

This chapter will build upon the work of the singly-connected domain. As for the singly-
connected chapter, 3D experimental data will be the primary data set, however, these will be 
supplemented with numerical data from MOBILE simulations. We will present a qualitative 
description of the dynamics of the multiply-connected domain by presenting experimental LIF 
data for a number of openings sizes. A 3D isosurface of the numerical density data will also be 
presented and discussed to demonstrate the similarities and differences between experimental 
data. Comparisons will be drawn to the dynamics of the singly-connected domain and, where 
differences are seen, these will be explained.

To understand the dynamics of mixing in the multiply-connected domain more quantitatively 
the mean concentration field and energetic profiles will be examined for both 3D experimental 
and numerical data. These results will be compared against one another, the singly-connected 
and unobstructed data presented in the previous chapter. As we find that, in some cases, the 
multiply-connected domain supports unidirectional flow through its openings, we look at the 
mean velocity through each of the openings, observing an apparent periodicity in its direction 
for a range of openings for both experimental and numerical data. Finally the dynamics for an 
asymmetric multiply-connected domain are discussed qualitatively.

7.2 Qualitative description

In this section we present a number of time series of LIF and PIV images for the multiply-
connected domain with symmetric openings of various sizes. The obstruction is created using a 
transparent polycarbonate sheet secured in the centre of the domain as shown in a schematic 
in figure 2.3. All LIF images presented within this chapter were post-processed using the 
photobleaching correction methods outlined in chapter 5. The method was modified slightly 
such that there was a weak vortex sheet applied in both openings, similar to that described in 
section 5.6.

7.2.1 Opening with $\gamma_1 = \gamma_2 = 0.25$

Figures 7.1 and 7.2 show LIF and PIV time series respectively for the multiply-connected 
domain with symmetric openings such that $\gamma_1 = \gamma_2 = 0.25$ and $\gamma = 0.50$. As for the singly-
connected domain, the RB is removed from left to right, evidenced by the increased growth 
of the RT mixing zone seen in the left-hand opening compared to the right at early times (see 
figure 7.1a). In figure 7.1a, at the right-hand opening, the distinctive mushroom shape structures
of early time RTI are still clearly visible. By contrast, the left-hand opening, where the interface is first exposed, looks distinctly more turbulent. Also visible in figure 7.1a is the initial jet (caused by finite removal of volume resulting from the removal of the RB), which has begun to propagate down the left-hand side wall. This jet is also visible in the early PIV images. For example, in figure 7.2a there is a large collection of long downward velocity arrows on the left-hand side wall in the lower layer, which propagate along the bottom boundary.

As for the singly-connected domain, the growth of the RT mixing zone results in a horizontal buoyancy gradient that draws unmixed fluid from above and below the fixed barrier (FB). The fluid is now able to flow from the FB into the two separate openings, as shown in figure 7.2a. This creates two bidirectional exchanges, one in each opening, which, as for the singly-connected case, carry mixed fluid via two wall plumes into each layer. This is made visible by the four distinct circulation cells seen above and below the openings in figure 7.2a, that bring fluid into the middle of the FB and then horizontally into each of the openings. This is made visible in the LIF image of figure 7.1b, we can see that the growth of the RTI increases with distance from the end of the FB in both openings. In addition, for the later time PIV image in figure 7.2b, the velocity arrows where the two layers meet are aligned horizontally in the direction of the FB.

As the wall plumes collide with the horizontal boundaries at the top and bottom of the tank they form gravity currents that begin propagating horizontally towards the centre at $x/L = 0.5$. These gravity currents collide and begin overturning away from the horizontal boundary towards the FB, as is visible in the upper layer of figures 7.1b and 7.2b. This strengthens the two circulation cells in each layer, such that there are in total four distinct circulation cells (two in each layer) that bring fluid from each layer onto each opening. These circulation cells act to draw fluid back towards the two openings. This effect is not as visible in the lower layer as the initial jet from the left opening propagates further to the right along the lower boundary than fluid from the right opening, causing the collision to be off-centre. There are, however, two distinct circulation cells in the lower layer with the left-hand circulation cell acting to draw some fluid back towards the left-hand opening, as made visible by the leftward pointing arrows beneath the FB in figure 7.2b.

The bidirectional exchange system seen thus far is, however, only metastable for the multiply-connected opening. The four circulation cells are unable to transport fluid equally to both openings. Eventually, the flux through one of the openings becomes unidirectional, as seen in the right-hand opening of figures 7.1c and 7.2c. This begins an overturning process where fluid from the lower layer is transported into the upper layer without significant mixing in the opening, resulting in a buoyant plume consisting primarily of lower layer fluid. This plume
Fig. 7.1 LIF data from the $\gamma = 0.5$ multiply-connected experiment with $A = 6.5 \times 10^{-3}$, with rhodamine dye added to the upper layer, at times (a) $\tau = 2.2 \ (t = 6 \ s)$, (b) $\tau = 4.4 \ (t = 12 \ s)$, (c) $\tau = 6.8 \ (t = 18 \ s)$, (d) $\tau = 9.0 \ (t = 24 \ s)$, (e) $\tau = 11.2 \ (t = 30 \ s)$, (f) $\tau = 13.4 \ (t = 36 \ s)$. The colour bar (in (g)) indicates intensity (density).
Fig. 7.2 Instantaneous PIV data from the \( \gamma = 0.5 \) multiply-connected experiment with \( A = 6.5 \times 10^{-3} \), at times (a) \( \tau = 2.2 \ (t = 6 \ s) \), (b) \( \tau = 4.4 \ (t = 12 \ s) \), (c) \( \tau = 6.8 \ (t = 18 \ s) \), (d) \( \tau = 9.0 \ (t = 24 \ s) \), (e) \( \tau = 11.2 \ (t = 30 \ s) \), (f) \( \tau = 13.4 \ (t = 36 \ s) \).
rapidly transports lower layer fluid to the upper boundary, beginning a process of anti-clockwise overturning.

This anti-clockwise circulation can be seen to extend around the full domain in figures 7.1d and 7.2d, with a unidirectional flow now evident in both openings. However, the circulation is limited to a narrow band around the perimeter of the domain and through each opening. This is unlike what was seen in the singly-connected domain, where the circulation was able to draw fluid from the horizontal boundaries back towards the FB such that each layer became well mixed. The circulation in this multiply-connected domain instead results in a significant volume of relatively unmixed fluid trapped on either side of the FB. Not all of the fluid in the boundary circulation is able to move through the opening, however, resulting in some fluid from the boundary circulation being deflected along the FB. For an anti-clockwise circulation, the deflected fluid is first present on the left-hand side beneath the FB and on the right-hand side above the FB such that it begins to establish a clockwise circulation around the FB (as is seen in figure 7.1e).

The fluid trapped on either side of the barrier is less well mixed than that carried by the boundary circulation (as shown by the brighter colours in figure 7.1e). The trapped fluid having a larger buoyancy magnitude when compared to the mixed fluid in the boundary circulation, forces itself against the direction of the boundary circulation in each opening. If there is sufficient trapped fluid this can actually reverse the direction of the flow through the opening. As figure 7.2e begins to show, in particular at the edge of the FB in the LHS opening, a stream of fluid is seen to move vertically upwards across the centre line of the tank. A similar, though opposite, effect is also observed at the right-hand edge of the FB. This process strengthens such that there is now a clockwise circulation established in the domain with fluid from the upper layer now moving downwards into the lower layer via the right-hand opening as visible in figures 7.1f and 7.2f.

At later times, not shown here, relatively unmixed fluid is again trapped either side of the FB and once more is transported towards the openings in a direction opposite to that of the global circulation. Once it reaches the opening again, the larger magnitude of buoyancy of the trapped fluid eventually reverses the circulation and the whole domain begins to circulate in the opposite direction. This process repeats while an unstable density difference continues to exists across the two layers.

### 7.2.2 Opening with $\gamma_1 = \gamma_2 = 0.125$

We now consider a case where the openings are much smaller, occupying, in total, only 25% of the domain width, with $\gamma_1 = \gamma_2 = 0.125$ ($\gamma = 0.25$). A time series of LIF data is shown in figure 7.3. Looking first at figure 7.3a, the RB has once again been removed from left to right,
Fig. 7.3 LIF data from the $\gamma = 0.25$ multiply-connected experiment at $A = 4.29 \times 10^{-3}$ with rhodamine dye added to the upper layer, at times (a) $\tau = 2.1 \ (t = 7 \ s)$, (b) $\tau = 3.3 \ (t = 11 \ s)$, (c) $\tau = 5.7 \ (t = 19 \ s)$, (d) $\tau = 9.0 \ (t = 30 \ s)$, (e) $\tau = 14.0 \ (t = 47 \ s)$, (f) $\tau = 21.1 \ (t = 71 \ s)$. The colour bar (in (g)) indicates intensity (density).
evidenced by the larger mixing zone visible in the left-hand opening when compared with the right. Looking at figure 7.3b we see the initial jet from the removal of the FB interacting with the lower boundary and spreading as a gravity current. The asymmetric influx of momentum and fluid into the lower layer begins a unidirectional exchange in both openings much earlier than that seen for the $\gamma_1 = \gamma_2 = 0.25$ case in figure 7.1.

Unlike for the $\gamma_1 = \gamma_2 = 0.25$ case a bidirectional exchange is not established in the opening at all. The lack of bidirectional exchange breaks the symmetry that created two circulation cells in each layer. Instead, as is seen in figure 7.3c, an overturning process occurs where fluid from each layer flows into the other, through one opening only, with very little RTI mixing due to the rapid vertical exchange. These vertical exchanges form highly buoyant wall plumes, composed primarily of unmixed fluid from the other layer. These plumes collide with the horizontal boundary and propagate as gravity currents, mixing with the ambient fluid as they move. This combined motion establishes an uni-directional, anti-clockwise circulation around the tank, similar to that seen in section 7.2.1.

The lack of small circulation cells in each layer, combined with the large obstruction, results in a significant volume of unmixed fluid trapped either side of the barrier. Due to the increased width of the boundary circulation, resulting from entrainment and mixing around the tank, not all of the fluid is able to be transported through the opening with some deflected along the barrier as was seen in section 7.2.1. This again forces unmixed fluid onto the opening. This unmixed fluid has a larger magnitude of buoyancy than the more mixed fluid of the boundary circulation and thus, as shown in figure 7.3d, we see that the trapped fluid forces its way through the opening and begins a clockwise circulation in the tank.

The large obstruction continues to trap relatively unmixed fluid either side of it, as this fluid is more (less) buoyant than the ambient fluid in the lower (upper) layer. Again it is displaced into the opening by the clockwise circulation and again its greater buoyancy is able to reverse the circulation direction as shown in figure 7.3e. This process continues even as the density difference between the two layers decreases and the circulation is weaker, as we can see in figure 7.3f.

### 7.2.3 Opening with $\gamma_1 = \gamma_2 = 0.375$

The next experimental scenario is that where the obstruction is much smaller than the domain width, occupying just 25% of the domain width such that $\gamma_1 = \gamma_2 = 0.375$ ($\gamma = 0.75$). A time series of the LIF data are shown in figure 7.4. In section 7.2.1 we saw that a bidirectional exchange existed in each opening for a significant period of time but that it was only metastable and soon transitioned to reversing unidirectional exchanges through the openings. In section 7.2.2 we saw that a larger obstruction prevented bidirectional exchanges from occurring
7.2 Qualitative description

Fig. 7.4 LIF data from the $\gamma = 0.75$ multiply-connected experiment at $A = 6.5 \times 10^{-3}$ with rhodamine dye added to the upper layer, at times (a) $\tau = 2.2$ ($t = 6$ s), (b) $\tau = 4.0$ ($t = 11$ s), (c) $\tau = 6.0$ ($t = 16$ s), (d) $\tau = 7.8$ ($t = 21$ s). The colour bar (in (e)) indicates intensity (density).
in either opening for any significant time and instead unidirectional exchanges through the openings were seen from early times with regular reversals. In this section, with a smaller obstruction, the volume of buoyant fluid able to trapped by the barrier will be less and as such we may expect fewer reversals.

Figure 7.4a shows a time at which the RB has just been removed and a RTI mixing region can be seen to grow in each opening. The increased size of each opening enables the RTI to grow for a greater distance and increases the horizontal buoyancy gradient between each opening and the unmix fluid trapped either side the barrier. This results in a larger torque applied in each layer such that the two circulation cells established in each layer are stronger. These four circulation cells effectively transport fluid from the horizontal boundaries towards the FB, displacing the fluid trapped on either side of the FB. Due to the symmetry of the four circulation cells the trapped fluid is almost equally displaced onto both openings such that a bidirectional exchange is able to continue (as shown in figure 7.4b).

The bidirectional exchange regime is longer-lasting in this case than in the other multiply-connected cases. The volume of fluid trapped by the FB is less than the volume of fluid able to pass through each opening. However, the FB is still able to trap some fluid that can be deflected preferentially through one opening (as shown in figure 7.4c). Interestingly the volume of trapped fluid moving through the right-hand opening is not large enough to block the whole opening. This results in a slower establishment of unidirectional flow through the opening, with significant variations in the direction of flow through each opening seen in the 3D scanned data. However, enough momentum and fluid is able to move through each opening that fluid is forced to circulate clockwise around the domain as shown by figure 7.4d. Note that this is the opposite direction to what was seen as the first circulation direction in the other cases presented.

7.2.4 MOBILE simulation with $\gamma_1 = \gamma_2 = 0.125$

Figure 7.5 shows a time series from a MOBILE simulation with opening $\gamma_1 = \gamma_2 = 0.125$ ($\gamma = 0.25$), Atwood number $A = 5 \times 10^{-3}$ at resolution $128 \times 128 \times 256$ with aspect ratio $H/L = 2$ (greater than the experimental value of $H/L = 1.25$). A small scale random perturbation is applied to the density interface at the start of the simulation, as discussed in chapter 3. The purpose of this simulation was to test the effect of the RB on the initial conditions and subsequent evolution of the flow, as well as to look at the impact of the slightly larger aspect ratio. In figure 7.5a we can see that the initial random noise perturbation gives way to bidirectional exchanges in each opening, with the fluid that is mixed in the openings transported equally away from the interface towards the horizontal boundaries by two narrow wall plumes. These plumes collide with the horizontal boundaries and form gravity currents that propagate...
7.2 Qualitative description

Fig. 7.5 MOBILE simulation of the $\gamma = 0.25$ multiply-connected domain at resolution $128 \times 128 \times 256$ with $A = 5.0 \times 10^{-3}$, at times (a) $\tau = 5.3$ ($t = 36$ s), (b) $\tau = 8.7$ ($t = 58$ s), (c) $\tau = 12$ ($t = 82$ s), (d) $\tau = 18$ ($t = 120$ s).

towards the centre of the horizontal boundary. At the centre they collide and overturn and are drawn down towards the FB in the middle of the tank by the two circulation cells that form in each layer.

Due to the turbulent nature of the motion in the domain, in particular that resulting from the collision and subsequent overturning of the gravity currents, there is not perfect symmetry in the four circulation cells, as was seen for the experimental data. As shown in figure 7.5b, the mixed fluid in the upper layer appears closer to the left-hand opening. This results in unmixed fluid being asymmetrically displaced into the left opening and this displaced fluid can be seen to establish unidirectional flow through each opening in an anti-clockwise direction. The larger aspect ratio does not appear to impact the qualitative dynamics of the multiply-connected domain. In particular the overturning fluid is seen to extend from the horizontal boundaries to the obstruction in the middle of the domain.
As for the experimental cases, the obstruction traps unmixed fluid on either side and not all of the fluid in the boundary circulation is able to pass through the opening. This results in some being deflected along the obstruction. This deflected fluid is forced into each opening against the circulation as shown in figure 7.5c. The buoyancy of this fluid overcomes the circulation and it is reversed such that there is a clockwise circulation. Through the same process we observe that the circulation reverses direction again in figure 7.5d. This process continues regularly for the remainder of the simulation as the same physical mechanisms persist even for smaller density differences. The regularity of this reversal will be looked at in more detail later.

Other simulations with \( \gamma_1 = \gamma_2 = 0.25 \) and \( \gamma_1 = \gamma_2 = 0.375 \) were run at the same resolution and with the same density differences. These again show qualitatively similar dynamics to the experimental results with a bidirectional exchange existing for longer with greater opening sizes and regular reversals of unidirectional exchanges. Thus, the circulation reversal does not appear to be solely caused by the initial conditions from removal of the RB, but is instead an intrinsic part of the dynamics arising due to the placement of an obstruction with two openings in the centre of unstably stratified domain. The small difference in the aspect ratio between the experimental and simulation data does not appear to significantly impact the dynamics.

### 7.3 Mean density concentration

In this section we discuss the mean concentration profile, \( \overline{C}(z,t) \), which is the average of the concentration in the horizontal plane. As for the singly-connected cases discussed in section 6.2, experimental and numerical data are shown for the multiply-connected symmetric cases with total opening sizes of \( \gamma = 0.75 \), 0.50 and 0.25 in figures 7.6 and 7.7 respectively.

We begin by discussing the concentration profile with the largest opening of \( \gamma = 0.75 \), shown in figures 7.6a and 7.7a for experimental and numerical data respectively. The first impression is that this concentration profile appears very similar to that of the singly-connected case in section 6.2. The growth of the initial RT mixing region can be seen to spread from \( z = 0 \) and is enveloped by the black line of \( \alpha = 0.05 \) for the experimental data. The numerical data is enveloped between the green and black lines (\( \alpha = 0.03 \) and 0.05). Indeed, this is true for the other two multiply-connected domains shown in figures 7.7b and 7.7c.

The mixing region can be seen to change the concentration significantly from its initial value as the large openings allow a lot of fluid to be transferred from each layer whilst also being mixed via the efficient bidirectional exchange mechanism. The small volume of fluid trapped by the FB is drawn into the openings where it is mixed and transported about each layer by the four circulation cells. As for the singly-connected domain, the first mixed fluid is seen to appear along \( |z/H| = 0.5 \) and spreads towards the FB at \( z = 0 \) for both experimental and
7.3 Mean density concentration

Fig. 7.6 Development of the mean concentration profile for the multiply-connected symmetric domain taken from 3D scanned LIF data, with openings of (a) $\gamma = 0.75$, (b) $\gamma = 0.50$ and (c) $\gamma = 0.25$. The colourbar for the mean concentration $C$ is shown in figure 6.2d. The superimposed coloured curves represent the quadratic growth of Youngs (1984) similarity law with $\alpha = 0.025$, 0.03 and 0.05 in red, green and black respectively.
Fig. 7.7 Development of mean concentration profile for the multiply-connected domain taken from MOBILE simulations at resolution $128 \times 128 \times 256$, with openings of (a) $\gamma = 0.75$, (b) $\gamma = 0.50$ and (c) $\gamma = 0.25$. The colourbar for the mean concentration $\overline{C}$ is shown in figure 6.2d. The superimposed coloured curves represent the quadratic growth of Youngs (1984) similarity law with $\alpha = 0.025$, 0.03 and 0.05 in red, green and black respectively.
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numerical data. At later times, the domain is fairly well mixed, with the mean concentration being close to 0.5 everywhere except at a few points along $|z/H| = 0.5$ for both figures 7.6a and 7.7a.

Looking at the $\gamma = 0.50$ multiply-connected concentration profile in figures 7.6b and 7.7b we can see that for early times, $\tau < 5$, the concentration profiles for both data sets are similar to the $\gamma = 0.75$ case. This is because, at early times, both cases exchange fluid between each layer via bidirectional exchange in a process similar to that of the singly-connected domain. The main difference between between the $\gamma = 0.50$ and 0.75 case, is that the larger obstruction traps more fluid, limiting the mixing that can occur. This is observable by the noticeably smaller change in $\bar{C}$ in the region $|z/H| < 0.25$ in figure 7.6b and the large (triangular) regions in $|z/H| < 0.3$ for $\tau = 2 - 6$ that have $\bar{C}$ equal to the initial value in figure 7.7b.

In figure 7.6b mixed fluid is seen to spread from $|z/H| = 0.5$ towards the interface at $z = 0$ up until $\tau = 11$. At around $\tau = 11$, we can see that along $|z/H| = 0.5$ the mean concentration changes from $\bar{C} = 0.5$ to $\bar{C} = 0.3$ and 0.7 for the upper and lower layer, respectively. The cause of this sudden change is a result of the collapse of the bidirectional exchange at $\tau = 9$. A similar effect is not as readily observable in the $\gamma = 0.50$ numerical data. We can observe at slightly later times that the mean concentration field in figure 7.7b changes significantly slower than for the $\gamma = 0.75$ data. Indeed, rather than the mean concentration field being well mixed along $|z/H| = 0.5$ and spreading into the layer, the whole concentration field gradually changes evenly through each layer. At late times ($\tau = 25$) there is a very weak stable stratification with $\bar{C} = 0.55$ and 0.45 along the lower and upper boundaries, respectively. The mean concentration profile demonstrates that this case has undergone an overturning motion, where fluid from one layer is transferred to the other without significant mixing. We can see that, at later times, the final concentration is not $\bar{C} = 0.5$ everywhere, as was true for all other obstructed cases considered so far (both singly and multiply connected).

The final case shown here is that with the smallest opening, $\gamma = 0.25$. The LIF timeseries of figure 7.3 demonstrated that there was little to no bidirectional exchange of fluid through the openings. Instead, unidirectional flows were established at early times and dominated as the primary exchange mechanism for most of the experiment, with a similar process seen in the numerical simulation. Looking at figure 7.6c, we observe that the $\alpha = 0.05$ curve is still a good envelope for the early time density change in each layer, while for figure 7.7c we observe that the best envelope lies between the green and black curves, as for the other numerical profiles.

The slower change in the concentration profile for early times in figures 7.6c and 7.7c is due to the reduced growth of the RTI mixing zone in the smaller openings. This results in narrow wall plumes that do not transport as much fluid as the larger openings, and as such, are not able to significantly alter the mean concentration in each layer. However, as before,
when these plumes interact with the horizontal boundaries, they form gravity currents that 
entrain ambient fluid, collide and overturn, resulting in the density difference spreading from 
$|z/H| = 0.5$ towards $z = 0$ in figures 7.6c and 7.7c. However, this mixed region is observed 
to not extend fully to $z = 0$ in figure 7.7c as the larger obstruction traps more fluid and the 
changing unidirectional exchanges prevent all of this fluid quickly being transported to the 
other layer. Indeed, there are still locations around the obstruction where the concentration has 
not changed from its initial value at $\tau = 15$. A similar pattern can be seen in the experimental 
data in figure 7.6c for $\tau < 11$.

The reversing direction of the unidirectional exchange is visible in figure 7.7c as regular 
patterns of mixed fluid appearing along $|z/H| = 0.5$, in particular at $\tau = 15$, 19 and 22. Here 
fluid from one layer is transported to the other, impacts with the horizontal boundary and mixes 
with the ambient resulting in the dark, well mixed structures that penetrate towards $z = 0$. These 
structures are stopped as the unidirectional flow changes direction, reversing the circulation and 
now the mixed fluid moves towards $|z/H| = 0.5$. This process can be seen to mix the two layers, 
however, it is not as efficient as other less obstructed case, as can be seen by a less uniform 
concentration field at later times in figures 7.6c and 7.7c. In particular we observe a significant 
stable final stratification in figure 7.6c, with a similar, though less clear, stable stratification in 
the numerical data of figure 7.7c (for a clearer image see digital copy of this thesis). Thus, for 
smaller multiply-connected openings the initial stratification is able to overturn and transfer 
fluid between each layer with less mixing.

### 7.4 Energetics

As for the singly-connected domain, more information about the mixing process can be gained 
by considering the different energy changes in the domain. Here we discuss the total potential 
energy (PE), kinetic energy (KE), available potential energy (APE) and background potential 
energy (BPE), as defined in section 1.3, for each of the three opening sizes for both experimental 
and numerical data (figures 7.8 and 7.9, respectively).

The simulations have one obvious benefit, in being able to provide insight into the early 
energetic changes that are obscured by the opaque RB in the experimental data. As for the other 
energy profiles seen in section 6.6, the early changes are driven by the growth of the RTI mixing 
region from the initial perturbations to the density interface. Thus, for the larger openings, the 
RTI mixing region is also larger, releasing more PE at a faster rate than for smaller openings, 
see figures 7.9a to 7.9c.

Looking at the $\gamma = 0.75$ energetic profiles in figures 7.8a and 7.9a, for experimental and 
numerical data, we see that after $\tau \approx 3$ and 4, respectively, there is a rapid decrease in the PE
Fig. 7.8 Energetics of experiments using the full 3D PIV velocity field and LIF density field, with openings of (a) $\gamma = 0.75$, (b) $\gamma = 0.50$ and (c) $\gamma = 0.25$. Initial data cannot be measured due to opaque RB.
Fig. 7.9 Energetics for the multiply-connected domain taken from MOBILE simulations at resolution $128 \times 128 \times 256$, with openings of (a) $\gamma = 0.75$, (b) $\gamma = 0.50$ and (c) $\gamma = 0.25$. 

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that is shared between an increase in BPE and KE. After this time the initial mixing zone has
grown sufficiently that bidirectional exchanges are established in each of the openings and the
initial perturbation no longer has an effect. Note that as for the singly-connected cases the
bidirectional exchange is very effective at mixing the two layers, resulting in the rapid decrease
in APE before $\tau = 6$ in figures 7.8a and 7.9a.

The KE can be seen to attain a maximum at $\tau = 6$ for both experimental and numerical data.
This is approximately the time that the bidirectional exchange is broken and the domain moves
to a unidirectional exchange, as was seen in figure 7.4. For both experimental and numerical
data in figures 7.8a and 7.9a the KE decreases slightly but remains relatively constant for a
significant period, until $\tau = 13$ and 14 respectively. Note that this is after the PE = 0 (the
point at which the domain is well mixed) at $\tau = 10$ and 12 for experimental and numerical
data respectively. The likely reason for this is that a lot of the energy is stored in the boundary
circulation that persists at later times. A small part of this remaining KE is used to further
increase the BPE, but a significant majority is simply dissipated.

With the smaller opening sizes, a unidirectional exchange was established earlier and
reversed direction more readily. In section 6.6.2, for singly-connected cases, when the bidirec-
tional exchange was disrupted the PE plateaued as mass was exchanged between each layer
without significant mixing. As expected, we see the same plateauing features in both the
$\gamma = 0.50$ and 0.25 energetic profiles (see figures 7.8a and 7.8c and figures 7.9a and 7.9c, for
experimental and numerical data respectively).

We now look in more detail at each of these cases, beginning with $\gamma = 0.50$ in figures 7.8b
and 7.9b. We see in figure 7.8b three clear peaks in the KE. These are the result of the
unidirectional flow reversing such that KE decreases as the direction is changing and then
increases again as the circulation begins moving in the opposite direction. Interestingly, despite
these reversals reducing the KE from its peak value, KE in the trough is still larger than zero,
suggesting that there is a significant amount of KE stored outside of exchanges through the
openings. These reversals are also not responsible for large increases in the BPE, as might be
expected from such turbulent directional changes on a density interface. At later times, the
majority of the KE appears to be dissipated rather than used for increasing the BPE. Despite a
similar dynamical regime observed in the numerical data the peaks in KE are not observable in
figure 7.9b.

In figures 7.8b and 7.9b, we see that there is a less rapid decrease in the APE than for the
$\gamma = 0.75$ profile. Indeed, the PE does not become zero until $\tau = 15$ and 23 for experimental
and numerical data respectively. This is 50% later than the same time for $\gamma = 0.75$, just as the
total $\gamma = 0.50$ opening is 50% smaller than the $\gamma = 0.75$. However, for the $\gamma = 0.25$ case, the
PE stops decreasing at $\tau = 15$ and 28 for experimental and numerical data respectively. Note
that when compared to the decrease in the opening size these times are not substantially longer than the similar $\gamma = 0.50$ time. This suggests that the $\tau_\gamma$ timescale (derived in chapter 6) is only appropriate when the layers are well mixed via a bidirectional exchange through a single opening.

The final energetic profiles, for $\gamma = 0.25$ are shown in figures 7.8c and 7.9c for experimental and numerical data respectively. As expected, for the smaller opening size, the PE change is the slowest of the three cases presented. The plateaus in the PE are very clear in both figures 7.8c and 7.9c and align well with the peaks in the KE as the unidirectional flow reverses regularly. The lower values of the PE and BPE are evidence of a final stable stratification, demonstrating once more that a unidirectional (overturning) exchange is less effective at mixing than a bidirectional exchange.

The unidirectional exchanges are responsible for the reduction in expected time to reach the final state (that state is not fully mixed but is stable). They enable the system to exchange fluid between each layer rapidly without mixing thoroughly. These also result in reductions of the PE with simultaneous growth in KE and a gradual increase in the BPE due to regular direction reversals of the unidirectional flow (as seen in figure 7.9c). The periodic nature of the peaks in KE are investigated further in the next section where the direction of the mean velocity in each opening is analysed.

### 7.5 Periodic exchange

For large openings, the multiply-connected domain exchange dynamics are similar to that for the singly-connected case. In such cases, mixing between each layer is primarily done via bidirectional exchanges in each opening. For smaller openings the bidirectional exchange appears to be only metastable, with unidirectional exchanges through each opening appearing to produce a more stable exchange mechanism. However, the direction of the flow is not stable and was seen in section 7.2 to reverse direction regularly. This observation was further supported by the periodic oscillation seen in the KE in section 7.4. In this section we look at the mean vertical velocity through each of the openings for both experimental and numerical data.

We consider 2D experimental PIV data (shown in figure 7.10). The use of 2D PIV data here is due the limited memory available for high speed recording, limited to just 70s for the 3D scanned data. We are able to record more 2D PIV data as the frame rate can be adapted to the velocities in the tank, such that at early times a high frame rate is used, whilst at later times, when the motion is slower, a lower frame rate can be used enabling recording to last for approximately 150 s.
7.5 Periodic exchange

7.5.1 Experimental

Figure 7.10 shows the mean vertical velocity over time for both openings with $\gamma = 0.25$ and 0.5. The first observation from looking at these is that the sign change of the vertical velocity has a very constant period. The next is that each opening’s profile is very close to the reflection of the other, despite these openings being disconnected. For early times, $\tau < 4$, the small (almost zero) mean velocity in each opening is evidence of bidirectional exchanges in both openings.

We now begin to look in more detail at each figures, starting with the $\gamma = 0.25$ case shown in figures 7.10a and 7.10b. Note the different Atwood number for each of these figures, $A = 5.5 \times 10^{-3}$ for (a) & (c), and $A = 1.2 \times 10^{-2}$ for (b) & (d). The Atwood number is twice as large for figure 7.10b as for figure 7.10a, resulting in the velocity scale being almost a factor of two different. In figures 7.10a and 7.10b we see that the bidirectional exchange gives way to a unidirectional exchange quickly, at $\tau = 1$ and $\tau = 2$ respectively. The first period of unidirectional flow has a fairly flat peak before the direction reverses at $\tau = 7$ and $\tau = 8$ for figures 7.10a and 7.10b respectively. After this the mean exchange speed increases for both cases, before changing direction again at $\tau = 12$ and 13 for respectively. Note that this means that the first and second unidirectional periods are the same for both cases.

After the peaks at $\tau = 13$ and $\tau = 14$ for figures 7.10a and 7.10b respectively, the subsequent peaks in velocity are seen to be significantly lower as the volume of initial density fluid trapped by the FB is greatly diminished, reducing the energy available for increased velocities. However, despite the decreasing density difference, the period of the reversing unidirectional flow remains surprisingly constant at $\Delta \tau \approx 5$ for the remainder of the mixing process. This results in highly symmetric velocity profiles between each opening, due to conservation of volume in each layer.

Considering the $\gamma = 0.5$ velocity exchanges, seen in figures 7.10c and 7.10d, we note again that the modified density difference (Atwood number) between these two experiments results in larger peak velocities in figure 7.10d. The first difference between the $\gamma = 0.25$ and 0.5 velocity profiles is the slightly longer bidirectional exchange period at the start of figures 7.10c and 7.10d. We see that a unidirectional exchange does not begin until $\tau = 3$ and $\tau = 4$ for figures 7.10c and 7.10d, respectively, compared to $\tau = 1$ and 2 for figures 7.10a and 7.10b. Thus for larger openings the initial bidirectional exchange appears to last longer. In addition we again see, for the larger density differences (higher Atwood number), that the initial bidirectional exchange appears to last for a slightly longer non-dimensional time.

Another feature of this case is that the first unidirectional flow through the right opening is negative in figure 7.10c, compared to a positive flow in all other cases in figure 7.10. This is particularly interesting as it demonstrates that the effect of the initial jet down the left-hand side does not always determine the direction of the initial circulation. The velocity is seen to reverse at $\tau = 9$ and 11 for figures 7.10c and 7.10d, respectively.
Fig. 7.10 Mean velocity through both left and right openings, respectively, from 2D experimental PIV data, with $\gamma = 0.25$ in (a) and (b), and $\gamma = 0.50$ in (c) and (d). The Atwood number of each figure is $A_0 = 5.5 \times 10^{-3}$ for (a) and (c), and $A = 1.2 \times 10^{-2}$ for (b) and (d).
The velocity then reverses at $\tau = 16$ and $\tau = 18$ for figures 7.10c and 7.10d, respectively, representing a reversal period of $\Delta\tau = 7$. Thus the reversal period also appears to be longer for the larger opening. After this time, the maximum speed is seen to decrease significantly, entering into a highly periodic velocity exchange, similar to that seen in figures 7.10a and 7.10b. The period of this exchange appears, again, to be fairly constant with a reversal period of $\Delta\tau \approx 7$ throughout, whilst the density difference between the two layers decreases significantly over the same period.

### 7.5.2 MOBILE

We now consider the same calculation from two MOBILE simulations with $\gamma = 0.25$ and $0.50$ (shown in figures 7.11a and 7.11b respectively). These simulations are initiated with small scale random perturbations in each opening. As such, the asymmetric initial conditions caused by the removal of the RB at the start of an experiment are not present here such that the direction of the unidirectional flow will be determined dynamically. Further details on the effect of the initial condition can be found in appendix A.

Beginning with the $\gamma = 0.25$ case (shown in figure 7.11a), we see that for early times there is a bidirectional exchange until $\tau = 2$. Then each opening gradually transitions to a unidirectional exchange, attaining a local maximum at of $|v| = 0.01 \text{ ms}^{-1}$ at $\tau = 9$. The circulation then accelerates in the opposite direction, attaining a much greater local maxima of $|v| = 0.03 \text{ ms}^{-1}$ at $\tau = 12$. However, this peak is far sharper than the previous maximum and the velocity is seen to change direction rapidly, achieving a slightly greater maximum of $|v| = 0.04 \text{ ms}^{-1}$ at $\tau = 16$. From this time onwards the velocity is seen to periodically change from positive to negative in each opening with period of $\Delta\tau = 5$. The maximum value of $|v|$ is seen to gradually decrease until $\tau = 30$.

From $\tau = 35$ in figure 7.11a the local maxima in $|v|$ are seen to be greatly reduced when compared to earlier times. This effect is comparable to what was seen in figures 7.10a and 7.10b for the experimental data. After this time, as for the experimental data, the velocity is seen to change direction, with a period of $\Delta\tau \approx 9$, until the end of the simulation when the density differences become almost negligible. At early times the fluid trapped by the FB at the initial density (thus allowing a large density difference to persist), moves into the opening, causing the sharp peaks in exchange velocity at early times. Eventually the trapped fluid is mostly displaced and replaced with fluid that is more mixed. Thus the density difference between the trapped fluid and the fluid moving through each opening is reduced, which in turn decreases the maximal exchange velocity.

Looking now at the $\gamma = 0.50$ case in figure 7.11b, the first thing to note is that the velocity scale here is greatly reduced compared to figure 7.11a. The reason for this is that the larger
Fig. 7.11 Mean velocity through both left and right openings for the multiply-connected domain taken from MOBILE simulations at resolution $128 \times 128 \times 256$, with openings of (a) $\gamma = 0.25$, (b) $\gamma = 0.50$, both at Atwood number $A = 5 \times 10^{-3}$.
opening sizes enable a more complicated three dimensional exchange, such that there are both upward and downward exchanges simultaneously in each opening, similar to what was seen in the energy plateaus of section 6.6.2. Thus, the mean velocity across an opening will be greatly reduced because of the two way exchange in each opening.

Looking at the early times, $\tau < 3$, in figure 7.11b, we see that the growth of the initial perturbation results in an equal exchange of fluid between each of the layers. After this, a weak unidirectional exchange appears to take place until $\tau = 17$. However, looking closely at the simulation data (not shown here) the flow appears to be largely bidirectional with the density interface in the openings shifting slightly from the $z = 0$ plane. Interestingly, despite primarily being bidirectional, these small deflections from the bidirectional flow (shown in figure 7.11b) occur on a near constant period of $\Delta \tau = 2$.

Eventually, as for the other multiply-connected domains, a unidirectional exchange through each opening becomes dominant. However, unlike the $\gamma = 0.25$ case, the exchange through each opening is not wholly in one direction. Despite this complicated two-way exchange, the mean direction of the exchange is seen to change periodically and symmetrically for each opening.

At $\tau = 28$ the flow through each opening appears to be changing direction, as expected from the periodicity. However, at $\tau = 29$ the change in direction halts and reverses, resulting in the double peak of the velocity profile in figure 7.11b. This is caused by the two-way exchange temporarily preventing the direction from reversing (as fluid is transferred against the prevailing direction in the opening). However, the influx of fluid onto each opening eventually overwhelms this mass flux and does reverse the direction of the unidirectional flow. This simulation then transitions to a very slowly varying unidirectional exchange from $\tau = 37$.

### 7.5.3 Fitted period

From the previous sections it appeared that the unidirectional flow changed direction over a near constant period for long times. This is a surprising result as one might expect that as the density differences between the two layers decreases, the timescales of the reversals would increase.

Within each layer it is known that there is a stable stratification (see section 7.3). It might be assumed that internal waves are the cause of the periodic oscillation through each opening. If we assume the waves have a characteristic lengthscale $l$, the frequency of these waves will scale as,

$$\omega \sim \sqrt{\frac{\rho U - \rho_L}{\rho} \frac{g}{g'} \frac{2\pi}{l}} = \sqrt{\frac{g'}{l}} \frac{2\pi}{l},$$  \hspace{1cm} (7.1)
where \( \overline{\rho U/L} \) represents the mean density of the upper and lower layer respectively and \( g' \) is the reduced gravity. Illustrated in figure 7.12 is the difference between the mean density of the upper and lower layer for a multiply connected domain with \( \gamma = 0.25 \). We use this domain wide density difference as an upper limit for the density difference in each layer. From figure 7.12 we see that the density difference decreases to approximately zero without there being a significant change in the observable period of the exchange velocity. For a constant time period, equation (7.1) requires the characteristic lengthscale of the waves to scale as \( l \sim g' \), such that the lengthscale would decrease as the velocity and density differences decay. This is the opposite of what is observed, where the characteristic lengthscale of the motion is seen to increase at later times.

Within the stable stratification of each layer it may be conjectured that the Brunt-Väisälä frequency,

\[
N = \sqrt{\frac{g}{\rho} \frac{d\rho}{dz}},
\]

sets a time scale for the oscillations, scaling as \( 1/N \). However, as figure 7.13 shows, \( N^2 \) evolves towards zero too quickly to be the cause of the constant period oscillation, suggesting an increase in period particularly between \( \tau = 0 \) and 30, which is not consistent with the data.

This leaves the initial Atwood number as the only remaining variable that can likely set a constant time period, (the instantaneous Atwood number decreasing too rapidly and the viscosity being insignificant compared to the inertia). In figure 7.14 we plot the reversal period.
Fig. 7.13 Layer averaged Brunt-Väisälä frequency, $N$, for multiply-connected MOBILE simulation with $\gamma = 0.25$.

Fig. 7.14 Fitted period, $t$ (s), for 2D experimental PIV data for various openings.
of mean velocity through each opening against the initial Atwood number. The period is calculated from the autocorrelation of the mean velocity data through each opening.

Dimensional analysis suggests the following timescale,

$$T \sim \sqrt{\frac{\mathcal{L}}{A_0 g}},$$

where $\mathcal{L}$ is an appropriate lengthscale. From looking at figure 7.14 we see that for a given $\gamma$ there is a fairly strong negative correlation on the initial Atwood number. This suggests that the lengthscale, $\mathcal{L}$, has some dependence on the opening size $\gamma L$, such that $\mathcal{L} \sim \gamma^q L$, for some $q$. However, there is not sufficient evidence to determine (or refute) the value of $q$ at this time, more experiments should be performed to investigate this further.

Whilst there is only a limited amount data plotted in figure 7.14 it does suggest that the constant period, even at late times, seen in figure 7.10 is determined by the initial density difference at the start of the experiment. This is quite a surprising result that suggests the initial Atwood number, rather than the instantaneous Atwood number, determines the regular period seen. This has the further implication that knowledge of the initial density stratification is stored in the system until late times despite significant mixing and turbulent motion occurring throughout the whole domain.

### 7.6 Asymmetric opening with $\gamma_1 = 0.125$ and $\gamma_2 = 0.375$

An asymmetric multiply-connected domain is defined as having $\gamma_1 \neq \gamma_2$, with the obstruction placed along $z = 0$ such that the geometry is centrally symmetric in $y$ and $z$ only. In this section we have included a 2D LIF time series using fluorescein dye as tracer, illuminated by a 2 mm thick light sheet created using two arc lamps beneath the tank. Unfortunately the dye concentration is too low for the image to be effectively corrected and thus to gather quantitative information. However, the key dynamics are visible and, crucially, are different from the other multiply-connected cases seen so far.

As discussed for the other multiply-connected cases, both openings support a bidirectional exchange for early times. As shown in figure 7.15a, the left-hand opening transitions to unidirectional flow from the lower to the upper layer. However, unlike for other multiply-connected cases, this does not appear to enforce a unidirectional flow through the right-hand opening. Indeed, a short time later the flow through the left-hand opening is seen to reverse in figure 7.15b. Throughout this process a bidirectional exchange is still seen to exist in the right-hand opening. The bidirectional flow is seen in figures 7.15c and 7.15d and is preserved.
7.6 Asymmetric opening with $\gamma_1 = 0.125$ and $\gamma_2 = 0.375$

Fig. 7.15 LIF time series for a multiply-connected domain at $A = 5 \times 10^{-3}$, with openings of $\gamma_1 = 0.125$ and $\gamma_2 = 0.375$ and fluorescein dye added to the upper layer, at times (a) $\tau = 4.4$ ($t = 14$), (b) $\tau = 5.6$ ($t = 18$), (c) $\tau = 7.8$ ($t = 25$), (d) $\tau = 10.0$ ($t = 32$).
in the right-hand opening for much longer than any other multiply-connected experimental setup considered.

Thus, for an asymmetric opening, a bidirectional exchange through the larger opening appears to be stable for long periods of time. The reason for this appears to be that the mass flux through the smaller opening is only a small perturbation when compared to that transferred through the larger opening. Thus, to a good approximation, the domain is almost singly-connected. The small mass flux through the left-hand opening is insufficient to impede or reverse the layer-wide circulation established by the bidirectional exchange in the larger opening. The regular reversals of the unidirectional flow in the left-hand opening are likely triggered by small, unequal exchanges of fluid from one layer to the other in the right-hand opening. Conservation of volume in each layer will result in fluid being exchanged to or from each layer via the smaller left-hand opening.

It may seem likely that if one opening were small enough that a bidirectional exchange could be seen in both openings for all times. However, “failed” singly connected experiments where the FB has not been secured tightly against the side wall, such that there was a small gap between the FB and the side wall, allowed small leaks of fluid from one layer to the other. This leak appeared as a very narrow unidirectional plume, whose direction changed regularly, whilst the motion in the larger opening was bidirectional.

The other limiting case is when the openings approach the same size and a bidirectional exchange is no longer stable in one opening. This is likely to dependent on ratio of $\gamma_1/\gamma_2$ as well as the total opening size $\gamma$. We saw earlier in the chapter that multiply-connected domains with large $\gamma$ sustained a bidirectional exchange for longer than smaller openings. To maintain a sustained bidirectional exchange, it seems likely that the smallest opening would have to be significantly smaller than the total opening size, such that the domain resembled a singly-connected domain as close as possible.

7.7 Summary

For both experimental and numerical data the opening size, $\gamma$, of the multiply-connected domain has a much more significant effect on the dynamics than was seen for the singly-connected domain. In the singly-connected domain, a bidirectional exchange was the only stable exchange mechanism. However, for a multiply-connected domain the bidirectional exchange was only metastable, with its duration dependent on the opening size. For larger openings, a bidirectional exchange was able to exist for longer times. The reason for the increased lifetime appears to be due to the smaller obstruction trapping less fluid and the exchange through the larger opening being impacted less by perturbations resulting from unequal buoyancy gradients.
The bidirectional exchange, for all obstruction sizes, gave way to a unidirectional exchange mechanism through each opening. Once established the unidirectional exchange does not return to the bidirectional exchange mechanism. However, neither does its direction remain constant. Instead, the direction of fluid passing through each opening was seen to repeatedly change direction over a constant period that appears to be determined by the initial density difference only. This has the further implication that knowledge of the initial density stratification is maintained until late times despite significant mixing and turbulent motion throughout the whole domain.

A unidirectional exchange is less effective at mixing fluid, enabling fluid to be transferred from one layer to the horizontal boundary of the other without being first well-mixed via the RTI. This results in a more stable, less well mixed final stratification for smaller openings where a unidirectional exchange process is established early. For larger openings a bidirectional exchange process, which is more effective at mixing fluid from each layer, is able to exist for longer. In this case less fluid is trapped either side of the obstruction further increasing the mixing.

The different dynamics of the asymmetric opening show that a multiply-connected domain can support a bidirectional exchange for long periods of time, so long as the flux through the smallest opening is sufficiently small compared to flux through the larger opening. This has significant implications for applications in ventilation as it suggests that relative the size of openings can affect the large scale dynamics and flux through each opening.
Chapter 8

Conclusions

8.1 Summary

A brief summary of the key ideas in this thesis are presented here for easy access. A more detailed discussion is presented in section 8.2

- The implementation and use of a novel 3D laser scanning system, discussed in section 2.5, introduces a new dimension to experimental fluid dynamics.

- Rhodamine 6G, used as a dye for LIF, is susceptible to bleaching by a laser. As the experimental setups of fluid dynamics experiments improve in search of greater accuracy, great care and corrections must be applied when using LIF for accurate density measurements. In chapter 5 we developed an innovative post-processing system that accurately compensates for the damage to dye caused by photobleaching and quenching.

- We saw in chapter 4 that the inclusion of a simple obstruction on the interface of two RT unstable layers results in dramatically different dynamics that are quasi-stable for long times resulting in total mixing times that are much longer than the classical unobstructed case. Fluid is exchanged through the opening via a bidirectional exchange, resulting in two circulation cells, one in each layer. These dynamics were observed for both experimental and numerical data.

- The circulation established by a singly-connected obstruction significantly increases the final mixing efficiency when compared to the classical case.

- In section 6.5 we developed a hierarchy of analytical models for the mean density change in each layer. The accuracy of these models increased with rank and we were able to accurately capture the density changes for long periods of time.
• In chapter 7 we saw that when the domain is multiply-connected, the early-time exchange dynamics are similar to the singly-connected case, with bidirectional flows in each opening. However, this exchange mechanism is only metastable and eventually a unidirectional flow is established through each opening.

• In section 7.5 we saw that the direction of the unidirectional flow in the multiply-connected domain appears to change over a regular period that is dependent on the initial Atwood number.

8.2 Review

This thesis began with the intention of investigating the effect of a material’s residual strength on the development of the RTI. The toy problem of introducing a thin obstruction along the interface of the classical RTI was proposed as a first step towards understanding RTI in materials with strength. The solid obstruction represents part of the flow that have solidified or, at least, not yet yielded. By using LIF and PIV data it became possible to observe how the RTI interacted with a solid obstruction and the impact this has on the development of the RTI. However, as can often be the case, this toy problem proved to be more interesting (and fun) than expected.

An innovative laser scanning system that could simultaneously capture the density field and velocity field in 3D was developed by Prof. Stuart Dalziel (as discussed in section 2.5). The 3D data presented in this thesis are the first data captured by the system and involved a significant amount of testing. From these experiments, it was shown (chapter 4) that an entirely new and unexpectedly interesting set of dynamics were observed. An initial RT mixing zone develops in the opening in a similar manner to what would be expected from the classical unobstructed RTI. However, unlike the classical instability the division of the mixing zone caused by the solid barrier results in a horizontal buoyancy gradient. This gradient acts to draw unmixed fluid from either side of the FB into the opening.

The influx of fresh fluid into the opening forces the mixing region into the side wall. A baroclinic torque across the opening forces the mixed fluid vertically from the interface to the horizontal boundaries at the top and bottom of the tank via two wall plumes. This motion establishes a layer wide circulation in each layer, whereby fluid is constantly drawn from either side of the barrier onto the opening. Here, a spatially varying RTI mixing zone develops, the height of which is proportional to the square of the distance from the end of the barrier. As the fluid moves across the opening it is mixed and transferred equally into each layer via a bidirectional exchange.
Away from the interface, the wall plumes collide with the horizontal boundaries and form gravity currents that propagate horizontally along the horizontal boundaries, entraining ambient fluid as they move. These gravity currents collide with the other side wall and overturn. The overturning fluid is drawn towards the obstruction against buoyancy forces, further than would be expected from previous work of overturning in a filling box (Kaye and Hunt, 2007). The overturning fluid mixes significantly with the ambient before it is drawn back onto the opening via the circulation in each layer. This fluid is drawn from either side of the barrier onto the interface. Despite mixing significantly with the ambient in each layer, the upper stream of fluid is still heavier than the lower (though at a reduced Atwood number from the initial value) and thus a RTI mixing zone continues to grow in the opening. This motion exists quasi-stably, taking much longer to reach a final quiescent state than the similar unobstructed classical RTI.

Experimental data were supplemented with a number of ILES calculations using MOBILE (described in chapter 3). With the ability to initialise each simulation with random small scale perturbations, the impact of the large scale perturbation caused by the removal of the RB could be investigated. Interestingly, unlike other RTI scenarios, the impact of the initial condition appears minimal as an almost identical dynamical regime to the experimental data was also observed in the numerical data. This is investigated further in appendix A. Knowledge of the initial condition is only present in the early evolution of the system and at mid-late times little difference is observable between small scale random noise and a larger sinusoidal perturbation as left by the RB (see section A.2). The horizontal buoyancy gradient forces the initial mixing region into the side wall, where it is mixed further through a turbulent boundary layer, such that any knowledge of the initial perturbation scales are lost.

Preliminary work by Davies Wykes (2014) suggested that the introduction of an obstruction to the interface reduced the cumulative mixing for two layers that were stably stratified with an unstable initial density difference at the interface. Using the same conductivity probe as used by Davies Wykes (2014), the final density profile was studied for two homogeneous statically unstable layers for various opening sizes in the singly-connected domain (section 6.4). These results showed that the inclusion of an obstruction resulted in a significantly more mixed final state, even when this obstruction was only a small percentage of the domain width. The increased mixing efficiency for the homogeneously stratified cases presented in this thesis is the result of the continuous recirculation of fluid about each layer. Fluid is continuously drawn from the vertical boundaries back onto the interface where it is subsequently mixed via the RTI. This process continues even at late times when the density difference between each of the layers is greatly diminished.

In chapter 5 we saw that the Rhodamine 6G (R6G) dye that was used as a tracer in the laser scanning system was permanently damaged by the laser, via a process known as photobleaching.
This is a quantum mechanical process that causes the intensity of fluoresced light from the R6G solution to decay exponentially with time. In order to get accurate density measurements a hierarchy of advection-diffusion post-processing corrections was developed. These correction models used recorded velocity data and estimated bleaching rates to model the distribution of bleached and unbleached dye in the domain.

The models that corrected only photobleaching were seen to accurately capture the late time decay, but failed to capture the early time rapid decay observed in experiments. The reason for this discrepancy was that another process known as quenching was also damaging the fluoresced intensity of the dye. The effect of quenching is temporary, with the rate of decay dependent on the concentration of NaCl in contact with R6G. By combining these two effects a new decay rate was presented that accurately captured the decay observed.

Having used these corrections to provide a more accurate 3D density field, the singly-connected domain dynamics were tested against some of the well developed analytical tools used extensively in previous studies of classical RTI (see sections 6.2 to 6.4). From these we saw that the singly-connected domain resulted in a more well-mixed final state for both the experimental and numerical data. From exploring the energetics of the singly-connected domain we observed a peculiar plateauing of the PE in section 6.6. These plateaus were seen to be caused by fluid being transferred in a large volume from each layer without significant mixing, in a series of unsteady periodic exchanges.

Furthermore, from these analytical tools it was observed that each layer was very close to homogeneous for long periods of time, with the density changing gradually across each layer. This enabled us to use the mean density of each layer as an accurate measure of the overall mixing. By using the non-dimensionalised time of $\tau = \gamma t \sqrt{Ag/H}$, it was observed (in section 6.5) that the mean density of all the obstructed cases collapsed onto a single curve. From this we derived a hierarchy of models that had increasing accuracy with rank, ultimately capturing the mean density change in each layer for long periods for both experimental and numerical data.

The effect of the aspect ratio on the dynamics of the singly-connected domain were also considered numerically in section 6.7. It was observed that for a high-aspect-ratio domain, with $H/L = 8$, the dynamics were very similar to the previously seen cases. For the low-aspect-ratio domain, with $H/L = 0.25$, the dynamics initially appear quite similar, the same horizontal buoyancy gradient drawing fluid into the opening from either side of the obstruction. However, the reduced height compared with the length of the opening prevented a layer-wide circulation from being established. Instead, fluid from each layer was able to easily move from one layer to the corresponding horizontal boundary of the other without mixing significantly.
The symmetry of the singly-connected domain ensured that the only stable exchange mechanism was via a bidirectional exchange through the opening such that equal volumes of well mixed fluid were transferred into each layer. The extension to this problem was to move the obstruction to the centre of the domain such that there were two openings connecting each layer, the multiply-connected domain in chapter 7. This scenario more closely represents the case where part of fluid with strength solidifies (or remains solid) in the centre of a domain away from other solid boundaries.

For the multiply-connected domain several different dynamical regimes were observed to occur throughout each experiment and simulation (in section 7.2). The initial mixing region that grows in each opening establishes two horizontal buoyancy gradients (as for the singly-connected domain) that draw fresh unmixed fluid from either side of the obstruction into each opening. This forces the mixed fluid into the side wall where two wall plumes transport well mixed fluid to the horizontal boundaries. However, this bidirectional exchange is only metastable, with its lifetime proportional to the size of each opening, such that for larger openings a bidirectional exchange lasts longer. The bidirectional exchange established four circulation cells, two in each layer.

Eventually the volume flux through one opening becomes greater in one direction such that the exchange through each opening becomes unidirectional. This establishes a large domain-wide circulation that connects both layers. However, not all of the fluid in the domain-wide circulation is able to pass through each opening, with some being deflected either side of the barrier. This deflected fluid displaces relatively unmixed fluid trapped by the obstruction onto each opening. As this occurs nearly symmetrically in each opening, the influx of buoyant fluid is sufficient to reverse the direction of the flow such that the circulation changes direction.

So regular was the reversal of unidirectional flow for both experimental and numerical data that the mean velocity through each opening was measured. It was observed that the direction of flow changed with an almost constant period that depended upon the initial (and not the instantaneous Atwood number). This has the surprising implication that knowledge of the initial density stratification is maintained until late times despite the majority of fluid being well mixed by highly turbulent motion.

The asymmetrical case considered experimentally in section 7.6 had one opening significantly larger than the other. We saw that the resulting dynamics were unlike the other symmetric multiply-connected cases. The larger opening was able to support a bidirectional exchange for long periods whilst the smaller opening supported a unidirectional exchange that regularly changed direction. The flux through the smaller opening is insignificant compared to the flux in the larger opening such that two circulation cells, one in each layer, were established, similar to that seen for the singly-connected domain in chapter 4.
8.3 Further work

There is a breadth of future work that could be built upon the simplicity of the experimental setup presented in this thesis. We will discuss some of these in this section.

8.3.1 Connecting RTI with natural ventilation

The dynamics considered in this thesis are new and previously unseen, with connections to both RTI and natural ventilation. They provide the possibility of connecting the two well-developed fields of the RTI and natural ventilation via one simple setup.

8.3.2 Further investigation of asymmetric opening

The damaged dye used in the asymmetric opening investigation in section 7.6 prevented quantitative data from being acquired. However, a qualitative understanding of the dynamics was achieved. The rather unexpected result that a bidirectional exchange through the larger opening appears to be stable for periods much longer than was observed for the other symmetric multiply-connected domains, warrants further investigation into the geometric factors controlling this time period. For example, how small can one opening be before the bidirectional exchange is fully stable, as was seen in the singly-connected domain. In addition to these interesting geometric quandaries, an asymmetric opening is more likely to reflect real-world obstructions, where openings are unlikely to be perfectly symmetric. As such further research into this scenario may improve upon the applicability of the results found in this thesis to other scenarios such as ICF.

8.3.3 RT with residual strength

The most obvious extension to this work is to continue with the original proposal of this thesis, which was to investigate the growth of the RTI in a material with strength. The ideas, models and insight gained through the work in thesis can hopefully be utilised to provide a jump start into understanding the effect of strength. Certainly, it is hoped, the work in this thesis could be used as an extreme limit when part of the flow has solidified. From this, the gap left between the obstructed and unobstructed domains could be filled. As a first step, experiments considering layers with differing viscosities could provide an interesting insight into some retarding effects to the growth of RTI. In particular, the organisation of the instability around areas that are still solid may decrease mixing. The viscosity could be increased to such a point that the growth is greatly inhibited.

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8.3.4 Impinging plumes

Two plumes impacting vertically onto a horizontal plate attached to one side wall is dynamically similar to that of the singly-connected domain. One positively buoyant plume from the base would impinge on the plate from the bottom whilst a negative buoyant plume would impinge on the other side from the top. This scenario is very similar to the singly-connected case discussed in chapter 6, and preliminary experiments suggest that the two plumes form two gravity currents that spread and begin to move off the end of the splitter plate. When the buoyancy of these two plumes was equally and oppositely matched, the motion moving off the barrier was very similar to that seen for the singly-connected domain. The two streams became unstable and developed into a RT mixing zone. The investigation of the impacting plumes could expand upon the results presented in this thesis; bringing them closer to natural ventilation problems. This includes scenarios such as in an office where computers and individuals produce hot plumes near the floor whilst an air conditioning unit (or similar) produces a cold plume from the ceiling. Investigating how these plumes interact may help make a more comfortable and less draughty temperature controlled environment.

8.3.5 Optimising mixing

The dynamics resulting from the singly-connected case produced significantly higher mixing efficiencies than the cases without an obstruction. Indeed significant improvements were observed with only a small obstruction. It would be important to investigate larger opening sizes to fully determine the point at which a regime change from classical to obstructed occurs. An extension to this is to investigate the effect of a cavity and whether this introduces as significant a change in mixing dynamics.

The potential to improve the mixing of two layers without inputting extra energy is a valuable result, especially when the industrial applications are considered. As such it would be useful to optimise the mixing process for different geometries, opening sizes and density differences. These applications would be highly relevant to industrial mixing.

8.3.6 Exchange on angle

One of the key geometric features of all the obstructions in this thesis was their simplicity, always being perpendicular to gravity. An interesting, simple extension would be to rotate the obstruction (or the tank itself) such that the obstruction and gravity are no longer perpendicular. This would disrupt the initial vertical symmetry that enabled the bidirectional flow seen for both singly and multiply-connected domains. Indeed, it would be expected that if the angle were
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sufficiently large the two layers would simply overturn. However, it is unclear how this would effect the mixing. Holford et al. (2003) showed that for a tilted interface, causing significant overturning, there was little change in the final mixing efficiency of the classical RTI with $\eta = 0.4$ at $\theta = 0$ (no tilting) to $\eta = 0.35$ at $\theta = 10\degree$. Via this extension, the work of this thesis could be expanded into other less simplistic areas of natural ventilation, with geometries that are more similar to real world environments.

8.3.7 Exchange past 3D objects

The work in this thesis has concentrated on planar objects that, whilst restricting the natural growth of the RTI and dramatically alter the dynamics, only occupy a small percentage of the total domain. By increasing the height of objects, interesting and unexpected boundary effects may occur, altering the dynamics from those seen in this thesis. The simplest scenario to consider would be to introduce a large cuboid both in a singly and multiply-connected domain. For the singly-connected domain this could probably break the circulation, for a large enough cuboid, as the initial mixing region would grow until its height were comparable to the height of the object. Once at this point, the horizontal buoyancy gradient would force fluid either side of the obstacle into the opening, but the initial mixing zone may have reduced the available potential energy so much that there is insufficient energy to establish layer-wide circulation as was observed in low-aspect-ratio results in section 6.7.

For the multiply-connected case, a large enough obstacle here too would change the expected dynamics from those discussed in this thesis. Again the initial perturbation would grow until its height was comparable to that of the object. At this point the initial mixing region is likely to be fairly well mixed. If the growth of the instability is symmetric on each side of the obstruction the mixed fluid is likely to displace and mix further with the trapped fluid. However, if the growth is not symmetric then it would be expected that the trapped fluid would be more likely to overturn than mix.

8.4 Final thoughts

This thesis began with the question of understanding Rayleigh-Taylor mixing in a material with residual strength. What was attempted first was to understand the simple problem of obstructing the classical RTI with a thin polycarbonate sheet. This in itself proved to be a dynamically interesting enough topic to study in depth. From a small modification to the classical, well-known problem, unexpected dynamics have been uncovered that may help with
some of the more complicated problems faced by the RT field (e.g. ICF) and other natural ventilation problems. To sum up this thesis in the words of another:

“Sometimes the questions are complicated and the answers are simple.”

Dr. Seuss

(Geisel, 1991)
Appendix A

MOBILE tests

A.1 Resolution testing

For numerical simulations it is important to investigate the effect of resolution. The mean density profile and energetic profiles for different resolution simulations of a $\gamma = 0.75$ singly-connected domain with $A = 5 \times 10^{-3}$ are shown in figure A.1. These simulations were all run at the same aspect ratio $1 \times 1 \times 2$ with resolution $n_x \times n_y \times n_z$. Looking at figure A.1a we see that all the mean density profiles are comparable, evolving at a similar rate and collapsing onto a value close to $\rho = 0$ at $\tau = 25$. Thus there is no clear trend with resolution for the evolution of mean density profile.

The different energetic profiles for the three resolutions are shown in figure A.1b. Again the three resolutions appear very similar, with comparable features in all three. In particular each of the three simulations displays two distinctive peaks in the KE, though at slightly different times, $\tau = 5$ for the lower resolution and $\tau = 6$ for the highest. These peaks coincide with a plateau in PE as discussed in section 6.6.2. There is a weak trend with increasing resolution, though overall, as for the mean density profiles in figure A.1a the effect of resolution on the evolution of the energetic profiles appears to be minor. Indeed the result of these resolutions tests appear to show that the simulations used within this thesis are not strongly dependent on the choice of resolution.

A.2 Initial perturbation

In this section we look at the effect of initiating an obstructed simulation with a perturbation comparable that to that left by the withdrawal of the RB in experiments. Previous research (Dalziel et al., 1999) has shown that different initial conditions can result in significant changes
Fig. A.1 Effect of resolution on a $\gamma = 0.75$ singly-connected domain for (a) mean density of the lower layer and (b) different energetic profiles. The three resolutions plotted are: $256 \times 256 \times 512$ solid line, $128 \times 128 \times 256$ dashed line and $64 \times 64 \times 128$ dotted line.
Fig. A.2 Time series of a large initial perturbation MOBILE simulation at resolution 128 × 128 × 256 with the density field rendered in 3D for the leftmost pairs of images and the y averaged density field in the right pairs of images at the times: (a,b) $\tau = 0$, (c,d) $\tau = 2.3$, (e,f) $\tau = 4.7$, (g,h) $\tau = 11.7$. 
in the mixing dynamics for the classical RTI. Here, we look at the effect of a large scale perturbation for a $\gamma = 0.50$ singly connected domain with a time series shown in figure A.2. The initial perturbation is visible in figures A.2a and A.2b. The simulation was run at a resolution of $128 \times 128 \times 256$.

Looking at figures A.2c and A.2d we can see that mixed fluid from the initial perturbation has spread fully towards $z = 1$ and spreads as a gravity current along the horizontal boundary. Looking at the lower layer, the mixed fluid only extends to $z = -0.75$ before it begins to spread horizontally. The reduced extent in this layer is due to the shape of the initial perturbation, with it being largest and positive along $x = 0$ before becoming negative and decreasing in amplitude with $x$. Unlike in the upper layer, the horizontal spreading of the fluid in the lower layer is not caused by the vertical wall plume being deflected by the horizontal boundary. Instead the vertical wall plume spreads horizontally as a result of the circulation established in each layer by the growth of the mixing region in the opening.

A short time later (see figures A.2e and A.2f) the effect of the initial large scale perturbation appears to have been entirely forgotten, with the evolving dynamics in each layer appearing largely symmetric. At later times, $\tau = 11.7$ in figures A.2g and A.2h, there is no observable evidence of the large scale perturbation to the interface. This result was expected, with knowledge of the initial condition being lost through a series of turbulent motions and the symmetry of the system enforcing equal fluxes of fluid between each layer.

We now look quantitatively at a comparison of the mean lower layer density profiles and energetic profiles between two $\gamma = 0.5$ singly-connected simulations at the same resolution, $128 \times 128 \times 256$, one with the large scale initial perturbation as discussed earlier and the other with small-scale random noise as used throughout thesis, as shown in figures A.3a and A.3b respectively. Looking first at the mean lower layer density profiles in figure A.3a, we see that the effect of the larger initial perturbation increases the initial mixing rate as the density of simulation with the larger perturbation is consistently larger than the random noise simulation. Interestingly the difference between the two density profiles decreases after $\tau = 10$ and the two curves are within 15% of one another by $\tau = 20$. This difference is seen to decrease significantly as time increases, with the two curves almost coalescing after $\tau = 25$. This implies that while the initial perturbation can “kick start” the mixing process it does not significantly increase the overall mixing rate.

Looking now at the energetic profiles in figure A.3b, we observe that, as for the mean density profile, a larger initial perturbation “kick starts” the mixing process, with the PE decreasing more rapidly than the random noise perturbation. We also see a larger and earlier peak in the KE, at $\tau = 4$, for the large initial perturbation case. However, this soon reduces and by $\tau = 10$ the KE is less than the random noise initial perturbation profile. This agrees with what was
Fig. A.3 Effect of modification of the initial condition on a $\gamma = 0.50$ singly-connected domain for (a) mean density of the lower layer and (b) different energetic profiles. The random noise initial condition used throughout this thesis is plotted as a solid line and the large scale initial perturbation is plotted as a dashed line. Both simulations are run at a resolution of $128 \times 128 \times 256$. Also plotted in (b), as a dotted line, are the energetic data from experimental 3D scanned data.
seen in figure A.3a where, after $\tau = 10$, the separation between the two mean density profiles decreases. This demonstrates that, at later times, it is the circulation in each layer that drives the resulting mixing and ultimately results in a more mixed final stratification than the classical unobstructed domain.

We also see from figure A.3b that introducing a perturbation similar to that observed in experiments results in a much closer agreement between experimental and numerical data for early times (compare the dashed and dotted lines). However, at around $\tau = 9$, the experimental potential energies changes more rapidly than the numerical data. This is likely the result of the significant differences in timescales as commonly observed between experimental and numerical investigations of the RTI (Dimonte et al., 2004). This is an area that is still under active investigation and beyond the scope of this thesis.

To summarise, the effect of a larger initial perturbation results in an initially faster mixing process. This was to be expected as introducing a large scale perturbation results in a more rapid growth of the RTI than for a flatter interface as the largest wavelengths are already present. The surprising result was that over the whole duration of the mixing process the larger initial perturbation has little to no effect on the final mean density of each layer. This suggests, ultimately, that it is the residual KE in the circulation cells of each layer that is responsible for the greater mixing efficiency observed for the singly-connected domain.

### A.3 Numerical errors

The difference between ILES and experimental timescales of RTI mixing is an ongoing investigation. The research of the Alpha Group collaboration of Dimonte et al. (2004) attempted to understand disparities in the RTI growth rate. They found a good agreement between all ILES algorithms used. However, there were still significant differences between the numerical and experimental timescales. Better agreement is observed to occur when experiment and numerical simulations are initiated with similar initial conditions as observed in section A.2 and by others (e.g. Dalziel et al. (1999)).

For turbulent mixing there is the additional complexity of the non-trivial dependency on Schmidt number (Zhou et al., 2017). For high Schmidt number flows of $\text{Sc} = O(10^3)$ a fine resolution is needed to capture the Bachelor scale

$$\eta_B = \frac{\eta_k}{\text{Sc}^{\frac{1}{2}}} \quad (A.1)$$

where $\eta_k$ is the Kolmogorov scale. As a result high Schmidt number simulations are prohibitively expensive to run, even for low $Re$. However, laboratory experiments using brine have
a high Schmidt number. This disparity between numerical and experimental Schmidt numbers is significant and a topic that is currently being actively investigated by others.

Despite the differences in timescales there is still plenty of evidence that demonstrates a good agreement between ILES, DNS and experimental data for a wide range of phenomena (Davies Wykes, 2014; Lawrie, 2009; Youngs, 2017). In addition to this, ILES has consistently been shown to capture the underlying fundamental dynamics (Aspden et al., 2009) and provides a useful tool for further investigation into areas not easily captured with laboratory research.
Appendix B

Experimental analysis

B.1 Discussion of 3D PIV/LIF system

Rayleigh-Taylor Instability mixing is typified by stratified turbulence where knowledge of both the velocity and density field are desired to allow a detailed understanding of the flow. Significant progress in understanding the three-dimensionality of RTI mixing has been made via DNS, LES and ILES simulations (Cook et al., 2004; Lawrie and Dalziel, 2011; Ramaprabhu et al., 2013). However, experimental results have struggled to produce three-dimensional results that are not just statistical measures. Experimental measurements are needed to complement numerical simulations due to the complexities in modelling physical boundaries and limits in realisable Reynolds numbers.

For the scenario presented in this thesis, the 3D laser scanning system enables far superior comparison between ILES and experimental data. Being able to qualitatively compare density fields and accurately identify similar structures in both experimental and numerical data reinforces confidence in the accuracy of the ILES results. By being able to build a strong visual foundation between ILES and experimental data, quantitative results can be fairly and accurately compared for differences. These include being able to calculate the full energetic field’s evolution with time, previously unachievable with 2D data.

One of the most significant advantages this thesis has gained from is using the three-dimensional scanning data to allow us to physically explain new phenomena identified in the data. For example we were able to further investigate the plateauing energy of section 6.6.2, which was initially first observed in numerical data and first thought to be a small rounding error in the numerical calculation. Only when the same phenomena was observed in experimental energetic profiles was it able to be further investigated and was observed to be caused by a physical phenomenon resulting from the equal and opposite exchange of mass between each layer.
The other significant result that required three dimensional density and velocity fields was the explanation for the periodic exchange in section 7.5. While this effect was observed clearly in 2D experimental PIV data, without the 3D scanning data it would not have been possible to confidently rule out other possible explanations for this effect, as discussed in section 7.5.3. As such the 3D scanning data was crucial in being able to accurately identify the same underlying phenomenon in both experimental and numerical data.

A quantifiable example of the efficacy of the 3D system versus the 2D system is to compare the BPE variation for the 3D field against that for a 2D slice. A representative example of this is shown in figure B.1. Here we are looking at the BPE variation taken from the $\gamma = 0.50$ singly-connected domain as discussed in section 6.6. The 2D slice data is taken at the same position for each full scan of the 3D field. Using same data set rather than a separate 2D experiment ensures that any differences between 2D and 3D data are not caused by different dynamics and are a true representation of the differences between a 2D and 3D data set.

Looking at figure B.1a we can see that there is quite good agreement for both the 3D and 2D calculation. In both cases the BPE begins around -0.3 J and follow a similar curve to finish near -0.05. However, the 2D data is significantly less smooth than the 3D as noise and random motion have a more dominant effect. Another significant difference is that the 2D consistently produces a more negative BPE than the 3D data, as shown in figure B.1b. We see in figure B.1b that using only a 2D slice produces differences in the BPE of more than 10 %, with spurious oscillations occurring particularly at late times. Having additional data in the form of 3D fields allows the averaging across multiple 2D slices. The differences between the 3D data and that taken from a single 2D slice are significant and would be expected to adversely affect the accuracy and usability of singular 2D data slices if taken as representative of the full domain.
B.1 Discussion of 3D PIV/LIF system

Fig. B.2 The instantaneous mixing efficiency, \( \eta_i \), of a \( \gamma = 0.50 \) singly-connected for a full 3D field (solid line) vs a 2D slice (dotted line) shown in (a), with their difference shown in (b).

Another quantitative scenario is to consider calculations of the instantaneous mixing efficiency, \( \eta_i \). Following Davies Wykes (2014) we define this as

\[
\eta_i = \left| \frac{BPE}{AE} \right| \tag{B.1}
\]

where \( AE \) is the available energy, \( AE = APE + KE \), and ‘\( \cdot \)’ represents the difference in energy between time steps. Using the same data set as for figure B.1 we plot the instantaneous mixing efficiency for the full 3D field against a 2D slice in figure B.2.

Looking at figure B.2 we see that two large spikes in the 2D data, at \( \tau = 4 \) and 11 respectively, dominate the instantaneous mixing efficiency and the difference between the 3D and 2D data set. Ignoring these spikes, looking at figures B.2a and B.2b, we see that for the overall trend there is a fairly good agreement between the two data sets. However, even excluding the large spikes, the instantaneous mixing efficiency calculated using the 2D slice is as much as 45 % larger than the average taken using the 3D data. This, along with the two large spikes, cast significant doubt on using 2D data for instantaneous mixing efficiency calculations as an accurate representation of the whole domain. Overall, we demonstrate that using a 3D field for such calculations provides vastly superior accuracy.

Overall the 3D scanning system has provided a number of valuable insights, providing greater accuracy and more robust data sets as shown above. The initial use of the 3D scanning system to investigate experiments of the singly-connected domain was motivated by the apparent two-dimensionality of the resulting dynamics such that the earliest diagnostics and test (even in its prototype condition) would still be able to produce meaningful and actionable results. The multiply-connected domain, being significantly more three dimensional, made much better use...
Experimental analysis

Overall, without such a system the conclusions of this thesis would be much less robust.

B.2 Additional discussion of errors

B.2.1 Conductivity probe

A detailed analysis of the potential errors resulting from the use of the conductivity probe to calculate the final mixing efficiency was performed by Davies Wykes (2014). A brief summary of the relevant results are presented here. For a more detailed explanation see appendix A of Davies Wykes (2014). In addition to the base accuracy of the conductivity probe, discussed in section 2.3, Davies Wykes investigated three further error sources that could result in $\Delta \rho$ errors.

The first of these is temperature changes, $\Delta T$, which can alter the measured conductivity. As discussed in section 2.3, temperature changes of $\pm 1$ K results in $0.1\%$ error in the density measured by the probe. Davies Wykes found the largest temperature change resulted from heating in the lab environment. This was an issue for Davies Wykes as her experiments had a long setup time. However, the experiments conducted in this thesis had a completion time of under 30 mins. In addition, each layer was filled from a large reservoir that had been allowed to reach thermal equilibrium with the laboratory environment. As such $\Delta T$ errors of this kind were not significant.

Another source of error were measurement height changes, $\Delta H$, which simply shift the measured conductivity vertically. The probe is not able to fully reach the bottom of the tank. As such measurements in height must be corrected by the distance of the probe from the base of the tank. This was measured to within an accuracy of $\pm 0.1$ mm. Davies Wykes observed that in a typical experiment between 10-20 ml of fluid can leak through the seal holding the RB. A loss of 20 ml can result in the free surface dropping by $0.25$ mm. The seal used in the experiments of this thesis was updated from that used by Davies Wykes and typically resulted in much smaller leakages of $< 5$ ml.

The final source of error is from volume changes, $\Delta V$. These can be considered errors that stretch or compress the vertical height of fluid. As the tank is filled with water, the walls bow outward, observed by Davies Wykes to result in a maximum height reduction of 0.40 mm, and, subsequently an increase in the volume of a full tank of $\delta V = 10^{-5}$ m$^{-3}$. Changes due to the non-linear equation of state when fresh and salt water are mixed result in $\delta V \approx 10^{-7}$ m$^{-3}$, which is small enough to be ignored. Additionally the compressibility of the lower layer results in $\delta V \approx 10^{-8}$ m$^{-3}$, which is again ignored. As the conductivity probe is traversed through the final stratification approximately 40 ml of fluid are removed, however, this is not considered
important as the probe traverses downward such that the removal of volume does not affect the stratification measured. The probe is not traversed through the initial stratifications which are a known density, well mixed and homogeneous.

### B.2.2 3D imaging: scanning PIV/LIF

An excellent description of the 3D laser scanning system used in this thesis is provided by Partridge et al. (2018). Here, we include a summary and discussion of errors produced by the laser scanning system.

At each $z$ location in a scan an estimate of the error from the stereo reconstruction can be found by projecting backwards the world velocities, $u$, onto the camera velocities (in pixels per frame). It is convenient to perform this calculation on a common grid to determine $U^*_i$ as

$$
\begin{bmatrix}
U^*_A \\
U^*_B
\end{bmatrix} = J^{-1} u
$$

(B.2)

where $J^{-1} = \frac{\delta X_i}{\delta F^{-1}_i}$ is the $(4 \times 3)$ Jacobian matrix of the inverse 3D mapping $F^{-1}_i$. Thus an error can be calculated by comparing the back-projected velocities with the real-world velocities calculated by the PIV algorithm. By assuming equal weighting among each component of the velocity it is possible to construct an error field

$$
E = \frac{1}{4} \left( ||U^*_A - U_A|| + ||U^*_B - U_B|| \right),
$$

(B.3)

where $U_i$ are the 2D pixel velocities for camera $i$. A typical value for the system used is $E < 10^{-3}$ pixels/frame. This error estimate is used as a further quality check by removing vectors where the error exceeds a threshold value.

When calculating stereo PIV velocities it is vital that the velocity vector calculated from one camera is coincident in world coordinates with the velocity vector from the other camera. While great care is taken to ensure that the initial calibration target is aligned perfectly with the laser light sheet, small discrepancies can produce large systematic errors in the stereo reconstruction. With the scanning system used in this thesis, a systematic error in positioning coordinates can be produced by any misalignment between the laser beam and optics. These errors are corrected for using an iterative two-step calibration refinement technique similar to Willert (1997). Simultaneously acquired raw particle images from each camera are mapped (using each camera’s coordinate mapping) onto world coordinates. In a perfect scenario, where the light sheet and calibration target are coincident and the light sheet is infinitesimally thin, the two particle images would be a perfect overlay of one another. Thus to determine how
well the real light sheet and coordinate system are aligned a disparity map is calculated from
cross-correlating the two images.

The first step of the refinement process is to iteratively refine the \( z \) position of the light
sheet, (for algorithmic details see Partridge et al. (2018)). The second step of refinement adjusts
for any residual misalignment between the light sheet position and the calibration target used
to create the original mappings. Any mismatch found by the algorithm is used to determine
the optimal transformation to align the particle images with the cameras. Unwanted outliers
are removed by calculating a polynomial fit to the disparity map over the \((x,y)\) plane and the
scanning direction using a least squares fit. This two step approach can be iterated until residual
correction is much less than the thickness of the light sheet. Typically only a single iteration is
required to achieve this.


