DOUBLE DIFFUSION IN LAKE KIVU

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Summary

Double diffusion enhances the vertical transport within a stratified water body by transforming gradual density gradients into staircases of convectively mixed layers separated by high-gradient and gravitationally stable interfaces. Those staircases can develop when two agents, which diffuse at different rates, contribute in opposing ways to the vertical density gradient. This study focuses on the diffusive regime of double diffusion, where the slower diffusing agent (here dissolved substances) is stabilizing. Estimating the vertical fluxes through double-diffusive staircases based on easily accessible parameters has been one goal of double diffusion research in the past. So far, flux laws are based on scaling arguments which are calibrated by empirical results from laboratory experiments and their validity in natural environments is questionable. Double-diffusive heat fluxes are of particular interest in the Arctic Ocean, where they control the heat exchange between a warm intrusion from the North Atlantic and the overlying sea ice. A more detailed understanding of double diffusion in natural environments is thus essential to test well-established theories.

In this study the presently most detailed in-situ measurements of natural double-diffusive staircases are combined with cutting-edge Direct Numerical Simulations (DNS) in order to improve our understanding of the dynamics between interfaces and mixed layers and to test existing flux laws.

Lake Kivu is an ideal study environment for double diffusion with up to 300 clearly distinguishable double-diffusive steps distributed almost over the entire permanently stratified water column below ~100 m depth. It is located close to the equator in the East African Rift Valley at the border between Rwanda and the Democratic Republic of the Congo.

During two field campaigns in 2010 and 2011, 225 microstructure profiles of temperature and conductivity were measured resulting in a total profiling length of ~55 km. Our data set comprises 9,401 fully resolved interfaces and adjacent mixed layers.

This study shows that a full resolution of the smallest interface thicknesses requires a correction for the responses of the microstructure sensors. The frequency responses of the FP07 temperature and the SBE-7 conductivity sensor are derived from observed differences in the statistical distributions of interface thicknesses at various profiling speeds. Heat and salt fluxes through double-diffusive staircases are found to be sensitive to the frequency response
corrections. This implies that the conductivity sensor is not “infinitely” fast, as previously assumed.

Temperature interfaces are shown to be thicker than salinity interfaces. The buoyancy stored in the resulting boundary layers is transported by plumes to the mixed layers. The interaction between the mixed layer and the boundary layers is time dependent and additionally influenced by mixed layer motions and thus cannot be understood by linear stability analysis.

The most common heat flux parameterization is tested and a correction introduced that depends on the Rayleigh number of the double-diffusive system. Applying the correction to studies in the Arctic reduces previous heat flux estimates by up to a factor of four.

Two-dimensional DNS is shown to reproduce the interface thicknesses of in-situ microstructure profiles and molecular heat fluxes through interfaces capture the total vertical heat fluxes for density ratios larger than three.

In summary, this study demonstrates the value of in-situ measurements, in particular in combination with DNS, for testing existing theories. With increasing computation power and sensor development, such interdisciplinary approaches will become even more attractive in the future and might eventually lead to new models and theories which are closer to reality than existing ones.
Zusammenfassung


In dieser Studie werden die bislang detailliertesten in-situ Messungen natürlicher doppeldiffusiver Treppen mit innovativen direkten numerischen Simulationen kombiniert. Das Ziel ist unser Verständnis der Dynamik zwischen den gemischten Schichten und deren Übergängen zu verbessern und existierende Flussgesetze zu testen.

Der Kivu-See ist in eine ideale Umgebung um Doppeldiffusion zu untersuchen, da bis zu 300 klar unterscheidbare doppeldiffusive Stufen existieren, welche fast über den gesamten permanent geschichteten Wasserkörper unterhalb von ~100 m Tiefe verteilt sind. Er befindet sich in der Nähe des Äquators im Ostafrikanischen Zentralgraben an der Grenze zwischen Ruanda und der Demokratischen Republik Kongo.


Diese Studie zeigt, dass für eine vollständige Auflösung der schärfsten Übergänge die Reaktion der Mikrostrukturen berücksichtigt werden muss. Die Ansprechzeit des FP07 Temperatursensors und des SBE-7 Leitfähigkeitsensors wird hier von den beobachteten


Nach dem Test der gebräuchlichsten Wärmeflussparameterisierung wird eine Korrektur eingeführt, welche von der Rayleighzahl im doppeldiffusiven System abhängt. Wird diese Korrektur für Studien in der Arktis angewendet, reduziert sie die bisherigen Wärmeflussabschätzungen um einen Faktor von bis zu vier.

Zweidimensionale DNS reproduziert die Übergangsicken, die in den in-situ Mikrostrukturprofilen im Kivu-See gemessen wurden und molekulare Wärmeflüsse durch Temperaturübergänge erfassen die totalen Wärmeflüsse für Dichteverhältnisse grösser als drei.

1 Introduction

The effect of double-diffusion on natural water bodies can easily be demonstrated in a simple experiment. We dump one tea spoon of sugar (without stirring) into a glass of hot coffee and add one tea spoon of coffee cream for visualization. After the internal waves (from adding the sugar and the cream) have died out, horizontal layers are forming (Fig. 1.1). This layering is caused by double diffusion. Double diffusion is, by itself, an extremely fascinating problem of fluid dynamics, because only few ingredients are necessary to display enormous complexity. But it is also a relevant process in a large range of natural settings because layering enhances the vertical transport of fluid constituents. This thesis sheds light on transport processes between the layers by measuring their small scale structure.

1.1 Phenomenon

For the formation of double-diffusive layers two agents are necessary which diffuse at different rates and contribute in opposing ways to the vertical density gradient. Let us call the faster and slower diffusing agents $T$ and $S$, respectively. In the coffee example, $T$ is temperature and $S$ dissolved sugar. The coffee is cooled from the top and the $T$ gradient is thus destabilizing. If there wasn’t the stabilizing $S$ gradient near the bottom of the glass, the entire coffee would be convectively mixed. Layers are forming if the stabilizing $S$ gradient slightly overcompensates the destabilizing $T$ gradient. The density ratio, which is the quotient of stabilizing to destabilizing (density) background gradient, is typically between one and ten in double-diffusively layered natural water bodies.

The configuration, where the slower diffusing agent ($S$) is stabilizing is called the “diffusive regime” of double diffusion. Layering is also observed when the faster diffusing agent ($T$) is stabilizing ($T$ decreasing with depth), which is then called the “finger regime”. Here we focus on the diffusive regime of double diffusion only and we henceforth omit the term “diffusive regime” for simplicity.
Double-diffusion is important, because it enhances vertical fluxes of $T$ and $S$ by transforming gradual gradients of $T$ and $S$ into staircases of convectively mixed layers separated by high-gradient and gravitationally stable interfaces (see Fig. 2.1).

Double-diffusive staircases are observed in oceans [Neal et al., 1969; Padman and Dillon, 1987; Timmermans et al., 2008] and lakes [Hoare, 1968; Schmid et al., 2004, 2010; Sánchez and Roget, 2007], where $S$ usually represents salt. Furthermore, double diffusion is relevant in stars ($S$ being helium) [Spruit, 2013], in magma chambers ($S$ being melted silica) [Huppert, 1984] and in industrial applications such as solar ponds [Newell and Boehm, 1982]. Comprehensive reviews on double-diffusion have been published by Turner [1973, 1974, 1985], Schmitt [1994] and Kelley et al. [2003] and a historic perspective of the discovery in the 19th century and its rediscovery in 1950s is given in Ruddick and Gargett [2003] and Schmitt [1995]. Double-diffusive heat fluxes are of particular interest in the Arctic Ocean, where they control the heat exchange between a warm intrusion from the North Atlantic [Carmack et al., 1997] and the overlying sea ice [Timmermans et al., 2008; Turner, 2010].

Fig. 1.1: Double-diffusive layering in a glass of coffee. Note the convective motions within the mixed layers.

1.2 Relevance and occurrence

Double-diffusion is important, because it enhances vertical fluxes of $T$ and $S$ by transforming gradual gradients of $T$ and $S$ into staircases of convectively mixed layers separated by high-gradient and gravitationally stable interfaces (see Fig. 2.1).

Double-diffusive staircases are observed in oceans [Neal et al., 1969; Padman and Dillon, 1987; Timmermans et al., 2008] and lakes [Hoare, 1968; Schmid et al., 2004, 2010; Sánchez and Roget, 2007], where $S$ usually represents salt. Furthermore, double diffusion is relevant in stars ($S$ being helium) [Spruit, 2013], in magma chambers ($S$ being melted silica) [Huppert, 1984] and in industrial applications such as solar ponds [Newell and Boehm, 1982]. Comprehensive reviews on double-diffusion have been published by Turner [1973, 1974, 1985], Schmitt [1994] and Kelley et al. [2003] and a historic perspective of the discovery in the 19th century and its rediscovery in 1950s is given in Ruddick and Gargett [2003] and Schmitt [1995]. Double-diffusive heat fluxes are of particular interest in the Arctic Ocean, where they control the heat exchange between a warm intrusion from the North Atlantic [Carmack et al., 1997] and the overlying sea ice [Timmermans et al., 2008; Turner, 2010].
1.3 Previous research and open questions

Numerous investigators have studied double-diffusion in laboratory experiments in the 1960s and the 1970s and one goal was to derive flux laws applicable to natural double-diffusive systems [e.g. Turner, 1965; Shirtcliffe, 1973; Marmorino and Caldwell, 1976; Linden and Shirtcliffe, 1978; Newell, 1984]. After a decrease of scientific activity in the 1980s and 1990s, double diffusion became attractive again after 2000, when the rapidly increasing computation power offered new opportunities to study the dynamics of double diffusion in numerical simulations [Worster, 2004; Noguchi and Niino, 2010a, 2010b; Gonzalez-Juez et al., 2011; Carpenter et al., 2012a; Flanagan et al., 2013; Wood et al., 2013; Zaussinger and Spruit, 2013]. However, the domains sizes of the simulations are still limited and their representativeness for double diffusion in natural systems is thus questionable. In the following we list some important unresolved questions accompanied by references to previous research on that topic.

(i) How do double diffusive staircases form from gradual background gradients in natural settings? Possible mechanisms are horizontal intrusions [Merryfield, 2000] or gradual evolution from vertical boundaries as observed in Lake Nyos [Wüest et al., 2012].

(ii) What determines the geometrical structure of the layering, i.e. the thicknesses and gradients of interfaces and mixed layers? Possible control parameters are the background gradients of $T$ and $S$ (defining the density ratio and the stability [Kelley, 1984]), the values of $T$ and $S$ at the boundaries and fluid properties such as viscosity and the molecular diffusivities of $T$ and $S$.

(iii) What are the evolutionary dynamics of layer merging and splitting within a staircase in natural systems? The time scales of these processes are not known, neither is the dominant mechanism. For example, many small steps could transform into few larger steps by decreasing either the distance between interfaces or the differences of $T$ and $S$ in the mixed layers [Huppert, 1971; Noguchi and Niino, 2010b].

(iv) What are the feedback mechanisms between double-diffusion and the lake/ocean stratification? If the double-diffusive layering caused vertically varying fluxes of $T$ and $S$, the background structure of $T$ and $S$ would be affected which then again has potential effect on the layering.
(v) How are mixed layer motions coupled to the interface? Various models have been developed to explain laboratory results [Linden and Shirtcliffe, 1978; Newell, 1984; Fernando, 1989; Kelley, 1990], but little is known about the coupling in natural systems.

(vi) Are laboratory derived flux laws valid in natural systems? [Kelley et al., 2003; Flanagan et al., 2013]

1.4 Approach

In this work we address questions (v) and (vi) by combining vertical microstructure measurements of temperature and conductivity in Lake Kivu (Central Africa) with Direct Numerical Simulations (DNS). This thesis greatly benefits from the work of Jeffrey R. Carpenter, who was Postdoc at Eawag and performed DNS parallel to the field work at Lake Kivu. However, the focus of the thesis are the microstructure measurements carried out during two campaigns in 2010 and 2011 at Lake Kivu.

1.5 Lake Kivu

Lake Kivu is located close to the equator in the East African Rift Valley at the border between Rwanda and the Democratic Republic of the Congo [Descy et al., 2012]. The surface area, the volume and the maximum depth are 2370 km$^2$, 580 km$^3$ and 485 m, respectively. It is well known for its impressive quantities of dissolved methane (60 km$^3$, at 0°C and 1 atm) that are stored together with dissolved carbon dioxide (300 km$^3$) in the deep water [Schmid et al., 2005]. Commercial extraction of the methane for energy production has recently started. Below ~65 m the lake is permanently stratified. Water density is determined by salinity, temperature, dissolved methane and dissolved carbon dioxide which all increase with depth. Whereas the temperature and methane gradients destabilize the water column, the permanent stratification is maintained by the gradients of salinity and carbon dioxide [Schmid et al., 2005; Pasche et al., 2009].

Several lakes on earth display double-diffusive layering in relatively confined, undisturbed and thus attractive study sites, e.g. Lake Nyos (Cameroon), Powell Lake (Canada), Lake Banyoles (Spain) or Lake Vanda (Antarctica). None of them, however, displays double-diffusive staircases in such clarity and quantity as Lake Kivu. With up to 300 clearly distinguishable double-diffusive steps distributed almost over the entire water column below 100 m depth, Lake Kivu is an ideal system for studying double diffusion.
1.6 Structure of thesis

This thesis is structured as follows. In chapter 2 [Sommer et al., 2013, published] we use double-diffusive structures to estimate microstructure sensor responses. It is shown, that a knowledge of the sensor responses is important for resolving interface thicknesses and for estimating heat and salt fluxes.

Having corrected interface thicknesses for the sensor responses, we are able to present the most detailed data set of natural double-diffusive staircases up to date in chapter 3 [Sommer et al., 2014, accepted]. We show that interfaces have a boundary layer structure and we estimate the “amount” of buoyancy that is stored in the boundary layers by means of a boundary layer Rayleigh number. Furthermore we suggest a correction for the most common heat flux parameterization which decreases previous heat flux estimates in the Arctic Ocean.

In chapter 4, we introduce the governing equations for the DNS, the approximations used to simplify those equations and we outline the limitations of the DNS.

In chapter 5 [Sommer et al., 2014b, submitted], we compare DNS to the Lake Kivu data and show that (i) the DNS reproduces the measured interface thicknesses of in-situ microstructure profiles, (ii) molecular heat fluxes through interfaces capture the total vertical heat fluxes for density ratios larger than three and (iii) the correction factor introduced in chapter 3 for heat flux estimates in the Arctic Ocean is supported by the DNS.

Chapter 6 summarizes the conclusions and in chapter 7, we outline future challenges and present our plans for upcoming research projects which attempt to address questions (iii) and (iv).

As Appendices we include the published manuscripts by Carpenter et al. [2012a] and Carpenter et al. [2012b] where we examine the stability of the double-diffusive interface and the interaction between the mixed layer and the interface.
2 Revisiting microstructure sensor responses with implications for double-diffusive fluxes

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2.1 Abstract

Thin high-gradient interfaces that occur naturally within double-diffusive staircases are used to estimate the response characteristics of temperature and conductivity microstructure sensors. The knowledge of these responses is essential for resolving small-scale turbulence in natural water bodies and for determining double-diffusive fluxes of heat and salt. Here, we derive microstructure sensor responses from observed differences in the statistical distributions of interface thicknesses at various profiling speeds in Lake Kivu (Central Africa). In contrast to the standard approach for determining sensor responses, our method is independent of any knowledge of the true in-situ temperature and salinity structure. Assuming double-pole frequency response functions, the time constants for the SBE-7 conductivity sensor and the FP07 thermistor are estimated to be 2.2 ms and 10 ms, respectively. In contrast to previous assumptions, the frequency response for the SBE-7 is found to be substantial, and dominates the wavenumber response for profiling speeds larger than 0.19 m s$^{-1}$. 


2.2 Introduction

Turbulent mixing in stratified water bodies generates small-scale structures on the order of millimeters or less. For in-situ turbulence studies, those naturally-occurring fluctuations need to be resolved as perfectly as possible [Gregg, 1999]. However, currently available sensors usually reach their measurement limits before a complete resolution of the finest turbulent scales is possible. In order to extract the maximum variance of those turbulent fluctuations, measured signals are routinely corrected for their sensor response properties.

In general, sensors have a frequency (temporal) response and a wavenumber (spatial) response. The frequency response is a consequence of temporal delays of the sensor to the environmental signal. The wavenumber response is a consequence of the finite size of the sensor, rendering it unable to resolve finer-scale features. It averages the signal over a certain volume determined by the spatial characteristics of the sensor.

Sensor responses are usually determined by comparing the “true” signal, to which the sensor is exposed, with the sensor’s measurement output. The response characteristics are modeled by a transfer function that is given by the ratio of the output to the input in the Laplace domain [Dorf and Bishop, 2010]. However, in practice, the true signal is usually not well known and has either to be estimated (Head 1983), or measured with another sensor with higher spatial resolution than the one being tested [Nash et al., 1999; Schmitt et al., 2005]. This is a potential source of error, in particular if the sensor being tested is already very fast.

Here, we take a different approach to finding sensor frequency responses which does not depend on a knowledge of the true input. Instead, we take advantage of the fact that, if the sensor shows a frequency response, the measured signal of a moving sensor is speed-dependent. Fast profiling will result in increased smoothing of the measured signal, as structures of a given spatial scale are detected over a short time scale. The shorter the time scale, the more the signal is affected by the frequency response. The frequency response can thus be found by correcting the signals, measured at different profiling speeds, such that they become identical. At the same time the true signal, initially unknown, is approximated with increasing accuracy. This approach assumes that either the true signal itself or the distribution of a certain characteristic of the true signal is stationary.

Lake Kivu offers an attractive natural environment for examining the frequency response characteristics of temperature ($T$, °C) and electrical conductivity ($C$, μS cm$^{-1}$) microstructure...
sensors. Depth profiles of the lake show more than 300 homogeneous layers separated by thin high-gradient interfaces, a phenomenon produced by double-diffusion of the diffusive type [Neal et al., 1969; Newman, 1976; Schmitt, 1994; Kelley et al., 2003; Timmermans et al., 2008]. Figure 2.1a shows background profiles of $T$ and $S$ in Lake Kivu and the close-up in Fig. 2.1b illustrates an example of the staircase structure consisting of a series of stable interfaces sandwiched between convectively mixed layers. Double-diffusive interfaces have previously been used to study the responses of CTD sensors [Schmitt et al., 2005; Johnson et al., 2007]. The goal of these studies was to match the $T$ and $C$ signals during post processing in order to avoid “salinity spiking” which would result in “density spiking”. However, those methods are not applicable to very fast microstructure sensors: The method by Schmitt et al. (2005) requires an assumption for the true signal, which for very fast microstructure sensors would strongly affect the deduced sensor response. The method by Johnson et al. (2007) is based on reconstructing the true signal from the measured signal [Fofonoff et al., 1974; Fozdar et al., 1985]. This requires the removal of high frequency instrument noise by smoothing the measured signal. However for fast microstructure sensors, those high frequencies contain essential information about the response and thus smoothing is problematic.

Our method, in contrast, only assumes that double-diffusive interface thickness distributions are stationary over the time of our measurement. We believe that this is a justified assumption, because the background profiles of $T$ and $S$ in Lake Kivu (Fig. 2.1a), on top of which the staircases are formed, are persistent both temporally and spatially. The variation between $T$ and $C$ profiles measured in 2004 by Schmid et al. (2010) and in 2010 and 2011 by us is largest near the lake bottom (excluding the top 60 m, which are affected by seasonal variation). At 450 m the ranges for $T$ and $C$ are $25.99 \pm 0.05 \, ^\circ\mathrm{C}$ and $5775 \pm 25 \, \mu\mathrm{S} \, \mathrm{cm}^{-1}$, respectively, corresponding to 0.4 % and 0.9 %. Thus, the statistical properties of the staircases are assumed to evolve slowly, and to be independent of profiling location in the open water. Here, we use this quasi-stationarity to explore the frequency response of two microstructure sensors by measuring interface thicknesses at three different profiling speeds. Our microstructure sensors are the FP07 thermistor (RSI, Canada and GE, USA), often used for the measurement of $T$, and the SBE-7 microconductivity sensor (Sea-Bird, USA) for the measurement of $C$. Differences in the distributions measured at those speeds are assumed to be caused by the sensor frequency response. The frequency response is then estimated by correcting individual interface thicknesses such that the corrected distributions collapse to a single distribution. In particular we show (i) that the SBE-7
sensor (in addition to the FP07 sensor) has a frequency response and (ii) that the deduced corrections result in improved estimates of vertical heat and salt fluxes as well as density flux ratios through double-diffusive staircases.

The paper is structured as follows: We first describe the vertical microstructure profiler (section 2.3.1), introduce the data set measured at Lake Kivu (section 2.3.2) and outline the method for interface detection (section 2.3.3). We then present our assumptions on the functional forms of the responses (section 2.4.1). Based on those responses we introduce the model approach for correcting interface thicknesses (section 2.4.2). In section 2.5 we show that measured interface thicknesses depend on profiling speed and how we remove this dependency by correcting for the frequency responses. In section 2.6 the estimated responses are discussed with respect to the findings by other researchers and in section 2.7 we investigate the effect of the sensor response correction on the estimates of physical parameters in Lake Kivu, such as vertical fluxes of heat and salt and the ratio of $T$ to $S$ interface thicknesses. We finally summarize our observations in section 2.8.
2.3 Methods

2.3.1 Vertical Microstructure Profiler

Profiles of $T$ and $C$ microstructure are measured with a loosely tethered, and thus quasi-free falling, vertical microstructure profiler (VMP, Fig. 2a) manufactured by Rockland Scientific International (RSI). The instrument is 163 cm long and weighs 340 N in air.

During profiling, the tether is released from a motor-driven winch slightly faster than the VMP descends, ensuring that it is not perturbed by any ship motions. The VMP descent is stabilized by two brushes, located at the rear, and a flotation collar. Three DC-response M4002 accelerometers (Precision Measurements Systems, USA) record pitch, roll and vibrations. Depth (m) is calculated by multiplying pressure (bar) by $10.213 \text{ m bar}^{-1}$, which accounts well for the density of Lake Kivu [Schmid et al., 2005] and has a maximum absolute error of 0.36 m at 250 m depth. The VMP profiling speed is computed from the low-pass filtered rate of change of pressure.

The VMP is optimized for slow profiling down to 0.1 m s$^{-1}$ and thus differs from e.g. the TurboMAP profiler in Wolk et al. (2002). For slow profiling the electronics were modified (as described below) and a flotation collar is mounted. The target profiling speed is then tuned by adding lead weights. We profile at three different speeds: $W = 0.19 \text{ m s}^{-1}$ (slow), 0.38 m s$^{-1}$ (medium) and 0.89 m s$^{-1}$ (fast). The cast properties for profiling at different speeds are summarized in Table 2.1.

Three pairs of microstructure sensors (Figs. 2.2b, c) are mounted at the nose of the instrument where they are exposed to the undisturbed water. As sensors, we use two fast FP07 (MicT) thermistors, two fast SBE-7 (MicC) conductivity micro-sensors (Fig. 2.1d) and two SPM-38-shear probes (RSI, Canada), sampled at a frequency $f_S = 512 \text{ Hz}$. 
Fig. 2.2. (a) Vertical Microstructure Profiler (VMP) with (1) orange tether cable, (2) stabilizing brushes, (3) yellow flotation collar, (4) lead and (5) Sea-Bird $C$ and $T$ sensors. (b) Six microstructure sensors mounted at the instrument nose and protected by a metal frame covered by black brushes. (c) Microstructure sensor arrangement when facing the instrument nose. (d) Conductivity sensor SBE-7. The electrodes are situated on the tips of the two needles. The distance between the tips defines the parameter $2\alpha$ of the response function by Hill and Woods (1988). Note the salt precipitations in white after deployment in Lake Kivu.

Microstructure sensors are very sensitive, but lack long-term stability. The temporal drifts of the signals are removed by calibrating the microstructure signals against the stable but slower $C$ and $T$ signals from a Sea-Bird SBE-4C and SBE-3F, respectively, sampled at 64 Hz, which are also mounted on the VMP (Fig. 2.2a). The calibration is done by linearly adjusting the microstructure signals to these slow CTD sensors over the depth interval from 100 m to the maximum depth of a profile. The fit error relative to the maximum variation of $T$ and $C$ over the entire profile is smaller than 1.7 % for both, $T$ and $C$. The flow through the glass cylinder of the
SBE-4C was enhanced by a submersible pump (SBE-5T) for most profiles. During the campaign in 2010, the glass cell of the SBE-4C was cracked which resulted in erroneous background data. For these profiles the MicC signal is mapped on an average background profile measured in 2011. This is unproblematic because time as well as horizontal variations of C from 2004 to 2011 are smaller than ~1%. In order to reduce quantization noise in the high frequency range, a pre-emphasis and deconvolution method [Mudge and Lueck, 1994] is applied to both microstructure sensors. The signal conditioning board of the internal electronics is optimized for slow profiling by increasing the pre-emphasis gain of the MicT about nine-fold compared to that used for normal profiling speeds ($W \sim 1$ m s$^{-1}$). The gain of the MicC is not enhanced, because the analog noise is already above the quantization noise and thus amplifying the signal at high frequencies would only cause amplification of analogue noise. The standard deviation of the noise signal of the two MicC sensors is 0.12 and 0.06 μS cm$^{-1}$, as well as 0.012 mK for both MicT sensors. Noise measurements were conducted in a laboratory tank under quiet conditions. The two MicC sensors have different noise levels because their transformers have different material in their cores.

Table 2.1. VMP operation and data acquisition. Values given for speed, pitch and roll were measured in the depth range of detected interfaces.

<table>
<thead>
<tr>
<th></th>
<th>Unit</th>
<th>Slow</th>
<th>Medium</th>
<th>Fast</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average profiling speed</td>
<td>m s$^{-1}$</td>
<td>0.19</td>
<td>0.38</td>
<td>0.89</td>
</tr>
<tr>
<td>Profiling speed (min / max)</td>
<td>m s$^{-1}$</td>
<td>0.10 / 0.28</td>
<td>0.30 / 0.42</td>
<td>0.70 / 0.96</td>
</tr>
<tr>
<td>Profiling speed (10th / 90th percentiles)</td>
<td>m s$^{-1}$</td>
<td>0.14 / 0.24</td>
<td>0.38 / 0.39</td>
<td>0.87 / 0.93</td>
</tr>
<tr>
<td>Time for 485 m downcast at average speed</td>
<td>min</td>
<td>43</td>
<td>21</td>
<td>9</td>
</tr>
<tr>
<td>Total number of detected interfaces</td>
<td>-</td>
<td>2199</td>
<td>5897</td>
<td>2141</td>
</tr>
<tr>
<td>Percentage of total interfaces</td>
<td>%</td>
<td>21</td>
<td>58</td>
<td>21</td>
</tr>
<tr>
<td>Floating collar mounted?</td>
<td>-</td>
<td>yes</td>
<td>yes</td>
<td>no</td>
</tr>
<tr>
<td>Lead added</td>
<td>kg</td>
<td>2.7</td>
<td>5.3</td>
<td>0</td>
</tr>
<tr>
<td>Pitch (10th / 90th percentiles)</td>
<td>degrees</td>
<td>-3.3 / -0.5</td>
<td>-1.9 / -1.5</td>
<td>-2.8 / -1.8</td>
</tr>
<tr>
<td>Roll (10th / 90th percentiles)</td>
<td>degrees</td>
<td>-2.2 / 3.4</td>
<td>0.2 / 0.5</td>
<td>-2.5 / -0.2</td>
</tr>
<tr>
<td>Vertical distance between measurement points</td>
<td>mm</td>
<td>0.4</td>
<td>0.7</td>
<td>1.7</td>
</tr>
</tbody>
</table>
The spatial resolution depends on sampling frequency, profiling speed and the wavenumber and frequency responses of the sensors and the internal electronics. Each aspect is discussed in detail in the following.

2.3.2 Lake Kivu data set

Measurements were carried out in Lake Kivu (surface area of 2300 km$^2$, maximum depth of 485 m and volume of 550 km$^3$), located at the border between Rwanda and the Democratic Republic of the Congo [Schmid et al., 2005; Descy et al., 2012]. During two field campaigns in 2010 and 2011 we measured 225 profiles covering a total profiling length of ~55 km, containing about 10,000 double-diffusive steps. Each step was simultaneously measured by four microstructure sensors, two MicT and two MicC. For a more detailed description of the lake and its double-diffusive staircases we refer to Newman (1976), Schmid et al. (2010) and Sommer et al. (2013, in preparation).

2.3.3 Interface detection

In order to manage the enormous data set, we developed an algorithm for automatic evaluation of the measured profiles. The algorithm detects double-diffusive interfaces and mixed layers in the measured profiles and extracts interface thicknesses, mixed layer thicknesses, step sizes of $T$ and $C$ between mixed layers and several more parameters. In this work, we focus on interface thicknesses defined by $h_T = \Delta T \left( \frac{\partial T}{\partial z} \right)^{-1} \bigg|_{z=z_0}$ for temperature and $h_C = \Delta C \left( \frac{\partial C}{\partial z} \right)^{-1} \bigg|_{z=z_0}$ for conductivity. Here $\Delta T$ (K) and $\Delta C$ (µS cm$^{-1}$) are the $T$ and $C$ steps across the interface (Fig. 2.3), respectively, $z$ (m) is depth (positive downward) and $z_0$ (m) is the depth of the interface center.

The detection algorithm is based on four mandatory conditions:

- **Condition (i)**: The interfacial gradient is large compared to the background gradient.
- **Condition (ii)**: The gradients of the two adjacent mixed layers are small compared to the background gradient.
- **Condition (iii)**: All four microstructure sensors detect the same interface based on arguments (i) and (ii).
**Condition (iv):** Profiles of $T$ and $C$ are close to linear in their interface core. More $C$ than $T$ interfaces are rejected by this condition, because the ratio of noise to step size for the MicC is larger than for the MicT, and because $S$ diffuses more slowly than $T$ and therefore disturbances in the $C$ interfaces persist over longer times.

Each of conditions (i) – (iv) is described in detail in appendix A. In total 17,619 $T$ interfaces and 9,489 $C$ interfaces passed all four conditions and are evaluated in the following.

### 2.4 Sensor response formulation

Measured interfaces are always smoothed out by the sensor responses and thus appear thicker than the true *in-situ* interfaces. If the sensor has a temporal response only, then this response is fully described by the impulse response function $h(t)$ with $t(s)$ being time, which is the output signal for a delta function input. In practice, the Fourier transform of $h(t)$, which we call frequency response $H(f)$, is often used to describe amplitude and phase changes as a function of frequency $f$ (Hz) [Dorf and Bishop, 2010]. In the spatial domain, we use the identical notation for the spatial impulse response $h(z)$ and the wavenumber response $H(k)$ with $k$ (cpm) being the wavenumber. For a given input, such as a model interface, we simulate the output (representing the measured signal) by a convolution of the input with $h(z)$ and/or $h(t)$. This way, we establish a
relation between the thickness of the input interface and the output interface and we use this relation to infer true interface thicknesses in Lake Kivu. In the following we introduce our assumptions for the sensor responses and then describe our method for correcting measured interface thicknesses.

### 2.4.1 Sensor responses

We distinguish between a wavenumber response and a frequency response and we explain each contribution briefly for both sensor types.

**Wavenumber response, MicT:** The FP07 thermoprobe is a tiny glass-coated thermistor bead with a diameter of ~180 μm. Because the smallest T-scales of interest are ~ 1 cm, the MicT wavenumber response is not a limiting factor, and it is omitted.

**Wavenumber response, MicC:** The SBE-7 conductivity sensor measures the conductivity of the fluid by applying a constant-amplitude sinusoidal voltage difference between its electrodes (Fig. 2.2d). This voltage difference drives a current through the fluid and the amplitude of the current is proportional to $C$. However, the current path-lines spread apart in the volume between and around the electrodes and the measured $C$ represents an average over this volume. The smoothing of the spatial $C$ fluctuations due to this averaging is described by a wavenumber response. We use the Hill and Woods (1988) form $H(k) = \exp(-2\pi ka)$ with $a = 0.23$ mm being half the distance between electrodes. The corresponding impulse response function is $h(z) = Qa(z^2 + a^2)^{-1}$, where $Q$ is a normalization constant.

**Frequency response, MicT:** The frequency response of the MicT depends on how fast heat is transported into the viscous boundary layer and diffused through the diffusive boundary layer as well as the glass coating to the thermistor. The frequency response characteristics of the FP07 are not known exactly and different findings are discussed in section 2.6.1. We follow Gregg and Meagher (1980) and use their double-pole frequency response function $H_{dp}(f) = (1 + j2\pi ft_{dp})^{-2}$ where $j$ is the imaginary unit, and $t_{dp}$ is the time constant specific for a double-pole response. Here, $t_{dp}$ is the single parameter that we use to characterize the temporal response, and one goal of this study is to determine this parameter. The time constant $t_{dp}$ was reported to depend on profiling speed $W$, because the water boundary layer around the sensor becomes thinner for higher $W$ and thus heat can diffuse faster to the sensor. For a velocity scaling of the form

$$t_{dp} = t_0(W/W_0)^\gamma$$  \hspace{1cm} (2.1)
with $W_0 = 1 \text{ m s}^{-1}$ and $\tau_0 = \tau_{dp}$ at $W = W_0$, the exponents $\gamma = -0.32$ [Gregg and Meagher, 1980] and $\gamma = -0.5$ [Vachon and Lueck, 1984; Hill, 1987] have been proposed. The corresponding impulse response function is $h(t) = \tau_{dp}^{-2} \exp(-t/\tau_{dp})$ for $t > 0$; $h(t) = 0$ otherwise. However, instead of convolving with $h(t)$, we filter twice with a first-order low-pass Butterworth filter with a cut-off frequency of $(2\pi\tau_{dp})^{-1}$, which is less time consuming and yields a better representation of $H_{dp}(f)$ for a discrete input signal.

**Frequency response, MicC:** The MicC sensor is usually considered infinitely fast and thus frequency response corrections are not applied to the $C$ signal [Gregg et al., 1978; Head, 1983; Hill and Woods, 1988; Washburn et al., 1996; Nash and Moum, 2002]. However, our observations (section 2.5.1) indicate that the MicC does have a frequency response. Both the delayed flushing of the viscous boundary layer by the flow and the processing of the signal can produce a frequency response and their contributions are discussed in sections 2.6.2. For the MicC, we assume the same double-pole frequency response function as for the MicT with variable $\tau_{dp}$. This is an arbitrary choice but facilitates direct comparison of the time constants.

### 2.4.2 Modeling interface thickness corrections

The relation between true ($h_{true}$) and observed ($h_{meas}$) interface thicknesses depends on the sensor response with the parameter $\tau_{dp}$ and on the profiling speed $W$. In the following, we derive six continuous functions $N(h_{meas}, \tau_{dp}, W)$ for this relationship for our two sensors and three profiling speeds. Here, $N$ corresponds to the fraction of $h_{meas}$, which must be subtracted from $h_{meas}$ in order to obtain $h_{true}$:

$$N(h_{meas}, \tau_{dp}, W) = 1 - h_{true}/h_{meas}. \quad (2.2)$$

The true thickness of an interface is then calculated (for each sensor and $W$) from the measured interface thickness by $h_{true} = (1 - N)h_{meas}$.

The functions $N$ are derived by simulating the sensor responses for a series of hypothetical model interfaces with thicknesses $h_{true}^*$ and $h_{meas}^*$ before and after the sensor response correction has been applied, respectively. The discrete correction factors $N^*(h_{meas}^*, \tau_{dp}, W)$ are then calculated for each pair of $(h_{meas}^*, h_{true}^*)$ from Eq. (2.2). Finally, continuous functions are fitted to $N^*$ to interpolate between the simulated $h_{meas}^*$. As a fit function, we use

$$N(h_{meas}, \tau_{dp}, W) = 0.043 + A\exp[B(h_{meas} + D)] + C(h_{meas} + D)^{-1}, \quad (2.3)$$

where the dependency on $\tau_{dp}$ and $W$ is included in the fit parameters $A$, $B$, $C$ and $D$. The combination of a constant term, an exponential term and a “$x^{-1}$” term on the right hand side of Eq.
(2.3) was found after testing various other relations, which did not provide a satisfactory fit to the modeled data. Apart from the purely empirical functional form, Eq. (2.3) is designed to fulfill three additional conditions: (i) The constant of 0.043 accounts for underestimating the gradient by fitting over the center 50% of the interface (Appendix A); (ii) forcing $B < 0$ ensures that the correction decreases for large $h_{\text{meas}}$; and (iii) the fit parameter $D$ in the “$x^{-1}$” term allows the fit function to rapidly increase at some $h_{\text{meas}}$, a behavior that was observed for all model runs.

As model $T$ and $C$ interfaces, we use error functions of the form

$$T(z) = 0.5 \Delta T \text{erf}(\pi^{1/2}(z-z_0)/h_{\text{true}})$$

and

$$C(z) = 0.5 \Delta C \text{erf}(\pi^{1/2}(z-z_0)/h_{\text{true}})$$

respectively. We use the error function form, because it is a solution of the diffusion equation, and its shape is close to observed interfaces (Fig. 2.3). The vertical spacing $\Delta z$ of the sampling for the modeled step was chosen as $W(4f_S)^{-1}$. The oversampling by a factor of four ensures that the Nyquist frequency $f_N = 0.5f_S$ is a few times larger than the half-power frequencies $f_h$, defined as $|H(f_h)|^2 = 0.5$, of the applied digital filters, and thus discretization errors are small. In our case $f_N > 6f_h$ is satisfied for all filters. We then apply the sensor responses of MicT and MicC to Eq. (2.4) and Eq. (2.5), respectively, in order to obtain individual $h_{\text{meas}}$ for each sensor and profiling speed, as described in the following.

MicT: We convert our model step $T(z)$ (Eq. 4) into a time series step $T(t)$ using $t = z/W$ and then apply the double-pole frequency response $H_{dp}(f)$ (section 2.4.1). Note that an interface of thickness $h$ is traversed in the time interval $\Delta t = h/W$. The larger $W$, the smaller is $\Delta t$ and the stronger is the smoothing of the frequency response function on the time series step. This effect of the frequency response causes measured interface thicknesses to be profiling speed-dependent. After back transformation into the spatial domain the interface thickness $h_{\text{meas}}$ of the filtered step is determined with the same method as used for interfaces measured in Lake Kivu (Appendix A). This is done for a series of 100 different values of $h_{\text{true}}$, which are logarithmically spaced between 0.1 mm and 1 m. The logarithmic scale ensures tight spacing at small interface thicknesses, where the correction is most important.

MicC: For the MicC, we follow the same procedure as for the MicT, but additionally account for the wavenumber response described in Hill and Woods (1988) before transforming the spatial model step into the time domain.
2.5 Results

2.5.1 Measured interface thicknesses

In Figs. 2.4a,b, the normalized histograms of measured $h_T$ and $h_C$ are shown for different profiling speeds with MicT results on the left and MicC on the right. No sensor response corrections are applied. Note that the distributions measured by the two MicT (Fig. 2.4a) and the two MicC (Fig. 2.4b) sensors are practically identical to each other. This is not necessarily expected for the MicT, as Nash and Moum (1999) as well as Gregg and Meagher (1980) found that individual sensors may have different response characteristics. Also note that the different noise levels of the MicCs do not affect the $h_C$ distributions. The algorithm for calculating interface thicknesses needs at least two points in the central 50% of the interface for fitting (appendix A), and thus interfaces containing fewer than four points are not detected. The thresholds corresponding to these conditions are indicated by vertical lines in Fig. 2.4 for each of the three profiling speeds. They are determined solely by the sampling frequency and the algorithm. Interfaces thinner than these thresholds are ignored by the algorithm and would result in a steep cut-off in the measured distributions. Since this is not seen in Figs. 2.4a,b we conclude that the distributions are unaffected by the thresholds, which indicates that a sufficiently fast sampling rate is used. The distribution of $h_C$ using fast profiling, however, is very close to its corresponding threshold (Fig. 2.4b).

For both sensors, the histograms of the thin interfaces exhibit a clear dependence on the profiling speed. We believe that this is caused by the frequency responses of the sensors. This is expected for the MicT, but a surprise for the MicC, as those sensors are commonly assumed to be infinitely fast [Meagher et al., 1982; Head, 1983; Hill and Woods, 1988; Washburn et al., 1996; Nash and Moum, 2002]. After applying the appropriate corrections for the interface thicknesses the histograms should be identical for all three profiling speeds.
Fig. 2.4. Effect of microstructure sensor responses on interface thickness distributions for different profiling speeds. All histograms are based on logarithmic bin sizes of 0.02 and are normalized by the total number of data points. The two almost identical lines for each profiling speed represent the individual measurements of the two sensors. (a,b) Measured distributions of $h_T$ and $h_C$; (c) $h_T$ after correcting according to the frequency response of Vachon and Lueck (1984); (d) $h_C$ after correcting according to the wavenumber response of Hill and Woods (1988); (e,f) Modified corrections eliminating most of the profiling speed-dependence. Vertical solid lines indicate the smallest measurable interface thickness (details in text). The two vertical dashed lines are Batchelor scales for dissipation rates of $\epsilon = 10^{-11}$ W kg$^{-1}$ (left) and $\epsilon = 10^{-9}$ W kg$^{-1}$ (right), corresponding to the range of $\epsilon$ observed in the mixed layers (Sommer et al. 2013, in preparation). The number of interfaces measured (by sensor 1, sensor 2) are (1865, 1828), (5069, 4993), (1941, 1907) for slow, medium and fast profiling, respectively. For $C$, these numbers are (899, 1075), (2370, 3002), and (985, 1149).
In Fig. 2.4c, \( h_T \) is corrected as described in section 2.4.2 using \( H_{dp}(f) \) with the \( \tau_{dp} \) of Vachon and Lueck (1984). They assume a velocity-dependent time constant \( \tau_{dp} = \tau_0(W/W_0)^{-0.5} \) with \( \tau_0 = 4.1 \) ms and \( W_0 = 1 \) m s\(^{-1} \). In Fig. 2.4d, \( h_C \) is corrected for the wavenumber response \( H(k) \) of Hill and Woods (1988) with \( a = 0.23 \) mm. After correction, both histograms still depend on profiling speed, indicating that the response characteristics of MicT and MicC are not yet captured adequately. This is obvious for the MicC because a wavenumber response alone does not introduce a profiling speed-dependency of the measured data and thus the corresponding correction cannot remove it. However, note that both corrections slightly decrease the thickness of the thinnest interfaces.

In our final correction (Figs. 2.4e,f), we keep the MicC wavenumber response of Fig. 2.4d constant, but include frequency responses \( H_{dp}(f) \) with variable \( \tau_{dp} \) for both sensor types. We then adjust \( \tau_{dp} \) separately for MicC and MicT to optimize the collapse of the corrected distributions for the three profiling speeds. We find that time constants \( \tau_{dp} \) of 10 ms and 2.2 ms for MicT and MicC, respectively, provide the best collapse based on visual inspection. Assuming \( \tau_{dp} \) to be speed-dependent, e.g. as in Vachon and Lueck (1984), results in either an insufficient correction for fast profiling or a large number of negative interface thicknesses for slow profiling, which can be understood by the following example. If we assumed a speed-dependent time constant, but still required that for slow profiling the time constant \( \tau_{dp,slow} \) is equal to the speed-independent time constant \( \tau_{dp} \) from above, then \( \tau_{dp,fast} \) must be multiplied by a constant factor \( > 0 \). But then the interfaces measured at slow profiling speed would be corrected more than without the velocity scaling. Because some corrected interface thicknesses are already close to zero without the velocity scaling (Figs. 2.4e,f), an increase of \( \tau_{dp,slow} \) would cause them to become negative. Therefore, we use a time constant \( \tau_{dp} \), which does not depend on profiling speed.

Even without velocity scaling, the corrections applied in Figs. 2.4e,f result in few negative interface thicknesses, namely 16 for \( T \) (out of 17,619) and 9 for \( C \) (out of 9,489). These are possibly caused by a slightly wrong shape of the response function or an overestimation of the interfacial gradients due to instrument noise or signal discretization. The few negative interface thicknesses are ignored. Note the proximity of the thinnest \( T \) and \( C \) interface thicknesses to the
Batchelor scales inferred from the approximate dissipation rates measured in the mixed layers (Sommer et al. 2013, in preparation).

The corrected histogram of \( h_C \) (Fig. 2.4f) shows two peaks, a main peak at ~6 cm and a small peak at ~3 mm. At the moment we are unsure whether the small peak is a physical feature that is characteristic of the \( C \) interfaces, or whether it is an artifact of the measurements, but we plan to address this question in a future publication by comparing our measurements to Direct Numerical Simulation.

Figure 2.5 shows the correction factor \( N \) for our final correction and the fit parameters of Eq. (2.3) are given in Table 2.2. For individual sensors, \( N \) increases with \( W \), indicating that faster profiling requires a larger correction. Note that for interfaces thicker than ~ 5 cm (Fig. 2.4), the correction is less than 10 \% \( (N < 0.1) \) except for MicT and fast profiling. The value of \( h_{\text{meas}} \) for
which $N \rightarrow 1$ indicates the smallest directly measurable interface thickness for a certain speed and sensor. For slow profiling this thickness is 6.5 mm for the MicT and 2 mm for the MicC. Note that for the MicC a few such interfaces were actually measured (Fig. 2.4b) which means that their true thickness was close to zero. This becomes an important issue in section 2.7 where we estimate the molecular fluxes through interfaces.

Table 2.2. Parameters of the function $N(h_{\text{meas}}) = 0.043 + A \exp[B(h_{\text{meas}} + D)] + C(h_{\text{meas}} + D)^{-1}$ used for interface thickness correction.

<table>
<thead>
<tr>
<th>Speed (m s$^{-1}$)</th>
<th>A (-)</th>
<th>B*10$^{-2}$ (m$^{-1}$)</th>
<th>C*10$^{4}$ (m)</th>
<th>D*10$^{3}$ (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$h_{C}$</td>
<td>0.19</td>
<td>-2.45</td>
<td>-38.67</td>
<td>4.33</td>
</tr>
<tr>
<td></td>
<td>0.38</td>
<td>-2.09</td>
<td>-25.13</td>
<td>6.21</td>
</tr>
<tr>
<td></td>
<td>0.89</td>
<td>17.90</td>
<td>-33.31</td>
<td>13.11</td>
</tr>
<tr>
<td>$h_{T}$</td>
<td>0.19</td>
<td>-2.96</td>
<td>24.53</td>
<td>7.71</td>
</tr>
<tr>
<td></td>
<td>0.38</td>
<td>-2.25</td>
<td>-9.91</td>
<td>16.67</td>
</tr>
<tr>
<td></td>
<td>0.89</td>
<td>0.40</td>
<td>-0.39</td>
<td>6.62</td>
</tr>
</tbody>
</table>
2.6 Discussion of the sensor responses

In section 2.5.2 we removed the profiling speed-dependence of measured $T$ and $C$ interface thickness estimates by correcting for a double-pole frequency response with the time constants $\tau_{dp} = 10$ ms and $\tau_{dp} = 2.2$ ms, respectively. We now discuss these time constants with respect to the findings of other researchers.

2.6.1 MicT sensor frequency response

The frequency response characteristics of the FP07 are not known exactly. An overview of the reported frequency responses, including the manufacturers specification, is given in Fig. 2.6, in which we compare half-power frequencies $f_{h,MicT}$ and their profiling speed-dependence. The findings differ in time constants, velocity scaling of the time constants and the shape of the response (double- or single-pole). We use here a double-pole response for which we deduced $\tau_{dp} = 10$ ms (without velocity dependence) and which has a half-power frequency of 10.2 Hz. Our half-power frequency is lower than the manufacturer’s specification but well within the range of findings of other researchers.

Different half power frequencies between sensors might be partly explained by different geometries of the glass coating surrounding the sensors, which are not perfectly identical for every individual sensor [Gregg and Meagher, 1980]. However varying time constants may also be a result of differences in the experimental setup. Therefore we discuss two different approaches for determining the frequency response of the MicT, in particular the methods of the manufacturer GE and Nash and coworkers [Nash et al., 1999; Nash and Moun, 2002].

GE states a “nominal” response time of 7 ms, determined by dropping the sensor from air into water (at $W < 0.1$ m s$^{-1}$) and measuring the time until the signal reaches 63% of the difference between initial and the final values (J. Lukie, GE Energy, 2012, personal communication). They do not specify the shape of the response, i.e., whether it is single- or double-pole response. The corresponding time constants for a single-pole and a double-pole frequency response are $\tau_{sp} = 7$ ms (corresponding to their nominal response time) and $\tau_{dp} = 3.3$ ms, respectively, with half-power frequency points at 22.7 Hz and 31 Hz. Dropping a dry sensor from air into water always underestimates the time constant.
because the water boundary layer (through which heat must be diffused) has not had time
to develop before the sensors first touch the water [Lueck et al., 1977]. Thus, it is not surprising that
our own measurements in water result in a larger time constant.

Nash and coworkers [Nash et al., 1999; Nash and Moun, 2002] use the T dependence of
the C signal to measure the in-situ T gradient spectrum $\psi_{Cz}$ with a four point conductivity
microstructure probe [Head, 1983]. The frequency response $H_{\text{MicT,Nash}}^2$ is then estimated by
$|H_{\text{MicT,Nash}}|^2 = \psi_{Tz} / \psi_{Cz}$, where $\psi_{Tz}$ is the T gradient spectrum measured with the MicT. This
procedure assumes that the conductivity sensor is infinitely fast. If this was not the case, the

\[ f_h = \text{Half-power frequencies} \]
\[ W = \text{profiling speed} \]
\[ |H_{\text{MicT,Nash}}|^2 = \psi_{Tz} / \psi_{Cz} \]

Fig. 2.6. Half-power frequencies $f_h$ of reported FP07 frequency responses and their
profiling speed-dependence. The legend indicates the defining parameters; dp and
sp are short for double-pole and single-pole responses, respectively. The length of
the lines indicates the investigated speed range. The grey bar on the left corresponds
to the specifications given by the manufacturer (details in text).
MicT half-power frequency response would be overestimated and the MicT would have to be corrected for the MicC response as \( |H_{\text{MicT,Nash,corr}}|^2 = |H_{\text{MicT,Nash}}|^2 |H_{\text{MicC}}|^2 \). For example if we assume \( |H_{\text{MicT,Nash}}|^2 \) to be a double-pole frequency response with a half-power frequency \( f_{h,\text{MicT,Nash}} \) of 18.7 Hz as in Nash and Moum (2002) and \( f_{h,\text{MicC}} = 47 \) Hz for \( H_{\text{MicC}} \) as determined for our MicC, \( H_{\text{MicT,Nash,corr}} \) would have a smaller half-power frequency of \( f_h = 17 \) Hz, but still larger than our MicT estimate of \( f_h = 10.2 \) Hz. A possibly neglected MicC frequency response thus does not explain the difference between our MicT half-power frequency and the one of Nash and Moum (2002). We expect this difference could rather be attributed to the large scatter in \( f_h \) between different FP07 sensors that results from manufacturing.

### 2.6.2 MicC sensor frequency response

The observed frequency response with a time constant of 2.2 ms might be induced by the signal processing or by the interaction of the moving sensor with the fluid environment. Possible contributions from the signal processing are the anti-aliasing (AA) filter and the pre-emphasis and its deconvolution [Mudge and Lueck, 1994]. The boundary layer over the sensor electrodes may be another possible cause for the observed frequency response. In the following we show that contributions from the signal processing are not large enough to explain the observed frequency response and that the delayed flushing of the viscous boundary layer reasonably predicts the time scale of the observed frequency response.

**AA-filter:** At very high frequency, the response is speed-dependent because anti-aliasing (AA) filters must be employed before the analog data are sampled. Spatial features with very small spatial scales will appear at high frequency and will be attenuated (and lagged) by the AA-filters, if the product \( W_k \) exceeds the half-power frequency of the AA-filters. The AA-filter is an 8-pole-low-pass Butterworth filter with a sharp cut-off at the half-power frequency \( f_{h,AA} = 98 \) Hz. Its transfer function is:

\[
H_{AA}(f) = \prod_{i=1}^{4} \left[ 1 + j\alpha_i \left( \frac{f}{f_{h,AA}} \right) - \left( \frac{f}{f_{h,AA}} \right)^2 \right],
\]

where \( \alpha_i = 1.9616, 1.6629, 1.1112 \) and 0.3902 for \( i = 1 \) to \( 4 \) (RSI, Fig. 2.7a, dashed line). Our double-pole frequency response \( H_{\text{MicC}}(f) \) has a half-power frequency \( f_{h,\text{MicC}} = 47 \) Hz.
Fig. 2.7. (a) Response functions for the MicC sensor. The relation between wavenumber (top axis) and frequency (bottom axis) corresponds to a profiling speed of 0.89 m s\(^{-1}\). Measured interface thicknesses were corrected for the frequency response \(H_{\text{MicC}}(f)\) and the wavenumber response \(H_{\text{MicC}}(k)\) as described in section 2.5.2. The expected frequency responses of the anti-aliasing filter \(H_{\text{AA}}(f)\) and the pre-emphasis and deconvolution method \(H_{\text{ML94}}(f)\) are also shown. Corresponding half power frequencies are indicated as vertical lines. (b) Frequency response of the MicT sensor \(H_{\text{MicT}}(f)\). Note that \(H_{\text{AA}}(f)\) and \(H_{\text{ML94}}(f)\) apply also for MicT but are not shown for clarity.

(Fig. 2.7a) which corresponds to \(\sim 0.5 \cdot f_{h,\text{AA}}\). Thus, the AA-filter does not explain the observed frequency response.
Signal pre-emphasis and its deconvolution: The microstructure signals are pre-emphasized and deconvolved [Mudge and Lueck, 1994]. Therefore, the signal and its pre-emphasized derivative are summed in the analogue domain before sampling. The pre-emphasis is equivalent to an “inverse” filter enhancing the high frequency portion of the signal. The subsequent deconvolution is achieved with a single-pole Butterworth low-pass filter in the discrete domain. The coefficients of this filter are derived using the bilinear transformation [Proakis and Manolakis, 1988]. The low-frequency characteristics of the discrete-domain filter match very closely to those of the equivalent continuous-domain filter, but their characteristics depart for frequencies larger than about one-third of the Nyquist frequency. Thus, the deconvolution filter is not the exact inverse of the pre-emphasis filter. The ratio of the deconvolution filter to that of the pre-emphasis filter can be considered as a frequency response, which is shown in Fig. 2.7a denoted by ML94 (dotted line). Its half-power frequency \( f_{h,ML94} \) is 148 Hz, much larger than \( f_{h,AA} \) and \( f_{h,MicC} \) and, thus, this part of the signal processing cannot explain our deduced frequency response for the C sensor.

Boundary layer: In the viscous boundary layer surrounding the sensor electrodes, the fluid velocity adjusts from its free-stream value down to zero at the sensor’s surface, satisfying the no-slip boundary condition. Thus, in the viscous boundary layer, the renewal of water by the ambient flow is delayed causing retardation of the measured signal relative to the free-stream. We use a simple model (appendix B), where the time scale of the response results from advection of fluid into the viscous boundary layer. Assuming a single-pole response function, the model predicts a time constant \( \tau_{sp} = 2 \) ms. Our measurements suggest \( \tau_{dp} = 2.2 \) ms for a double-pole response, which corresponds to single-pole time constant of \( \sim 6 \) ms. Considering the simple assumptions made for our model, the agreement is reasonable. In addition, we estimate that 44% of the measured signal is from the viscous boundary layer and thus processes within the viscous boundary layer as described above are important. Hill and Woods (1988) have previously suggested that the conductivity sensor has only a wavenumber response. They used faster profiling speeds of 0.54 m s\(^{-1}\) to 1.89 m s\(^{-1}\) with a larger electrode spacing of \( a \sim 2 \) mm. For their configuration the viscous boundary layer contribution to the measured signal is much smaller than it is for our MicC and ranges between 10% and 17%, depending on \( W \). This may explain why we observe a frequency response while Hill and Woods (1988) did not.

The frequency response of the MicC becomes important when the size, and spacing, of the electrodes is reduced in an attempt to reach extremely small spatial resolution. The frequency
response due to the viscous boundary layer negates the benefit of finer spatial resolution. The spatial resolution of the MicC increases with slower profiling, if only the frequency response is considered. At some transition profiling speed $W^*$, the wavenumber response, which is independent of $W$, exceeds the spatial resolution. We estimate $W^*$ by $f_{h,MicC}/k_{h,MicC}$, where the half-power wavenumber $k_{h,MicC}$ is given by $|H_{MicC}(k_{h,MicC})|^2 = 0.5$. For $\tau_{dp} = 2.2$ ms and $a = 0.23$ mm we have $f_{h,MicC} = 47$ Hz, $k_{h,MicC} = 240$ cpm and consequently $W^* = 0.19$ m s$^{-1}$, which is our slow profiling speed. For faster profiling speeds, the frequency response will dominate the spatial smoothing and consequently the spacing between the electrodes should be increased in order to reduce the effect of the frequency response.
2.7 Implications for double-diffusive fluxes

2.7.1 Molecular fluxes through interfaces

Heat and salt fluxes through double diffusive staircases are often approximated by the molecular fluxes through interfaces [Timmermans et al., 2008]. For their quantification it is thus important to determine the gradients within the interface cores. According to the definition of \( h_T \) and \( h_S \) these gradients can be expressed as \( \Delta T/h_T \) and \( \Delta S/h_S \). Because \( T \) has an influence on the measured \( C \) signal, this needs to be corrected for when estimating the fine-scale salinity field. For the computation of \( S \) from \( T \) and \( C \) and the conversion from \( h_C \) to \( h_S \) we refer to Sommer et al. (2013, in preparation). In Lake Kivu the conductivity gradient \( \partial C/\partial z \) is mainly determined by \( \partial S/\partial z \), with a contribution of only \( \sim 10 \% \) by \( \partial T/\partial z \). Consequently, \( h_C \) and \( h_S \) are similar with \( h_C \) being only 3.5 \% larger than \( h_S \) on average. Mean interface thicknesses (with 10\(^{\text{th}}\) and 90\(^{\text{th}}\) percentiles in brackets) are: \( \bar{h}_S = 6.8 \text{ cm (0.6, 14.4)} \) and \( \bar{h}_T = 9.9 \text{ cm (3.1, 17.8)} \). This indicates that a gravitationally unstable boundary layer is present on either side of the interface as predicted by Linden and Shirtcliffe (1978), Worster (2004) and Carpenter et al. (2012a).

By definition of \( h_T \) and \( h_S \) molecular heat and salt fluxes through interfaces are then:

\[
\begin{align*}
F_H &= c_p \rho \kappa_T \Delta T h_T^{-1} \quad (\text{W m}^{-2}) \\
F_S &= \rho \kappa_S \Delta S h_S^{-1} \quad (\text{g m}^{-2} \text{s}^{-1})
\end{align*}
\]

where \( c_p \) (\( \text{J kg}^{-1} \text{K}^{-1} \)) is the specific heat capacity of water, \( \rho \) (\( \text{kg m}^{-3} \)) is its density, \( \kappa_T \) (\( \text{m}^2 \text{s}^{-1} \)) and \( \kappa_S \) (\( \text{m}^2 \text{s}^{-1} \)) are the molecular diffusivity of heat and salt, respectively. Molecular fluxes through interfaces are inversely proportional to the interface thickness. Consequently, small interface thicknesses cause large fluxes, and the average values are sensitive to the occurrence of those individual thin interfaces. Because the sensor response correction reduces interface thicknesses disproportionately for small interface thicknesses (Fig. 2.5), the correction is important for calculating average fluxes. Small absolute errors in the thin interface thicknesses can cause large absolute errors in the fluxes. Therefore, we excluded the first percentile of \( h_T \) (\( h_T < 1.5 \text{ cm} \)) and \( h_S \) (\( h_S < 0.16 \text{ cm} \)) from flux calculations, but, for completeness we also provide the values without this restriction.

The molecular heat flux through the double-diffusive interfaces, averaged over all measured interfaces in Lake Kivu staircases, is 78 mW m\(^{-2}\) (11, 173) and 81 mW m\(^{-2}\) including the first percentile of \( h_T \). The average heat flux increase due to interface thickness correction for
slow, medium and fast profiling is 5.8 %, 6.9 % and 22.3 %, respectively. For comparison, the correction of Vachon and Lueck (1984) yields increases of 4.8 %, 6.1 % and 8.1 %, respectively and thus underestimates the heat flux in particular for fast profiling. The average salt flux is 0.81 μg m⁻² s⁻¹ (0.09, 1.59) and rises to 1.04 μg m⁻² s⁻¹ if we include the first percentile. The interface thickness correction increases the average salt flux by 9.6 %, 12.1 %, and 28.0 % for slow, medium and fast profiling, respectively. If only the wavenumber response of Hill and Woods (1988) is corrected for, increases of 6.9 %, 4.4 % and 1.0 %, respectively are obtained. This is in agreement with our expectations and Figs. 2.4b,d. The smallest measured interface thicknesses are detected for slow profiling, because measured interfaces are influenced by the frequency response. The smaller the interface thickness, the larger is the correction by the wavenumber response, which increases the average flux foremost for slow profiling.

In summary, our findings show that average fluxes through interfaces are sensitive to both the response characteristics of the sensors and the large contribution by a few very thin interfaces.

### 2.7.2 Interface thickness ratio

The interface thickness ratio $r = h_T/h_S$ is another important physical parameter for double-diffusion. It can be used for testing theories of double-diffusive boundary layers [Carpenter et al., 2012a] and it appears in the density flux ratio $R_F$ (-) of molecular fluxes through interfaces, defined as

$$R_F = \frac{\beta \kappa_S \Delta S h_S^{-1}}{\alpha \kappa_T \Delta T h_T^{-1}} = \tau R_\rho,$$

where $\beta$ (kg g⁻¹) is the haline coefficient of contraction, $\alpha$ (K⁻¹) is the thermal coefficient of expansion, $\tau = \kappa_S/\kappa_T \sim 0.01$ is the diffusivity ratio and $R_\rho = \beta \Delta S/\alpha \Delta T$ is the density ratio.

Because the correction for both $T$ and $C$ interfaces reduce the interface thickness in a non-linear way, the effect of the correction on the ratio $r$ is less clear. The average $r$ is $\bar{r} = 2.6$ (0.9, 5.5) and rises to 2.9 by including the first percentile. Note that $\bar{r}$ is much larger than $\bar{h}_T/\bar{h}_S = 1.5$ because $r$ is very sensitive to the occurrence of small $h_S$ (Fig. 2.4f). Here, $\bar{r}$ increases by 4.3 %, 6.6 % and 5.2 % for slow, medium and fast profiling, respectively.
2.8 Conclusion and Outlook

The distributions of interface thicknesses of the double-diffusive staircases in Lake Kivu have been used to estimate the frequency responses of conductivity and temperature microstructure sensors. Our method does not rely on a knowledge of the “true” $T$ and $C$ structure but takes advantage of the speed-dependency of the frequency response on the spatial resolution. Double-diffusive interfaces provide distinct step changes in $T$ and $C$ for measuring the response of very fast sensors. In particular for $C$, the thickness of the thinnest interfaces was smaller than 1 mm and thus close to the estimated Batchelor scales. Such sharp transitions are difficult to maintain in laboratory experiments. The response time constant of the SBE-7 conductivity sensor was found to be 2.2 ms assuming a double-pole frequency response. This is, to our knowledge, the first observation of a frequency response for conductivity microstructure sensors that is thought to result from the interaction of the moving sensor with its fluid environment. The time constant of the frequency response is of the same order as the advection time scale of salt into the viscous boundary layer on the sensor. For the FP07 the time constant of the double-pole frequency response was found to be 10 ms (omitting any velocity scaling) which is in the range of previously observed values.

Measured $T$ and $C$ interface thicknesses were corrected for the sensor responses and the effect of these corrections on the heat flux ($F_H$), the salt flux ($F_S$) and the ratio of the temperature to salt interface thickness ($r$) was studied. We showed that all three parameters are sensitive to the sensor response correction.

Determining the frequency response of a sensor by measuring physical structures at different speeds is not restricted to double-diffusive interfaces. Turbulence in stratified water bodies might also provide the small-scale structures needed to infer sensor responses. In particular the integrals over gradient spectra of $T$ and $C$, $\chi_T$ and $\chi_C$, respectively, might be an appropriate choice for testing sensor responses. The distributions of $\chi_T$ and $\chi_C$ should be profiling-speed independent, if the sensor response corrections were applied correctly. If speed-dependency is observed, a frequency response might have been neglected, over- or underestimated. However it is well possible that this requires a larger data set than the one used in Lake Kivu in order to assume representative and constant distributions of $\chi_T$ and $\chi_C$ for a particular study area, the time period of the study and for each profiling speed. When the instrument design and the measurement time frame allows, it might be worth designing field
experiments such that more than one profiling speed is used. This will increase the confidence in microstructure frequency responses and finally also in turbulent flux estimates.

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2.9 APPENDIX

2.9.1 A) Interface detection algorithm

We explain the four conditions of the interface detection algorithm using three consecutive $T$ interfaces shown in Fig. 2.8, but identical arguments hold for $C$. In Fig. 2.8, the middle interface $I_m$ is sandwiched between two mixed layers ML$_a$ (index $a$ stands for above) and ML$_b$ ($b$ for below), respectively, followed by two more interfaces $I_a$ and $I_b$.

Condition (i): Whenever

\[
\frac{\partial \bar{T}/\partial z}{\partial T/\partial z} > 1.8
\]

(with both $\partial \bar{T}/\partial z > 0$ and $\partial T/\partial z > 0$) the data are considered a candidate interface and delineated by circles. Here $\bar{T}$ is the slightly smoothed $T$ obtained by applying a first-order Butterworth filter with a cut-off frequency of $f_c = W/\theta$, where $\theta$ is a length scale much smaller than the average mixed layer thickness $H$; $\bar{T}$ is the background profile, determined by a moving average of over a vertical distance $\Theta >> H$. For Lake Kivu $H \approx 0.8$ m and we chose $\theta = 0.04$ m and $\Theta = 6$ m. The interfacial points (Fig. 2.8) appear almost as a single thick line because their spacing is tight. Below we define the staircase parameters to be determined by the algorithm for $I_m$ and ML$_b$. Identical notation is valid for $I_a$, $I_b$ and ML$_a$ with adjusted indices.

$(T_{I,m,\text{first}}, D_{I,m,\text{first}})$: temperature and depth of the first point of the series of interface points $I_m$

$(T_{I,m,\text{last}}, D_{I,m,\text{last}})$: temperature and depth of the last point of the series of interface points in $I_m$

$(T_{ML,b}, D_{ML,b})$: temperature and depth of ML$_b$

$H_{b}^*$: preliminary thickness of ML$_b$
The individual staircase parameters are then calculated as follows, starting from the points determined by condition (i):

- \( D_{ML,b} = (D_{I,m,\text{last}} + D_{I,b,\text{first}})/2 \)
- \( H_b^* = D_{I,b,\text{first}} - D_{I,m,\text{last}} \)
- \( T_{ML,b} \) is calculated by averaging the temperature within the interval \( D_{ML,b} \pm H_b^*/2 \).
- Steps one to three are carried out identically for \( ML_a \), defining \( D_{ML,a}, H_a^*, T_{ML,a} \)
- \( \Delta T_m = T_{ML,b} - T_{ML,a} \)
- \( T_{I,m} = (T_{ML,a} + T_{ML,b})/2 \)
- \( D_{I,m} \) is determined by averaging the depths of the points within the interval \( T_{I,m} \pm \Delta T_m/4 \).

Because measurement points are approximately equally spaced for a free-falling profiler with constant sampling frequency, averaging is unproblematic.
• \((\partial T/\partial z)_{\text{fit},I,m}\): A straight line is fitted to the data within the interval \(T_{I,m} \pm \Delta T_m/4\). At least two fit points are necessary. The slope of this line determines \((\partial T/\partial z)_{\text{fit},I,m}\).

• \(h_m = \Delta T_m/(\partial T/\partial z)_{\text{fit},I,m}\)

• The interfaces thicknesses \(h_a\) and \(h_b\) are calculated identically according to the previous steps.

• The final mixed layer thicknesses \(H_b\) and \(H_a\) (replacing the preliminary mixed layer thicknesses \(H_b^*\) and \(H_a^*\)) are given by \(H_b = (D_{I,b} - D_{I,m}) - (h_b + h_m)/2\) and \(H_a = (D_{I,m} - D_{I,a}) - (h_m + h_a)/2\). This definition ensures that the thickness of all layers and interfaces sum to the total vertical length of the staircase.

Condition (ii): Both mixed layer gradients adjacent to the interface are small compared to the background gradient. For the mixed layer ML\(_b\), this can be written as:

\[-0.4 < \left(\frac{(\partial T/\partial z)_{\text{fit},ML,b}}{(\partial T/\partial z)_{ML,b}}\right) < 0.4\]

Here, \((\partial T/\partial z)_{\text{fit},ML,b}\) is the slope of a linear fit through the mixed layer points within the interval \(D_{ML,b} \pm H_b/2\); \((\partial T/\partial z)_{ML,b}\) is the background gradient averaged over the same interval.

Condition (iii): Only if all four sensors detect the same interface according to arguments (i) and (ii), the step parameters, as defined in (i), are saved. The condition for detecting the same interface is that all four interface centers are located within a vertical interval of 10 cm, which is the minimum distance between interface centers.

Condition (iv): The definition of an interface thickness only makes sense if the interfaces are approximately linear in their cores. Therefore, we introduced the rejection parameter \(M = T_{rms}/\Delta T\) where \(T_{rms}\) is the root-mean-squared deviation of the measured \(T\) from the linear fit through the central 50% of the interface. Based on visual inspection we chose to discard steps with \(M > 0.03\). Figure 2.9 shows two typical examples of rejected \(C\) interfaces, whereas both \(T\) interfaces are accepted. In Fig. 2.9a, the inversion in the \(C\) interface is probably caused by a physical disturbance of the interface, which has
already diffused out in the $T$ interface. In Fig. 2.9b, the inversions are caused by noise from the MicC sensor. As a result of the rejection criteria, the total number of steps decreased by 14% and 54% for $T$ and $C$, respectively. Conductivity was more affected by this rejection criteria because inversions in $C$ persist longer due to the smaller diffusivity of salt compared to $T$ (Fig. 2.9a), and because the ratio of noise to step size is about ten times larger for $C$ than for $T$ (Fig. 2.9b).

### 2.9.2 B) A simple model of the MicC frequency response

The MicC consists of two electrodes with a constant-amplitude sinusoidal voltage difference applied between them. The resulting electric field drives a current through the fluid which is inversely proportional to its resistance. The spatial distribution of the field lines determines the measurement volume, which consists of a free stream portion, a viscous boundary layer portion and a diffusive boundary layer portion, where the latter is negligible. Conductivity changes in the free-stream are sensed immediately, whereas in the viscous boundary layer the flow is delayed. This delay causes the sensor to have a frequency response. However the frequency response is only observed if the contribution of the viscous boundary layer to the total resistance is significant. Our model consists of two parts: (i) We estimate the time scale of how fast changes in $C$ are advected into the viscous boundary layer and (ii) we estimate the contribution of the boundary layer to the total resistance.
(i) Figure 2.10a shows our model setting for part (i). We only consider one of the two MicC electrodes, which is represented by a solid plane located at \((x,y,z=0)\). The electrode starts at \(x = 0\) and ends at \(x = d\) with the flow in the \(x\)-direction. We only consider horizontal advection into the viscous boundary layer and neglect molecular diffusion, because it can be shown to be small. At \(t = 0\), the front of a rapid change of strength \(C_0\) is taken to be located at \(x = 0\) and is then advected across the sensor. We neglect the change in boundary layer thickness \(\delta_v\) over the length of the sensor and just look at the changes in the concentration profile at \(x = d/2\) (Fig. 2.10b), which is assumed to be representative of the mean along \(x\). Furthermore, we assume a linear velocity profile \(u(z)\) in the boundary layer and constant velocity \(W\) in the free stream (Fig. 2.10a), so that

\[
 u(z) = \begin{cases} 
 W, & z > \delta \\
 \frac{Wz}{\delta}, & 0 < z < \delta 
\end{cases}
\]

At any time, the horizontal location \(X\) of the front at height \(z\) within the viscous boundary layer (Fig. 2.10b) is given by

\[
 X = \frac{Wz}{\delta} t
\]

The sensor will see a concentration profile with front of concentration \(C_0\) moving downwards as the front is advected horizontally past the point \(x = d/2\), which happens after the time \(t = t_0 = d/(2W)\) (Fig. 2.10c). The height of the front above the sensor, \(Z\), at \(x = d/2\) is then given by

\[
 Z = \frac{d\delta}{2Wt}
\]

with \(t > t_0\). Note that the speed \(dZ/dt\) of the front is decreasing with \(t^2\). The mean \(C\) in the viscous boundary layer as a function of time is then

\[
 C_m(t) = \frac{1}{\delta} \int_0^\delta C(z,t) dz = \frac{1}{\delta} C_0(\delta - Z) = C_0 \left[ 1 - \frac{d}{2Wt} \right]
\]
for $t > t_0$. Note that $C_m(t)$ is independent of $\delta$. This relation allows estimating the time scale of the frequency response for concentration changes within the viscous boundary layer. Setting $C_m(\tau_{sp}+t_0)/C_0 = 1-e^{-1}$ provides a single-pole time constant $\tau_{sp}$ of

$$\tau_{sp} = \frac{d}{2W} (e-1)$$

For $d = 0.9$ mm (diameter of the MicC electrode) and $W = 0.38$ m s$^{-1}$, we get $\tau_{sp} = 2$ ms. Our double-pole frequency response with $\tau_{dp} = 2.2$ ms fulfills the same condition at $\tau_{sp} \sim 6$ ms. This simple model thus appears to provide the approximate time scale of the MicC frequency response, but it also predicts a velocity scaling $\tau_{dp} \sim W^{-1}$, which is not supported by our data (section 2.5.2). In the following we show that the viscous boundary layer represents a significant fraction of the measured signal.

(ii) The MicC sensor measures the electric current $J$ (A) while applying a constant-amplitude sinusoidal voltage difference $\Delta V$ (V) between the electrodes. The current is given by $J(t) = \Delta V/R(t)$ where $R(t)$ (Ω) is the resistance between the electrodes, which changes over time depending on the conductivity $C$ in the measurement volume. We divide the measurement volume and the resistance into a free stream portion and a viscous boundary layer portion.

$$R = R_{FS} + R_\delta$$
We assume that the resistance of the free stream is instantaneously reacting to changes of $C$ in the flow, whereas the resistance in the viscous boundary layer is only changing after the $C$ variations of the free stream have been advected into the viscous boundary layer by the process described in $(i)$. The time constant determined in $(i)$ is only observed, if the contribution $P_{\delta} = R_{\delta}/R$ to the total resistance $R$ is significant. The resistance of the viscous boundary layer is proportional to the electric potential difference $\Delta V_{\delta}$ across this layer and therefore

$$P_{\delta} = \frac{R_{\delta}}{R} = \frac{\Delta V_{\delta}}{\Delta V}$$  \hspace{1cm} (2.6)

The electric potential $V (V)$ is given by the geometry of the electrodes. Here, we represent the electrodes by two metal spheres of diameter $d$ with their centers at $y = -a - d/2$ and $y = a + d/2$. The electrodes carry the charges $q$ (C) and $-q$ and are surrounded by a viscous boundary layer. The viscous boundary layer thickness is

$$\delta \approx \frac{2}{\sqrt{\text{Re}}}$$

where $\text{Re} = Wd/\nu$ is the Reynolds number with profiling speed $W$ and the kinematic viscosity of water $\nu$ (Schlichting and Gersten 2003, p. 173, Fig. 7.3).

The charges cause an electric potential outside the spheres which we assume to be equal to the potential of two hypothetical point charges $q$ and $-q$ located at the centers of the spheres. We simplify the problem further by only considering $V$ on the line connecting the two electrodes. The potential $V$ evaluated on this line at $-a-d/2 < y < a+d/2$ is:

$$V(y) = \frac{q}{4\pi \varepsilon} \left( \frac{1}{a + d/2 - y} - \frac{1}{a + d/2 + y} \right)$$  \hspace{1cm} (2.7)

where $\varepsilon$ ($\text{A s m}^{-1} \text{ V}^{-1}$) is the permittivity, which is assumed to be constant. The potential is anti-symmetric relative to $y = 0$ and therefore we restrict the problem to $y > 0$. The potential differences across the free-stream layer and the viscous boundary layer are then

$$\Delta V_{FS} = V(0) - V(a - \delta)$$

$$\Delta V_{\delta} = V(a - \delta) - V(a)$$

where $\Delta V = 2(\Delta V_{FS} + \Delta V_{\delta})$ and $V(0) = 0$ by symmetry. Substituting Eq. (2.7) into Eq. (2.6) gives:

$$P_{\delta} = \frac{\Delta V_{\delta}}{\Delta V_{FS} + \Delta V_{\delta}} = \frac{1}{1 - \frac{(2a + d/2 - \delta)^{-1} - (d/2 + \delta)^{-1}}{(2a + d/2)^{-1} - (d/2)^{-1}}}$$
For \( a \to \delta \), \( P_\delta \to 1 \), as the viscous boundary layer occupies the entire spacing between the electrodes. For \( a \gg \delta \gg \rho \), \( P_\delta \to 1 - d/(2\delta) \). This means that, even when the electrode spacing is large, the resistance in the viscous boundary layer contribution is still significant, if the electrodes are small compared to the viscous boundary layer thickness.

For \( d = 0.86 \text{ mm}, a = 0.23 \text{ mm}, W = 0.38 \text{ m s}^{-1}, v = 9 \times 10^{-7} \text{ m}^2 \text{ s}^{-1} \) we get \( \text{Re} = 363 \), \( \delta = 90 \mu \text{m} \) and \( P_\delta = 0.44 \). Thus the resistances of the fluid in the viscous boundary layer and in the free stream are almost equal and consequently processes occurring in the viscous boundary layer such as described in (i) are important.
3 Interface structure and flux laws in a natural double-diffusive layering

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3.1 Abstract

The diffusive regime of double-diffusive convection generates staircases consisting of thin high-gradient interfaces sandwiched between convectively mixed layers. Simultaneous microstructure measurements of both temperature and conductivity from the staircases in Lake Kivu are used to test flux laws and theoretical models for double diffusion. Density ratios in Lake Kivu are between one and ten and mixed layer thicknesses on average 0.7 m. The larger interface thickness of temperature (average 9 cm) compared to dissolved substances (6 cm) confirms the boundary-layer structure of the interface. Our observations suggest that the boundary layer break-off cannot be characterized by a single critical boundary layer Rayleigh number, but occurs within a range of $O(10^2)$ to $O(10^4)$. Heat flux parameterizations which assume that the Nusselt number follows a power law increase with the Rayleigh number $Ra$ are tested for their exponent $\eta$. In contrast to the standard estimate $\eta = 1/3$, we found $\eta = 0.20 \pm 0.03$ for density ratios between two and six. Therefore, we suggest a correction of heat flux estimates which are based on $\eta = 1/3$. The magnitude of the correction depends on $Ra$ in the system of interest. For Lake Kivu (average heat flux 0.10 W m$^{-2}$) with $Ra = O(10^8)$, corrections are marginal. In the Arctic Ocean with $Ra = O(10^8)$ to $O(10^{12})$, however, heat fluxes can be overestimated by a factor of four.
3.2 Introduction

The vertical transport of heat and dissolved substances, such as salt, nutrients, oxygen are of high importance in natural water bodies. Double diffusion enhances the vertical transport within a stratified water body by transforming gradual density gradients into staircases of convectively mixed layers, separated by high-gradient and gravitationally stable interfaces (Fig. 3.1). Such staircases can develop when two agents that diffuse at different rates, contribute in opposing ways to the vertical density gradient [Schmitt, 1994; Kelley et al., 2003]. In this work, we focus on the diffusive type of double-diffusion, where the faster diffusing agent (temperature \( T \) in our case) is destabilizing and the slower diffusing agent (dissolved substances DS in our case) is stabilizing.

Double-diffusive staircases are found in polar oceans [Neal et al., 1969; Foster and Carmack, 1976; Padman and Dillon, 1987], the Mediterranean and Black Seas [Özsoy and Besiktebe, 1995] and a variety of lakes of very different environments in Antarctica [Hoare, 1968], North America [Osborn, 1973], Europe [Sánchez and Roget, 2007; Boehrer et al., 2009] and Africa [Newman, 1976; Schmid et al., 2004, 2010; for a review see Wüest et al., 2012]. Double-diffusive heat fluxes are of particular interest in the Arctic Ocean, where they play a role in the heat exchange between a warm intrusion from the North Atlantic [Carmack et al., 1997] and the overlying sea ice [Timmermans et al., 2008; Turner, 2010].

Flux estimates and theoretical models for double diffusion are usually based on laboratory experiments with rigid (and often unrealistic) boundary conditions. How well they apply in large and dynamic natural systems is still an open question, which we address with our measurements at Lake Kivu.

The double-diffusive staircases in Lake Kivu consist of up to 300 steps (Fig. 3.1), distributed almost over the entire water column between 110 m and the maximum depth of 485 m [Schmid et al., 2010]. With its manageable size, permanent stratification, small horizontal gradients, weak currents, weak Coriolis forcing and slowly evolving water properties, Lake Kivu is an ideal study environment for double-diffusion [Schmid and Wüest, 2012] and represents an intermediate system between small-scale laboratory experiments and the ocean.
We extend previous observational studies of double diffusion [Padman and Dillon, 1987; Sánchez and Roget, 2007; Timmermans et al., 2008; Schmid et al., 2010] by simultaneously measuring the microstructure of conductivity $C$ (μS cm$^{-1}$) in addition to $T$ that allows us to estimate also the density profiles. Our goal is to shed light on the density structure of the interfaces and to test existing flux laws by measuring molecular fluxes through interfaces. In particular, we address the question of whether interfaces have a double boundary-layer structure, and whether there is an associated critical boundary layer Rayleigh number, as proposed by Linden and Shirtcliffe [1978] and Worster [2004]. Then we test a basic assumption of many flux parameterizations, i.e. that the heat flux through double-diffusive staircases is independent of the mixed layer thickness [Turner, 1965]. Finally we compare the Lake Kivu flux measurements to the often cited flux parameterizations of Kelley [1990].

The manuscript is structured as follows. In section 3.3, we introduce Lake Kivu, the vertical microstructure profiler, the evaluation algorithm and our method for calculating water density. In section 3.4, we summarize the theoretical background essential for this work. In section 3.5, we present histograms of the measured staircase parameters and in section 3.6 we compare our data set to theoretical models and discuss the influence of our findings on heat flux estimates in the Arctic Ocean and Lake Kivu.

Fig. 3.1. (a) Typical Lake Kivu profile of temperature and salinity (1° 47' 28" S, 29°13' 30" E, 2 February 2011). (b) Double-diffusive staircases within the 20 m long section marked by the rectangle in (a). Adapted from Sommer et al. [2013].
3.3 Methods

3.3.1 Lake Kivu

Lake Kivu is located at the border between Rwanda and the Democratic Republic of the Congo (Fig. 3.2). The surface area, the volume and the maximum depth are 2370 km$^2$, 580 km$^3$ and 485 m, respectively [Descy et al., 2012]. Below ~65 m the lake is permanently stratified. Water density is determined by four agents, which all increase with depth: Salinity $S$ (‰), $T$ (°C), dissolved methane CH$_4$ (mol L$^{-1}$) and dissolved carbon dioxide CO$_2$ (mol L$^{-1}$). Whereas $T$ and CH$_4$ gradients destabilize the water column, the permanent stratification is maintained by the gradients of $S$ and CO$_2$ [Schmid et al., 2005; Pasche et al., 2009].

3.3.2 Vertical Microstructure Profiler

During two field campaigns from 18 April to 2 May 2010 and 19 January to 4 February 2011, we measured 225 profiles of $T$ and $C$ with a loosely tethered, free-falling Vertical Microstructure Profiler (VMP) manufactured by Rockland Scientific International (RSI, Fig. 3.3a) [Sommer et al., 2013]. The profiling length of the total data set is ~55 km. Three pairs of microstructure sensors were mounted at the nose of the instrument where they were exposed to the undisturbed natural water (Figs. 3.3b,c). For this work we exploit only the $T$ and $C$ signal of two fast FP07 (MicT, RSI, Canada and GE, USA) thermistors, and two fast SBE-7 (MicC, Sea-Bird, USA) conductivity micro-sensors, sampled at 512 Hz. Responses and noise levels of the sensors have been studied in detail by Sommer et al. [2013]. They concluded that the time response of the MicT has a half-power frequency of 10.2 Hz and a root mean square noise level of 1.2 x 10$^{-5}$ K. The half-power frequency of the MicC is 47 Hz and in addition to the time response, a spatial response must be accounted for with a half-power wavenumber of 240 cycles per meter. The two MicC sensors have noise levels of 0.12 μS cm$^{-1}$ and 0.06 μS cm$^{-1}$, respectively. The profiling speeds were: 0.19 m s$^{-1}$ (for 21 % of the measured interfaces), 0.38 m s$^{-1}$ (58 %) and 0.90 m s$^{-1}$ (21 %). We include data measured at all three speeds for analysis, since speed has only a minor influence on the spatial resolution, if the frequency responses of the microstructure sensors are correctly accounted for [Sommer et al. 2013].
Fig. 3.2. Profiling locations on Lake Kivu. Black dots indicate the 225 profiles collected in 2010 and in 2011. Bathymetric lines denote 100 m depth intervals; the thick line corresponds to the lake surface. The dotted line indicates the border between the neighboring countries.

3.3.3 Evaluation algorithm

The important staircase parameters for this study are the interface thicknesses $h_T$ (m) and $h_C$ (m) the step sizes across interfaces $\Delta T$ (K) and $\Delta C$ (µS cm$^{-1}$), and the mixed layer thicknesses $H_T$ (m)
and $H_C$ (m) (Fig. 3.4). The ratios $\Delta T/ h_T$ and $\Delta C/ h_C$ represent the interfacial gradients and are used to calculate molecular fluxes through interfaces; $H_T$ is needed for estimating the Rayleigh number. The interface thicknesses of $T$ and $C$ are defined by

$$h_T = \Delta T(dT/dz)^{-1} \quad (3.1a)$$

and

$$h_C = \Delta C(dC/dz)^{-1} \quad (3.1b)$$

where $z$ is depth (m, positive downward) and gradients are determined at the depth of the interface center [Sommer et al., 2013].

Fig. 3.3. (a) Vertical Microstructure Profiler (VMP). (b) Six microstructure sensors mounted at the instrument nose and protected by a metal frame covered by black brushes. (c) Microstructure sensor arrangement when facing the instrument nose (for abbreviations, see text). Adapted from Sommer et al. [2013].
In order to manage our enormous data set, we developed an interface detection algorithm to extract the staircase parameters from measured $T$ and $C$ profiles. The algorithm is described in detail in Sommer et al. [2013] and is based on four criteria:

(i) The interfacial gradient is large compared to the background gradient.

(ii) The gradients in the two adjacent mixed layers are small compared to the background gradient.

(iii) All four microstructure sensors (two MicT and two MicC) detect the same interface based on arguments (i) and (ii).

(iv) Profiles of $T$ and $C$ are close to linear in their interface core.

In total 9,401 interfaces passed all four criteria and form the basis for this work.

Measured interface thicknesses are always larger than their real values because of the smoothing effect of the sensor responses. Sommer et al. [2013] estimated the MicT and MicC sensor responses and developed a method to correct each measured interface thickness to obtain its true value. Here we use this corrected data set for further analysis.

### 3.3.4 Density steps

Having evaluated the $T$ and $C$ profiles, we now present our method to deduce the corresponding information for $S$, $DS$ and density. In most studies of double diffusion density is defined by two
agents only that diffuse at different rates. Those two agents are typically $T$ and $S$, corresponding to the oceanic case [Linden and Shirtcliffe, 1978; Newell, 1984; Timmermans et al., 2007], or sugar and salt in laboratory experiments [Shirtcliffe, 1973; Stamp et al., 1998]. In Lake Kivu four agents contribute to density: $T$, $S$, $CO_2$ and $CH_4$ [Schmid et al., 2005]. The fastest diffusing agent is $T$ (molecular diffusivity $\kappa_T = 1.4 \times 10^{-7}$ m$^2$ s$^{-1}$), whereas the molecular diffusivities of $S$ ($1.2 \times 10^{-9}$ m$^2$ s$^{-1}$), $CO_2$ ($1.9 \times 10^{-9}$ m$^2$ s$^{-1}$) and $CH_4$ ($1.8 \times 10^{-9}$ m$^2$ s$^{-1}$) (at the in-situ $T$ of ~25 °C) [Lide, 2012] are similar and approximately one hundred times smaller than the molecular diffusivity of $T$. We thus group the $S$, $CO_2$ and $CH_4$ together to form the slower diffusing agent DS. The diffusivity of $S$ is approximated by the weighted average of the most abundant Lake Kivu salts, which have molecular diffusivities in the range of (0.71 to 1.96) x $10^{-9}$ m$^2$ s$^{-1}$ [Yuan-Hui and Gregory, 1974]. The “artificial” molecular diffusivity $\kappa_{DS} = 1.43 \times 10^{-9}$ m$^2$ s$^{-1}$, which we use from now on for DS, is the average of the diffusivities of $S$, $CO_2$ and $CH_4$, weighted by their individual contribution to the density gradient, which is ~79%, 32% and -11%, respectively [Schmid et al., 2003]. Including the destabilizing $CH_4$ into the stabilizing component DS is not of concern based on the experimental findings of Griffiths [1979].

As DS is a mixture of components that have slightly different molecular diffusivities, each individual component might contribute to the interfacial density structure and thus the dynamics of the double-diffusive layering. However, experiments by Griffiths [1979] showed, that this effect is minor for $2 < R_\rho < 4$, which contains 51% of our data. Here, the density ratio $R_\rho = \Delta \rho_{DS}/\Delta \rho_T$ is the ratio of the fractional density steps of DS and $T$ across an interface. Because the dynamics of multicomponent convection are still not well understood [Turner, 1985], we treat DS as a single component with molecular diffusivity $\kappa_{DS}$.

For studying the structure of double diffusive interfaces, knowledge on the contributions of $T$ and DS to density is essential. This would require microstructure information on $T$, $S$, $CO_2$ and $CH_4$, of which only $T$ is obtained directly from our measurements. Having both, $T$ and $C$ information it is possible to calculate $S$ [Wüest et al., 1996]. For $CO_2$ and $CH_4$ we have only the large-scale profiles [Schmid et al., 2005], which contain no information on the double-diffusive steps. We thus estimate the microstructure of $CO_2$ and $CH_4$ by making three assumptions: (i) The large-scale profiles of $CO_2$ and $S$ are related; (ii) the large-scale profiles of $CO_2$ and $CH_4$ profiles are proportional to each other; and (iii) assumptions (i) and (ii) are also valid for the microstructure of $CO_2$ and $CH_4$. 

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Assumptions (i) and (ii) are based on observations of Schmid et al. [2005]. The large-scale structure of CO$_2$ is well described as a function of $S$ by a 2$^{nd}$ order polynomial $CO_2 = p_0 + p_1 S + p_2 S^2$ with $p_0 = -0.0182$ mol L$^{-1}$, $p_1 = 0.0062$ mol L$^{-1}$‰$^{-1}$, $p_2 = 0.0023$ mol L$^{-1}$‰$^{-2}$, where the coefficients are obtained by a least square fit of the background $S$ profile to the CO$_2$ profile below a depth of 100 m ($R^2 > 0.99$). The CO$_2$ profile agrees with the fit within 10% in the staircase region. Furthermore, a constant gas ratio of $\gamma_g = [CO_2] / [CH_4] = 4.8$ (2) was shown to agree well with direct CH$_4$ measurements below 100 m depth [Schmid et al., 2005]. Assumption (iii) is acceptable because $S$, CO$_2$ and CH$_4$ diffuse at similar rates and convective mixing in the homogeneous layers affects all three DS ingredients approximately in the same way.

In Eqs. (3.1a, b) we defined interface thicknesses for $T$ and $C$. The same definitions hold for $S$, CO$_2$, CH$_4$ and as well for their density contributions $\rho_T$, $\rho_S$, $\rho_{CO_2}$, $\rho_{CH_4}$ and $\rho_{DS}$. The parameters $\Delta T$, $h_T$, $\Delta C$ and $h_C$ are directly extracted from the measurements. Step sizes and interface thicknesses of the other agents are derived from the $T$ and $C$ parameters as described below.

**Step sizes**: The salinity step size $\Delta S$ is calculated from the mixed layer $C$ and $T$ using a typical ionic composition for Lake Kivu water and following the methodology of Wüest et al. [1996]; $\Delta CO_2 = (p_1 + 2p_2 S_{int}) \Delta S$, where $S_{int}$ is the salinity at the depth of the interface; $\Delta CH_4 = \Delta CO_2/\gamma_g$; $\Delta T = \rho_0 \alpha \Delta T$, where $\rho_0 = 1000.6$ kg m$^{-3}$ is the average water density below 100 m depth and $\alpha = (2.43$ to $2.78) \times 10^{-4}$ K$^{-1}$ [Chen and Millero, 1986] is the $T$-dependent thermal expansion coefficient; $\Delta DS$ is not defined because DS consists of three different agents; $\Delta \rho_S = \rho_0 \beta_S \Delta S$, where $\beta_S = (7.50$ to $7.55) \times 10^{-4}$ kg g$^{-1}$ [Chen and Millero, 1986] is the haline contraction coefficient, $\Delta \rho_{CO_2} = \rho_0 \beta_{CO_2} \Delta CO_2$ and $\Delta \rho_{CH_4} = \rho_0 \beta_{CH_4} \Delta CH_4$, where $\beta_{CO_2}$ (0.0125 L mol$^{-1}$) and $\beta_{CH_4}$ (-0.020 L mol$^{-1}$) are the contraction coefficients of CO$_2$ and CH$_4$, taken as constants over this small $T$ range. Finally $\Delta \rho_{DS} = \Delta \rho_S + \Delta \rho_{CO_2} + \Delta \rho_{CH_4}$.

**Interface thicknesses**: For the $S$ interface thickness $h_S = \Delta S(dS/dz)^{-1}$, we use $\Delta S$ as explained above and we determine the $S$ gradient by
\[
\frac{dS}{dz} = \frac{dC}{dz} \frac{\partial C}{\partial T} \bigg|_S \frac{dT}{dz} - \frac{\partial C}{\partial S} \bigg|_T
\]

(3.3)

Here, per definition \( dC/dz = \Delta C/h_C \) and \( dT/dz = \Delta T/h_T \) and the subscripts of the gradients indicate the parameter which is kept constant. From Eqs. (3.1, 3.2) and assuming that CO\(_2\) is proportional to \( S \) for small changes of \( S \) (such as \( \Delta S \)), we get \( h_S = h_{\text{CO}_2} = h_{\text{CH}_4} = h_{\text{DS}} \). Assuming a linear approximation of the equation of state we further get \( h_T = h_{p,T} \) and \( h_{DS} = h_{p,DS} \).
3.4 Theoretical background

Predicting vertical fluxes through double-diffusive staircases has been the focus of many laboratory studies in the past [Turner, 1965, 1973; Marmorino and Caldwell, 1976; Newell, 1984; Fernando, 1989; Kelley, 1990]. One of the goals was always to estimate fluxes based on easily measurable parameters, such as step sizes or mixed layer thicknesses. For that purpose, the heat flux $F_H$ (W m$^{-2}$) is usually parameterized directly and the salt flux is expressed as a function of the density flux ratio $R_F$ (-) and $F_H$. In our case, salt is replaced by DS and the flux of DS is expressed in density units. The density flux ratio $R_F$ is thus defined as

$$R_F = \frac{F_{\rho,DS}}{(\alpha/c_\rho)F_H}$$

(3.4)

with $c_\rho$ (J kg$^{-1}$ K$^{-1}$) being the specific heat capacity of water. Laboratory experiments showed that $F_H$ as well as $R_F$ both strongly increase when $R_\rho$ becomes small, whereas for large $R_\rho$ the dependence on $R_\rho$ is weak. The most common parameterization for $F_H$ and $R_F$ was introduced by Kelley [1990], who used the scaling relation of Turner [1965] and an empirical fit to various laboratory data sets. In order to predict $F_H$ and $R_F$ for certain ranges of $R_\rho$, a number of models [Linden and Shirtcliffe, 1978; Newell, 1984; Fernando, 1989; Stamp et al., 1998] have been developed. We focus on the model by Linden and Shirtcliffe [1978], because it is valid for the intermediate $R_\rho$ usually observed in natural waters and it assumes a double-boundary-layer structure of the interface that can be directly tested by our measurements.

We first point out some interesting aspects of the boundary-layer theory of Linden and Shirtcliffe [1978]. Then we introduce the “4/3 law” of Turner [1965] that is the basis of many theoretical models [Marmorino and Caldwell, 1976; Linden and Shirtcliffe, 1978; Kelley, 1990; Worster, 2004] and finally we focus on the parameterization by Kelley [1990] that is often applied to calculate double-diffusive fluxes in oceans and lakes [Schmid et al., 2004, 2010; Sánchez and Roget, 2007; Polyakov et al., 2012]. For each theory we briefly mention which aspect we will test using the Lake Kivu data set.

3.4.1 Boundary layer model by Linden and Shirtcliffe [1978]

The model of Linden and Shirtcliffe [1978] is valid in the range of $1 < R_\rho < (\kappa_S/\kappa_T)^{1/2} = \tau^{1/2} \approx 10$ and agrees with experimental data for $2 < R_\rho < 7$ within a factor of two. The model assumes steady-state and a double-boundary-layer structure of the interface. Within the diffusive core of
the interface the gradients of $T$ and $S$ are constant and heat and salt are transported by molecular diffusion. Outside this core, marginally unstable boundary layers develop which are characterized by a boundary layer Rayleigh number $Ra_{bl}$ (-). When a critical boundary layer Rayleigh number $Ra_{bl,c}$ (-) is exceeded, the boundary layers are assumed to break off into the mixed layer. The steady-state assumption requires that the molecular transport through the core is balanced by the advective flux of heat and salt into the mixed layers. This leads to a constant density flux ratio

$$R_{F,LS} = \tau^{1/2} \approx 0.1.$$  \hfill (3.5)

The sole adjustable parameter of this model is the critical boundary layer Rayleigh number $Ra_{bl,c}$. \textit{Linden and Shirtcliffe} [1978] took $Ra_{bl,c} = 1629$ in line with \textit{Howard}'s [1964] model for high Rayleigh number thermal convection. \textit{Worster} [2004] derived $Ra_{bl,c}$ by matching an extended model of \textit{Linden and Shirtcliffe} [1978] to the experimental data of \textit{Turner} [1965] and determined $Ra_{bl,c} = 8801$ for a heat-salt system ($\tau \approx 0.01$). Interestingly, for a sugar-salt system ($\tau \approx 0.3$), he found $Ra_{bl,c} = 738$, suggesting $Ra_{bl,c}$ being a function of $\tau$.

In previous field studies, the stabilizing component (DS) was ignored and $Ra_{bl}$ was only calculated based on the destabilizing agent ($T$), because instrumentation did not allow for resolution of the interface structure of the stabilizing agent \cite{Padman and Dillon, 1989; Sánchez and Roget, 2007}. We calculate $Ra_{bl}$ based on the density structure of the interface that is derived from both $T$ and DS. We expect the histogram of $Ra_{bl}$ to cut-off at $Ra_{bl,c}$, if the theory of \textit{Linden and Shirtcliffe} [1978] is appropriate.

We briefly introduce the definition of $Ra_{bl}$ by \textit{Linden and Shirtcliffe} [1978] with the notation of \textit{Carpenter et al.} [2012a, 2012b] which is used here. We define $Ra_{bl}$ for an individual interface as the average $Ra_{bl}$ of the upper and the lower boundary layer. For the lower boundary layer

$$Ra_{bl} \equiv \frac{g\delta p b^3}{\rho_0 \nu \kappa_T}.$$ \hfill (3.6)

where $g$ (m s$^{-2}$) is the gravitational acceleration, $b \equiv (h_T - h_{DS})/2$ (m) is a representative thickness of the boundary layer, and $\delta p$ (kg m$^{-3}$) is a representative boundary layer density scale defined by

$$\delta p b = \int_{z_{bl}}^{z_{bl,T/2}} [\rho(z) - \rho_{ml}] dz$$ \hfill (3.7)

Here $\rho_{ml}$ (kg m$^{-3}$) is the average density of the lower mixed layer (determined over the mid 50% of the mixed layer), $z_{bl}$ (m) is the closest $z$ below the interface center which fulfills $|\rho(z) - \rho_{ml}| = 0$. 59
and \( z_{H,T/2} \) (m) is the center of the lower mixed layer adjacent to the interface. In Fig. 3.5a, \( \delta \rho b \) corresponds to the gray area. In practice, we assume an error function profile of \( T \) and \( S \) with the same \( h_T, h_D, \Delta \rho_T, \Delta \rho_D \) as measured. This allows us to write \( Ra_{bl} \) as a function of \( Ra_{bl} = \frac{h_T}{h_S}, \Delta \rho_T, h_T, \kappa_T, \nu, \rho, g \) and \( H_T \) (see Carpenter et al. [2012b] for details), which are all available for Lake Kivu. For the upper boundary layer, \( Ra_{bl} \) is calculated identically. Because we assume symmetry of the upper and lower boundary layer, the only difference between the two \( Ra_{bl} \) is caused by the dependence on \( H_T \). This dependence on \( H_T \) is small as long as \( H_T/h_T > 5 \) [Carpenter et al., 2012b].

### 3.4.2 The 4/3 law by Turner [1965]

Turner [1965] used laboratory experiments to investigate an \( S \) interface which was heated from below. The relevant physical parameters of the system are assumed to be \( g \alpha \Delta T, g \beta_S \Delta S, \kappa_T, \kappa_S, \nu \) and the layer thickness \( H = H_T + h_T \). Out of these four dimensionless control parameters can be formed. They are

\[
Ra = \frac{g \alpha \Delta T h^3}{\nu \kappa_T}, \quad R_p = \frac{g \beta_S \Delta S}{g \alpha \Delta T} = \frac{\Delta \rho_S}{\Delta \rho_T}, \quad \tau = \frac{\kappa_S}{\kappa_T}, \quad Pr = \frac{\nu}{\kappa_T},
\]

(3.8)
corresponding to Rayleigh number, density ratio, diffusivity ratio and Prandtl number, respectively. One important key system response is the dimensionless heat flux described by the Nusselt number \( Nu = \frac{F_H}{c_p \rho_0 \kappa_T \Delta T/H} \) where \( F_H \) (W m\(^{-2}\)) is the total vertical heat flux across the interface. For constant \( \tau \) and \( Pr \), \( Nu \) is expected only to depend on \( Ra \) and \( R_p \). Turner [1965] suggested the functional from

\[ Nu = C(R_p) Ra^\eta \]

(3.9)
with \( \eta = 1/3 \), which removes the dependence on \( H \). The \( R_p \) dependent proportionality factor \( C(R_p) \) must be determined experimentally. Solving Eq. (3.9) for \( F_H \), we get

\[ F_H = C(R_p) c_p \rho_0 \left( \frac{\kappa_T^2 g \alpha}{\nu} \right)^{1/3} \Delta T^{4/3} \]

(3.10)

This law is often called the “4/3 law” due to the exponent on \( \Delta T \).

We will estimate the exponent \( \eta \) in Eq. (3.9) by subdividing our data set into bins of \( R_p \), so that \( C \) becomes approximately constant. \( Nu \) and \( Ra \) will be calculated directly from our measurements assuming molecular transport through interfaces. The slope of a linear fit through
the data (on a double-logarithmic scale) then determines \( \eta \). For calculating Ra we use

\[
H = \overline{H_T} + h_T,
\]

where \( \overline{H_T} \) is the mean thickness of the mixed layers above and below the interface.

### 3.4.3 Parameterization by Kelley [1990]

Kelley [1990] questioned the exponent \( \eta = 1/3 \) of Eq. (3.9) based on a model for thermal convection that leads to \( \eta = 0.27 \pm 0.02 \) and is between \( \eta = 2/7 \) [Castaing et al., 1989; Kerr, 1996; Sommeria, 1999] and \( \eta = 1/4 \) (\( Ra < 10^{11}, Pr \approx 7 \)) [Grossmann and Lohse, 2000] of previous scaling laws for single-component convection. For double-diffusive convection, however, Kelley [1990] recommended to retain \( \eta = 1/3 \) as long as observations do not provide evidence for a
different exponent. Assuming \( \eta = 1/3 \) he introduced an improved fit function to \( C_{\text{Kel}}(R_p) = \text{NuRa}^{-\eta} \) by compiling numerous available laboratory data sets and found:

\[
C_{\text{Kel}}(R_p) = 0.0032 \exp \left( \frac{4.8}{R_p^{0.72}} \right)
\]  
(3.11)

The density flux ratio \( R_F \) as a function of \( R_p \) was obtained from an empirical fit to the same experimental data used for \( C_{\text{Kel}}(R_p) \). The form of the fit function was based on the theory of Linden [1974] assuming that the total flux across the interface is a composition of a “diffusive flux” and an “entrainment flux” relevant for large and small \( R_p \), respectively. Kelley [1990] then optimized the numerical values of the proposed form and got:

\[
R_{F,\text{Kel}}(R_p) = \frac{R_p + 1.4(R_p - 1)^{3/2}}{1 + 14(R_p - 1)^{3/2}}.
\]  
(3.12)

Both Eqs. (3.11) and (3.12) increase strongly when \( R_p \to 1 \) reflecting the increasing influence of advection across the interface when the stability of the interface decreases.

Equations (3.11) and (3.12) will be compared to our Lake Kivu observations by assuming that the total fluxes are well represented by molecular fluxes through the interfaces. The molecular fluxes of heat \( F_{H,\text{mol}} \) (W m\(^{-2}\)) and the density fluxes of dissolved substances \( F_{\rho,\text{DS, mol}} \) (kg m\(^{-2}\) s\(^{-1}\)) through interfaces are defined by

\[
F_{H,\text{mol}} = c_p \rho_0 \kappa_T \Delta T h_T^{-1}
\]  
(3.13a)

\[
F_{\rho,\text{DS, mol}} = \kappa_{\text{DS}} \Delta \rho_{\text{DS}} h_{\text{DS}}^{-1}
\]  
(3.13b)

where \( c_p = (4168 \text{ to } 4177) \) J kg\(^{-1}\) K\(^{-1}\) for Lake Kivu water. The molecular density flux ratio is then

\[
R_{F,\text{mol}} = \frac{F_{\rho,\text{DS, mol}}}{(\alpha/c_p) F_{H,\text{mol}}} = \tau R_p
\]  
(3.14)

with \( \tau = \kappa_{\text{DS}}/\kappa_T \approx 0.01 \). For constant \( \tau \), \( R_{F,\text{mol}} \) thus only depends on \( r \) and \( R_p \), which are both measured in Lake Kivu.

It has been suggested that molecular fluxes might underestimate the total fluxes, in particular for low \( R_p \) [Linden and Shirtcliffe, 1978; Newell, 1984]. We have tested this by comparing two-dimensional Direct Numerical Simulations with the Lake Kivu measurements (T. Sommer, J. R. Carpenter and A. Wüest, Representativeness of Direct Numerical Simulations for double diffusion in natural systems, submitted to Geophysical Research Letters). For \( R_p \geq 3 \), \( F_{H,\text{mol}} \) underestimates the total heat flux by less than 10% and \( R_{F,\text{mol}} \) underestimates the density
flux ratio by less than 27%. We emphasize that condition \textit{iv} of the algorithm is important to achieve good agreement between the two estimates, in particular for small $R_\rho$.

In summary, all theories described in this section contain properties that can be directly compared to our measurements. Specifically, the histogram of $R_{ab}$ will shed light on the existence of a critical $R_{abl,cr}$ as assumed by Linden and Shirtcliffe [1978] and Worster [2004] and molecular fluxes through interfaces will serve to test the 4/3 law of Turner [1965] and will be compared to the semi-empirical flux law of Kelley [1990].
3.5 Results

In this section we present histograms of staircase parameters measured in Lake Kivu between 111 m and 451 m depth. Most of the data (58%) is from the gradients between 180 m and 200 m as well as 300 and 330 m depth. Each histogram contains 9,401 data points. Arithmetic means and 10th and 90th percentiles are indicated in the top left corner of the panels. Histograms for the following staircase parameters are presented: Step sizes across interfaces for $T$ and $S$, density ratios $R_\rho$, interface thicknesses $h_T$ and $h_S$, their ratio $r$, mixed layer thicknesses for temperature $H_T$, Rayleigh numbers $Ra$, molecular fluxes of heat ($F_{H,mol}$) and density fluxes of DS ($F_{\rho,DS,mol}$) through interfaces and finally density flux ratios $R_{F,mol}$.

3.5.1 Step size

Histograms of the step size $\Delta T$ and $\Delta S$ are shown in Figs. 3.6a, c. The arithmetic means are 11 mK (3, 20) and 0.013 ‰ (0.002, 0.024). The step sizes $\Delta CO_2$ and $\Delta CH_4$ are numerically estimated as functions of $S$ and are not shown.

The histogram of $R_\rho$ for Lake Kivu is shown in Fig. 3.6e. The average is 4.0 (2.4, 5.6) and thus the Lake Kivu staircases are within the usually observed range of $R_\rho$ between one and ten [Kelley et al., 2003].

3.5.2 Interface thickness

Interface thicknesses $h_T$ and $h_{DS}$ are on average 9.2 cm (2.5, 16.5) and 6.4 cm (0.4, 13.5), respectively (Figs. 3.6b,d). The minimum interface thicknesses for DS and $T$ are $h_{DS,\text{min}} \approx 1$ mm and $h_{T,\text{min}} \approx 1$ cm, emphasizing our excellent spatial resolution, in particular of the $S$ measurements. The time scale of diffusion of those smallest interfaces is $h_{DS,\text{min}}^2 (4\pi\kappa_{DS})^{-1} \approx h_{T,\text{min}}^2 (4\pi\kappa_{T})^{-1} \approx 1$ min. Such a short time scale proves the existence of active processes which effectively maintain interfaces. In Fig. 3.6d, we observe a gap between the frequency of the thin interfaces (thicknesses ~3 mm, for an example see Fig. 3.7a) and the thick interfaces (~6 cm, see Fig. 3.7c). Interfaces with thicknesses in between the two peaks are usually disturbed and often show small mixed segments within the interface (Fig. 3.7b). Such interfaces are rejected by the algorithm resulting in the separation of the two peaks in Fig. 3.6d. The small mixed segments within the interface could be a signature of interfacial waves as described by Stamp et al. [1998]. We plan to investigate this phenomenon in more detail in a future publication (see above), where we compare the Lake Kivu observations to Direct Numerical Simulations.
The interface thickness ratio \( r \) is an important parameter for computing density flux ratios (Eq. 3.14) and for studying the interfacial boundary layer (section 3.4.1). The theoretical range of \( r \) is between one and \((\kappa_T/\kappa_D)^{1/2} \approx 10\). An interface thickness ratio smaller than one is unlikely, because in that case \( h_D > h_T \), which would imply that the \( T \) interface is eroded more effectively.

Fig. 3.6. Histograms of (a,c) step sizes, (b,d) interface thicknesses, (e,f) their respective ratios, (g) temperature mixed layer thicknesses and (h) Rayleigh numbers for all profiles over the entire depth range. Logarithmic scale is used for the x-axis. Arithmetic means are indicated by short vertical lines and bootstrapped 95% confidence intervals of the mean are within the width of the lines. The numbers inside each panel indicate the arithmetic mean (bold) with the 10th and 90th percentiles in parentheses. Each histograms contains 9,401 data points.
than the $S$ interface. An interface with $r = 1$ might exist directly after an erosion event before $h_T$ and $h_{DS}$ begin growing again by molecular diffusion. The upper limit $r = (\kappa_T/\kappa_{DS})^{1/2}$ is the long-term asymptotic value for the molecular diffusion of $T$ and DS interfaces.

Figure 3.6f shows the histogram of $r$ for Lake Kivu. For the investigated interfaces, $r$ is on average 3.3 (1.0, 7.7) and thus within the theoretical range explained above. However we also detect few interfaces with $r < 1$ (12 %) and $r > 10$ (7 %), which are the result of slightly non-linear interfaces, of which an example is shown in Fig. 3.7c. Here, the DS interface (approximated by $C$) has a slight kink close to the interface center, which decreases the measured gradient in the interface and therefore increases the calculated interface thicknesses so that $h_{DS} > h_T (r = 0.85)$.

### 3.5.3 Mixed layer thickness and Rayleigh number

Average mixed layer thicknesses $H_T$ and $H_S$ are 0.72 m (0.33, 1.17) and 0.75 m (0.36, 1.22), respectively and we only show the histogram of $H_T$ in Fig. 3.6g, because the differences between the two are marginal.

The average Rayleigh number $Ra$ is 2.4 (0.1, 5.2) x $10^8$ and the corresponding histogram is shown in Fig. 3.6h.
3.5.4 Molecular fluxes through interfaces

Arithmetic means of $F_{H,mol}$ (Eq. 3.13a) and $F_{DS,mol}$ (Eq. 3.13b) for all measured interfaces are 0.10 W m$^{-2}$ (0.02, 0.21) and 0.89 $\mu$g m$^{-2}$ s$^{-1}$ (0.07, 1.63), respectively, and the corresponding histograms are shown in Figs. 3.8a,b. The distribution of $R_{F,mol}$ (Eq. 3.14) is shown in Fig. 3.8c and its arithmetic mean is 0.11 (0.03, 0.21).

In 2004 the average molecular heat flux through interfaces was estimated to be 0.02 W m$^{-2}$ [Schmid et al., 2010], a factor of five less than our estimate. This difference is mainly caused by the different profile evaluation methods. We distinguish between four major differences of the two methods that all result in smaller heat fluxes for the estimate of Schmid et al. [2010]. The approximate contribution to the total difference (factor 5) is given in parentheses. (i) Both methods imply different interface thickness definitions (factor 2). Schmid et al. [2010] determined the interface thickness by visually estimating the depth of the upper boundary of one mixed layer and the lower boundary of the adjacent mixed layer above and subtracting the two values, whereas our definition is based on the gradient at the interface center. (ii) The manual evaluation of Schmid et al. [2010] is more efficient in detecting interfaces with small $\Delta T$ (factor 1.4). (iii) Schmid et al. [2010] did not account for the sensor response (factor 1.1) (iv) No rejection criteria was used for disturbed interfaces (factor 1.2). The remaining factor of 1.4 might be caused by the temporal variation and the horizontal heterogeneity of the heat fluxes which we plan to investigate in a future publication.
Fig. 3.8. Histograms for (a) the molecular heat flux through interfaces, (b) the molecular density flux of dissolved substances through interfaces and (c) the density flux ratio. Arithmetic means are indicated by short vertical lines and bootstrapped 95% confidence intervals of the mean are within the width of the lines. The numbers inside each panel indicate the arithmetic mean (bold) with the 10\textsuperscript{th} and 90\textsuperscript{th} percentiles in parentheses.
3.6 Discussion

Having outlined the relevant theories for this work in section 3.4, we now compare them to the Lake Kivu measurements. We present a histogram of $Ra_{bl}$ and compare it to the predictions of Linden and Shirtcliffe [1978] and Worster [2004]. We test the exponent $\eta$ in Eq. (3.9), which for $\eta = 1/3$ results in the 4/3 law and discuss the heat flux and density flux ratio parameterizations of Kelley [1990]. Finally we estimate corrections for heat flux estimates in the Arctic Ocean.

3.6.1 Critical boundary layer Rayleigh number

In the theories of Linden and Shirtcliffe [1978] and also Worster [2004] the boundary layer water adjacent to the double-diffusive interface is assumed to be entrained into the mixed layer when a critical boundary layer Rayleigh number $Ra_{bl,cr} = 1629$ or $Ra_{bl,cr} = 8801$ is exceeded, respectively. The histogram of $Ra_{bl}$ is shown in Fig. 3.5b with the average $Ra_{bl}$ being 609 (0.6, 1277). Most of the interfaces have $Ra_{bl} \approx 100$, which agrees well with the Direct Numerical Simulations of Carpenter et al. [2012a]. The histogram of $Ra_{bl}$ does not show a sharp cut-off at a certain $Ra_{bl,cr}$, but instead continuously decreases between $O(10^2)$ and $O(10^4)$. We provide three possible explanations for this smooth decrease. (i) Carpenter et al. [2012b] show that the instability of the boundary layers is time-dependent and thus linear stability theory with its prediction of $Ra_{bl,cr}$ is not applicable to double-diffusive interfaces. (ii) The Direct Numerical Simulations of Carpenter et al. [2012b] indicate that the boundary layers are rather swept away at variable time intervals by the mixed layer flow than being released from the interface after they have accumulated enough excess buoyancy. (iii) Measurement uncertainties in $Ra_{bl}$ (especially in parameter $b$ that enters Eq. (3.6) to the third power) might contribute to the smooth decrease of $Ra_{bl,cr}$ at large $Ra_{bl}$.

However, the models of Linden and Shirtcliffe [1978] and Worster [2004] only require an estimate for $Ra_{bl,cr}$ at which the boundary layers are released into the mixed layers, the reason for the break-off is not essential to the model. Both estimates of $Ra_{bl,cr} = 1629$ and 8801, respectively, are in the range of the observed drop-off in the histogram of $Ra_{bl}$ and are thus reasonable choices within the model limitations.

The histogram of $Ra_{bl}$ in Fig. 3.5b has a long tail toward small $Ra_{bl}$, for which we now provide an explanation. Therefore, we model the growth of $T$ and DS interface thicknesses by molecular diffusion from initially identical thicknesses. In the simulation, both interfaces are
represented by error function profiles and have the initial thickness \( h_T = h_{DS} = h_0 \). At equal time steps, \( \text{Ra}_{bl} \) is calculated until a maximum \( \text{Ra}_{bl,cr} = 10^3 \) is reached. Our choice of \( \text{Ra}_{bl,cr} \) is arbitrary between \( 10^2 \) and \( 10^4 \). The histogram of the simulated \( \text{Ra}_{bl} \) is then scaled to contain the same number of data points as the Lake Kivu data set. The results of two simulations with \( h_0 = 1 \) mm and \( h_0 = 100 \) mm are indicated by the two lines in Fig. 3.5b. The simulation, in particular for \( h_0 = 100 \) mm, reproduces the tail toward small \( \text{Ra}_{bl} \) and thus supports the idea of Linden and Shirtcliffe [1978] that the \( T \) and DS interfaces periodically grow by molecular diffusion from initially the same thickness until they are released into the mixed layer at \( \text{Ra}_{bl} \) between \( 10^2 \) and \( 10^4 \).

### 3.6.2 Testing the 4/3 law

In section 3.4.2 we introduced the 4/3 law as a basic assumption for heat flux parameterizations. The 4/3 law is based on \( \text{Nu} \sim \text{Ra}^{\eta} \) with \( \eta = 1/3 \). Whereas for single-component convection, \( \eta \) has been widely studied and deviations from 1/3 have been found, experiments are complex for double-diffusive convection, because \( \text{Nu} \) additionally depends on \( R_p \) (Eq. 3.9) and it is difficult keeping \( R_p \) constant while varying \( \text{Ra} \).

By assuming molecular fluxes through interfaces we estimate the exponent \( \eta \) for double-diffusive convection. We use two independent estimates for \( F_H \) in the definition of the Nusselt number: (i) \( F_H = F_{H,mol} \) for \( \text{Nu} = \text{Ra}^{\eta} \) and (ii) \( F_H^* = (c_p/\alpha)F_{\rho,DS,mol}R_{F,Kel}^{-1} \) for \( \text{Nu}^* = \text{Ra}^{\eta^*} \). For the starred quantities the heat flux is calculated from the density flux of dissolved substances and \( R_{F,Kel} \), which only depends on \( R_p \) (Eq. 3.12). In order to estimate \( \eta \) (and \( \eta^* \)) we first sort the Lake Kivu interfaces into bins of \( R_p \) of interval 0.5 to ensure that \( R_p \) (and therefore also \( R_{F,Kel} \)) is approximately constant within each bin. We then estimate \( \eta \) (and \( \eta^* \)) bin-wise from the slope of a least-square fit of \( \text{Nu} \) against \( \text{Ra} \) in double logarithmic space. Varying bin-sizes between 0.1 and 1.0 has only marginal effect on the estimates of \( \eta \).

In Figs. 3.9a,c we show fit examples (thick solid lines) for the bin \( 4 < R_p < 4.5 \). The prediction of Kelley [1990] is indicated by the thin dashed line. In Fig. 3.9b,d, the fit slopes \( \eta \) and \( \eta^* \) are plotted together with their 95% bootstrapped confidence intervals as a function of \( R_p \).

We find that for the entire range of \( R_p, \eta < 1/3 \). For \( 2 < R_p < 6, \eta = 0.20 \pm 0.03 \), where 0.20 is average \( \eta \) and 0.03 the average confidence interval in that range in Fig. 3.9a. At large \( R_p > 7 \), \( \eta \) decreases and crosses zero at \( R_p \approx 8 \). Note that the two independent estimates \( \eta \) and \( \eta^* \) yield
similar results, except at small $R_\rho < 3$, where we expect disturbed interfaces, in particular for DS, because $\kappa_{DS} \ll \kappa_T$.

We emphasize that linear fits of $y$ (here $\log_{10} Nu$) on $x$ (here $\log_{10} Ra$) assume that the entire uncertainty is in $y$, which is not the case here because both $Nu$ and $Ra$ are subject to measurement errors and natural fluctuations, with the latter being the dominant effect in Fig. 3.9.

Fig. 3.9. Dependence of the Nusselt number $Nu$ on the Rayleigh number $Ra$. (a) $Ra$ is plotted against $Nu$ for $4 < R_\rho < 4.5$ on double logarithmic scale. The thick solid line is the linear fit through the data, while the thin dashed line represents the parameterization by Kelley [1990] with a slope of 1/3. (b) Fit slopes determined as in (a) for successive bins of $R_\rho$ of interval 0.5 within the range $1 < R_\rho < 10$. The circle represents the fit in panel (a). Error bars indicate bootstrapped 95 % confidence limits. Panels (c) and (d) are identical to (a) and (b), respectively, but the heat flux in $Nu^*$ is expressed as $F_{H,mol} = (c_p/\alpha)F_{\rho,DS,mol}R_{F,Kel}^{-1}$. 
Attributing uncertainties to $x$ can severely increase the slope of the fit. Following the methodology of Ricker [1973], we studied the sensitivity of the fit slope toward uncertainties in $x$ and found that our values of $\eta$ are unaffected by uncertainties in $x$ as long as the uncertainty in $y$ is at least twice as large as the uncertainty in $x$. Based on thermistor data (not yet published), we expect that the time scale of layer merging and splitting (causing changes in $\Delta T$ and $H$ and therefore in $Ra$) is at least several days, whereas the time scale for interface diffusion (causing changes in $Nu$) is several hours. Thus the uncertainty in $Nu$ is much larger than the uncertainty in $Ra$ and our result $\eta = 0.20 \pm 0.03$ is unaffected.

In section 3.4.3 we mentioned that $\eta < 1/3$ has been found for single-component convection. We now show that $\eta \approx 0.2$ does not contradict previous double-diffusive experiments. In double-diffusive experiments $C(R_p) = NuRa^{\eta}$ with $\eta = 1/3$ is often plotted as a function of $R_p$ for intercomparison between different experiments and in order to obtain a continuous empirical fit function for $C(R_p)$ such as $C_{Kel}(R_p)$ (Eq. 3.11). The observed scatter in $C(R_p)$ [e.g. Fig. 4 in Kelley et al. 2003] for fixed $R_p$ could be the result of systematic errors in $\eta$ in addition to random measurement errors and varying experimental boundary conditions. If we assume error-free experiments with identical boundary conditions and a true $\eta \neq 1/3$, then we can estimate the deviation $\Delta \eta = \eta - 1/3$ that is needed to reproduce the same scatter as observed. We express the scatter in $C$ (at constant $R_p$) as

$$\frac{C_{Ra_1,\eta=1/3}}{C_{Ra_2,\eta=1/3}} = \left( \frac{Ra_1}{Ra_2} \right)^{\Delta \eta} \equiv \xi$$

where the left-hand-side is the ratio of $C$ for two different Rayleigh numbers $Ra_1$ and $Ra_2$ and assuming that $\eta = 1/3$ is the exponent that deviates from the true exponent by $\Delta \eta$. Note that measuring $Nu$ and $Ra$ over a larger range of $Ra$ (at constant $R_p$) increases the confidence in the estimate of $\eta$. Kelley et al. [2003] estimated the scatter in $C$ to be 40% ($\xi = 1.4$) and took $Ra_1/Ra_2 = 1/20$ based on experiments of Marmorino and Caldwell [1976], which yields $|\Delta \eta| \approx 0.11$. This is close to our estimate of $|\Delta \eta| = |0.2 - 1/3| \approx 0.13$. If our estimate was true, it would mean that most of the observed scatter in experiments is indeed caused by the choice of $\eta$ and the effects of measurement errors and boundary conditions are small. However, a scatter of 40% is a rather small estimate [Fig. 4 in Kelley et al., 2003] and the estimate of $Ra_1/Ra_2$ is uncertain, because the previous literature does not provide explicit values for this ratio at fixed $R_p$. Therefore $|\Delta \eta|$ might be larger in reality. For example, taking $Ra_1/Ra_2 = 1/10$ and $\xi = 2$ yields $|\Delta \eta| = 0.3$. Our finding of
η ≈ 0.2 is thus realistic and using $C(R_\rho) = \text{NuRa}^{-0.2}$ instead of $C(R_\rho) = \text{NuRa}^{-1/3}$ should result in a better collapse of the experimentally derived $C(R_\rho)$. Recently, an exponent $\eta < 1/3$ in double-diffusive convection has gained some additional support from the three-dimensional Direct Numerical Simulations of Flanagan et al. [2013]. However, it should be mentioned that they tested the exponent Eq. (3.10) instead of Eq. (3.9) and thus ignored the dependence of $F_H$ on $H$.

The parameterization of Kelley [1990] is based on $\eta = 1/3$ which we have shown might not be the appropriate value. Figure 3.9a shows that this does not necessarily affect heat flux estimates. For $Ra = Ra_{\text{int}} = O(10^8)$, where both lines in Fig. 3.9a intersect, both Kelley [1990] and our estimate yield the same Nu and thus identical heat fluxes if applied to the same double-diffusive step. For $Ra > Ra_{\text{int}}$, however, $F_{H,\text{Kel}}$ overestimates and for $Ra < Ra_{\text{int}}$ underestimates the true heat fluxes. We suggest to correct heat fluxes by $F_{H,\text{corr}} = F_{H,\text{Kel}} \xi_{\text{corr}}$, where the correction factor $\xi_{\text{corr}}$ accounts for the choice of $\eta$ and is defined by Eq. (3.15) with $Ra_2 = Ra_{\text{int}}$. In Fig. 3.9c, $Ra_{\text{int}}$ is smaller than in Fig 3.9a, because $F_H^*$ depends on $R_{F,\text{Kel}}$ and at $4 < R_\rho < 4.5$, $R_{F,\text{Kel}}$ deviates from $R_{F,\text{mol}}$ by almost factor of 2, which offsets the solid line vertically. The slope $\eta^*$, however, is not affected by the choice of $R_F$ and is an independent estimate for the exponent $\eta$.

### 3.6.3 Comparison to Kelley [1990]

In this section we compare heat flux and density flux ratio estimates of Kelley [1990] to our measurements. In Lake Kivu the average $Ra = O(10^8)$ (Fig. 3.6h) and we thus expect good agreement between $F_{H,\text{Kel}}$ and $F_{H,\text{mol}}$. The comparison is shown in Fig. 3.10a. Here $F_{H,\text{Kel}}$ and $F_{H,\text{mol}}$ are calculated for each interface and arithmetic means (thick black lines) as well as 10th and 90th percentiles (thin grey lines) are shown bin-wise (interval of 0.4, overlap 0.2) as a function of $R_\rho$. For $2 < R_\rho < 4$ the agreement is excellent confirming our expectation. For $R_\rho > 4$, $F_{H,\text{Kel}}$ is 10% to 40% smaller than $F_{H,\text{mol}}$ and for small $R_\rho < 2$ the molecular heat fluxes do not follow the increase of $F_{H,\text{Kel}}$. This is because at such small $R_\rho$, the molecular flux assumption breaks down. The arithmetic means of $F_{H,\text{Kel}}$ and $F_{H,\text{mol}}$ are 0.09 W m$^{-2}$ and 0.10 W m$^{-2}$, respectively.
In Fig. 3.10b we compare $R_{F,mol}$ from Eq. (3.14) to $R_{F,Kel}$ and in Fig. 3.10c, $r$ is shown as a function of $R_p$. For all three panels, the Lake Kivu data set is subdivided into bins of $R_p$ of interval 0.4 with 0.2 overlap and for each bin we calculate the arithmetic mean (black lines) and the 10th and 90th percentiles (grey lines). In panels (a) and (b) the results from the Kelley [1990] parameterization are shown for comparison.

In Fig. 3.10b we compare $R_{F,mol}$ from Eq. (3.14) to $R_{F,Kel}$ and in Fig. 3.10c, $r$ is shown as a function of $R_p$. The bins of $R_p$ are identical to Fig. 3.10a. For $6 < R_p < 10$, $R_{F,mol} \approx R_{F,Kel} \approx 0.15$, which is the value initially found by Turner [1965] for $R_p > 2$, but slightly larger than $R_{F,LS} = \tau^{1/2} \approx 0.10$. For $1 < R_p < 6$, $R_{F,mol}$ is smaller than $R_{F,Kel}$, because we only account for molecular transport through interfaces. Interfacial entrainment, which is included in $R_{F,Kel}$, increases the transport of salt relative to heat and thus leads to a larger $R_F$. This is most evident for $R_p < 2$,
when $R_{F,Kel}$ steeply increases whereas $R_{F,mol}$ decreases. Another interesting feature is the different trends for $4 < R_{p} < 10$. Whereas $R_{F,Kel}$ decreases, $R_{F,mol}$ increases with $R_{p}$ in a similar way as predicted by Newell [1984] and observed in the simulations by Carpenter et al. [2012a]. The increase of $R_{F,mol}$ (Eq. 3.14) with $R_{p}$ is only possible because the decrease of $r$ with $R_{p}$ is very small (Fig. 3.10c). The fit function chosen by Kelley [1990] does not allow for an increase of $R_{F}$ at large $R_{p}$. It was chosen to map the strong change of $R_{F}$ at small $R_{p}$, where most of the experimental data points were located [Fig. 2 in Kelley, 1990]. The observed increase of $R_{F}$ with $R_{p}$ at large $R_{p}$ is thus not in contradiction with the experimental data in Kelley [1990].

### 3.6.4 Implications for Arctic heat fluxes

Vertical heat fluxes are of particular interest in the Arctic Ocean, where warm (and salty) water from the North Atlantic intrudes at a depth of 200 – 400 m [Carmack et al., 1997] with the potential of melting the overlying sea ice [Turner, 2010]. Double diffusive staircases are found at the upper boundary of this intrusion. In Table 3.1, we summarize the staircase properties of four different locations within the Arctic Ocean, provide the literature estimates for $F_{H,Kel}$ and $F_{H,mol}$, compute correction factors $\xi_{corr}$ and finally calculate the corrected heat fluxes $F_{H,corr}$. Even though each of the parameters in Table 3.1 varies by up to two orders of magnitude, we provide average values in order to simplify comparison.

We discuss the Canada Basin (CB) [Timmermans et al., 2008] and the Beaufort Sea (BS) [Padman and Dillon, 1987] separately from the Amundsen Basin (AB) [Sirevaag and Fer, 2012] and the Laptev Sea Slope (LS) [Polyakov et al., 2012] because of their difference in $R_{p}$ and the geographical separation by the Lomonosov Ridge. The staircase parameters and heat fluxes for CB and especially BS are surprisingly similar to Lake Kivu. Correction factors of 0.68 and 1.01 for CB and BS, respectively, result in corrected heat fluxes of $F_{H,corr} = 0.15$ W m$^{-2}$ and 0.06 W m$^{-2}$ that agree with $F_{H,mol}$ within 50 %. Note that Turner [2010] used $F_{H,Kel} = 0.22$ W m$^{-2}$ from CB for estimating the contribution of double-diffusive heat fluxes to the melting of Arctic sea ice. For AB and LS, correction factors are 0.71 and 0.24, respectively, corresponding to $F_{H,corr} = 0.43$ W m$^{-2}$ and 1.95 W m$^{-2}$. Even though the correction reduces $F_{H,Kel}$ significantly, $F_{H,corr}$ for AB and LS is still much larger than $F_{H,corr}$ for CB and BS. Furthermore $F_{H,corr}$ at AB and LS is 9 and 33 times larger than the corresponding estimate of $F_{H,mol}$, respectively. The large difference between $F_{H,mol}$ and $F_{H,corr}$ for AB and LS is not understood. One reason could be that $F_{H,mol}$ underestimates the total flux, because advective transport across interfaces becomes important at $R_{p} < 2$. Another
possibility is that the applied correction is not large enough, because the uncertainty in $\eta$ (Fig. 3.9) increases for small $R_p$. However, exponents of $\eta = -0.65$ and -0.13 are needed for AB and LS, respectively, to reduce $F_{H,\text{Kel}}$ to $F_{H,\text{mol}}$, and such small $\eta$ are not supported by our data. A third possibility is that the earth’s rotation reduces turbulent fluxes in the mixed layers [Kelley, 1987; King et al., 2009, 2012]. This effect is only important for interface thicknesses larger than a certain threshold that inversely depends on the Coriolis parameter. This condition is fulfilled for both LS and AB, but not for CB, BS or Lake Kivu [Carpenter and Timmermans, 2013].

In summary, we found that correcting heat fluxes for the choice of $\eta$ in Eq. (3.9) reduces heat flux estimates in the Arctic by up to a factor of four and levels the extreme variability of heat fluxes measured at different locations in the Arctic ocean.
Table 3.1. Comparison of staircase properties and heat fluxes in the Arctic Ocean and Lake Kivu.

<table>
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<tbody>
<tr>
<td>Lake Kivu</td>
<td>m</td>
<td>110 - 485</td>
<td>200 - 300</td>
<td>320 - 430</td>
<td>200 - 260</td>
<td>160 - 220</td>
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<tr>
<td>Depth range</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>$R_p$</td>
<td>-</td>
<td>2.4 - 5.6</td>
<td>2.0 - 7.0</td>
<td>4.0 - 6.0</td>
<td>2.2 - 3.8</td>
<td>1.2 - 3.0</td>
</tr>
<tr>
<td>$\Delta T$</td>
<td>mK</td>
<td>11</td>
<td>40</td>
<td>10</td>
<td>65</td>
<td>300</td>
</tr>
<tr>
<td>$H_T$</td>
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<td>1.3</td>
<td>15.0</td>
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<tr>
<td>$h_T$</td>
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<td>0.07</td>
<td>0.73</td>
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<td>6.4x10^{-5}</td>
<td>6.0x10^{-5}</td>
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<tr>
<td>$\nu$</td>
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<td>9.1x10^{-7}</td>
<td>1.8x10^{-6}</td>
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<td>1x10^{8}</td>
<td>1x10^{9}</td>
<td>4x10^{12}</td>
</tr>
<tr>
<td>$(Ra/Ra_{int})^{\eta}$</td>
<td>-</td>
<td><strong>0.98</strong></td>
<td><strong>0.68</strong></td>
<td><strong>1.01</strong></td>
<td><strong>0.71</strong></td>
<td><strong>0.24</strong></td>
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<tr>
<td>$F_{H,mol}$</td>
<td>W m^{-2}</td>
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<td>0.20</td>
<td>0.09</td>
<td>0.05</td>
<td>0.06</td>
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<tr>
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<td>W m^{-2}</td>
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<td>0.60</td>
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<td>0.15</td>
<td>0.06</td>
<td>0.43</td>
<td>1.95</td>
</tr>
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</table>

*For all sites, we use $Ra_{int} = 10^8$, $\Delta \eta = (0.2 - 1/3)$, $g = 9.81$ m s$^{-2}$ and $\kappa_T = 1.4x10^{-7}$ m$^2$ s$^{-1}$. Note that $F_{H,Kel}$ for Padman and Dillon [1987] and Timmermans et al. [2008] is based on the parameterization of Marmorino and Caldwell [1976] and not Kelley [1990]. However for $4 < R_p < 8$ both parameterizations are almost identical and both use $\eta = 1/3$. 

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3.7 Conclusion

We have presented the most detailed study of double-diffusive interfaces in a natural system up to date. The 9,401 interfaces used in this study were detected in Lake Kivu between 111 m and 451 m depth with most of the interfaces being located in the gradients between 180 m and 200 m as well as 300 and 330 m depth. Average interface thicknesses were 9 cm and 6 cm for temperature and dissolved substances, respectively, and 0.7 m for the mixed layers, with molecular heat fluxes through interfaces of 0.10 W m$^{-2}$. The smallest observed interface thicknesses are ~1 mm and ~1 cm for dissolved substances and temperature, respectively.

The larger interface thickness of temperature compared to dissolved substances confirms the boundary-layer structure of the interface as assumed by Linden and Shirtcliffe [1978]. The histogram of boundary layer Rayleigh numbers has a long tail at small boundary layer Rayleigh numbers, peaks at O(10$^2$) and continuously decreases between O(10$^2$) and (10$^4$). The long tail confirms the idea of Linden and Shirtcliffe [1978] that the $T$ and DS interfaces periodically grow by molecular diffusion from initially the same thickness. However, the boundary layer break-off does not occur at a single critical boundary layer Rayleigh number.

Heat flux estimates based on the parameterization of Kelley [1990] agreed well with molecular fluxes through interfaces, in particular for $2 < R_p < 4$. However the Kelley [1990] parameterization should only be applied to double-diffusive systems with Rayleigh numbers O(10$^8$), similar to Ra in the laboratory experiments used by Kelley [1990]. For different Rayleigh numbers, the exponent $\eta$ in the scaling $Nu \sim Ra^\eta$ becomes important. We estimated $\eta = 0.20 \pm 0.03$ for density ratios between two and six, which is different from $\eta = 1/3$ as proposed by Turner [1965] and used by Kelley [1990]. We thus suggest to correct heat flux estimates based on the parameterization of Kelley [1990] by multiplication with the factor $\xi_{corr} = (Ra/10^8)^{(\eta-1/3)}$, where Ra is the Rayleigh number of the system of interest and $\eta$ is the true exponent.

We studied the effect of this correction on heat flux estimates in the Arctic Ocean. There, double-diffusive staircases form at the upper boundary of the warm North Atlantic intrusion between 200 m and 500 m depth and the heat flux through these staircases contributes to the melting of the Arctic sea ice [Turner, 2010]. For Arctic staircases, Rayleigh numbers are generally larger than O(10$^8$) and therefore $\xi_{corr} \leq 1$. This leads to up to four times smaller heat fluxes compared to previous estimates based on Kelley [1990].
Acknowledgments:

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4 Direct Numerical Simulations

4.1 Introduction

So far, we used the natural step functions of temperature $T$ and salinity $S$ in Lake Kivu to determine microstructure sensor responses (chapter 2) and tested several theories of double-diffusion by comparing to the Lake Kivu data set (chapter 3). However, profiles of $T$ and $S$ represent only one-dimensional snap-shots of a double-diffusive system and lack information about the horizontal structure and the temporal dynamics. Direct Numerical Simulations (DNS) can provide this information.

Parallel to the field-oriented work at Lake Kivu, Jeffrey Richard Carpenter, Postdoc at Eawag, used DNS to simulate double-diffusive steps similar to those found in Lake Kivu. The resulting two publications are found in the attachment. The first one (A1) studies the stability of the double-diffusive interface by combining linear-stability theory with two-dimensional (2-D) DNS [Carpenter et al., 2012b]. The second one (A2) examines the structure of the double-diffusive interface and the adjacent mixed layers in three-dimensional (3-D) DNS [Carpenter et al., 2012a]. A direct comparison between the DNS and the Lake Kivu measurements is presented in chapter 5 (C5).

In this chapter we provide a general introduction to the equations of motions that are solved by the DNS and summarize our choices on dimensionality, domain size, grid spacing, boundary conditions and initial conditions.

4.2 Governing equations

The two governing equations are the conservation of mass (continuity equation) and the conservation of momentum (Navier-Stokes equation). Several approximations are made to simplify the problem. Those are $(i)$ incompressibility, $(ii)$ linearized equation of state, $(iii)$ no rotation, $(iv)$ Boussinesq approximation.

4.2.1 Conservation of mass

The conservation of mass states that the density changes over time at a certain point are either caused by a divergence of the advective flux or of the diffusive flux.

\[
\frac{\partial \rho}{\partial t} = -\mathbf{\nabla} \cdot (\rho \mathbf{u}) + \kappa \nabla^2 \rho
\]  

(4.1)
Here $\rho$ is the fluid density ($\text{kg m}^{-3}$), $t$ is time ($\text{s}$), $\vec{u}$ ($\text{m s}^{-1}$) is the fluid velocity and $\kappa$ ($\text{m}^2 \text{s}^{-1}$) is the molecular diffusivity (here assuming that the fluid density is entirely determined by one scalar, such as temperature $T$ for example). Using the identity $\tilde{\nabla} (\rho \vec{u}) = \vec{u} \tilde{\nabla} \rho + \rho \tilde{\nabla} \vec{u}$ results in

$$\frac{\partial \rho}{\partial t} = -\vec{u} \tilde{\nabla} \rho - \rho \tilde{\nabla} \vec{u} + \kappa \nabla^2 \rho \quad (4.2)$$

Incompressibility of the fluid is expressed by

$$\tilde{\nabla} \vec{u} = 0 \quad (4.3)$$

Equation (4.3) is already the first of the final set of equations used for the DNS. With Eq. (4.3), Eq. (4.2) reduces to

$$\frac{\partial \rho}{\partial t} = -\vec{u} \tilde{\nabla} \rho + \kappa \nabla^2 \rho \quad (4.4)$$

We further assume a linearized equation of state

$$\rho = \rho_0 + \rho_T + \rho_S \quad (4.5)$$

where $\rho_0$ is the background density (constant in space and time), $\rho_T = -\alpha \rho_0 (T - T_0)$ and $\rho_S = \beta \rho_0 (S - S_0)$ are density fluctuations caused by anomalies of temperature $T$ and salinity $S$ from the background $T_0$ and $S_0$, respectively. Here $\alpha$ ($\text{K}^{-1}$) and $\beta$ ($\%_0^{-1}$) are the thermal expansion coefficient and the haline contraction coefficient, respectively. Inserting Eq. (4.5) in Eq. (4.4) results in two separate equations for $\rho_T$ and $\rho_S$

$$\frac{\partial \rho_T}{\partial t} = -\vec{u} \tilde{\nabla} \rho_T + \kappa_T \nabla^2 \rho_T \quad (4.6a)$$

$$\frac{\partial \rho_S}{\partial t} = -\vec{u} \tilde{\nabla} \rho_S + \kappa_S \nabla^2 \rho_S \quad (4.6b)$$

Because both agents $T$ and $S$ contribute to density but diffuse at different rates, the molecular diffusivity $\kappa$ in Eq. (4.4) was replaced by the diffusivities $\kappa_T$ and $\kappa_S$ of heat and salt, respectively, in Eqs. (4.6a,b). Equations (4.3), (4.5) and (4.6a,b) are four out of the five final equations.

**4.2.2 Conservation of momentum**

This equation states that momentum variations of a fluid at a fixed point are either caused by advection of fluid of different momentum, earth rotation, pressure gradients, gravity or friction.

$$\rho \frac{\partial \vec{u}}{\partial t} = -\rho (\vec{u} \tilde{\nabla}) \vec{u} - 2 \vec{\rho} \vec{\Omega} \times \vec{u} - \tilde{\nabla} p - \rho \vec{g} + \rho \kappa \nabla^2 \vec{u} \quad (4.7)$$
Here, $\Omega$ (s$^{-1}$) is the angular velocity of the earth, $p$ is pressure (kg m$^{-1}$ s$^{-2}$), $g$ (m s$^{-2}$) is gravitational acceleration, and $\nu$ (m$^2$ s$^{-1}$) is kinematic viscosity. The non-linear advection term $-(\vec{u}\vec{V})\vec{u}$ is one of the reasons why Eq. (4.7) can only be solved numerically. We omit rotation and set $-2\Omega \times \vec{u} = 0$, which is justified for Lake Kivu because of its location close to the equator [Carpenter and Timmermans, 2013]. For the Boussinesq approximation we decompose $\rho$ and $p$ into their background states $\rho_0, p_0$ and fluctuations $\rho'$, $p'$, respectively.

$$\rho = \rho_0 + \rho' \quad (4.8)$$

$$p = p_0 + p' \quad (4.9)$$

Taking the gradient of $p$ results in

$$\nabla p = \nabla p_0 + \nabla p' = -\rho_0 g + \nabla p' \quad (4.10)$$

where the hydrostatic relation $\nabla p_0 = -\rho_0 g$ was used in Eq. (4.10). We then substitute Eqs. (4.8, 4.10) into Eq. 4.7 and divide by $\rho_0$.

$$\left(1 + \frac{\rho'}{\rho_0}\right) \frac{\partial \vec{u}}{\partial t} = -\left(1 + \frac{\rho'}{\rho_0}\right) (\vec{u}\vec{V})\vec{u} - \frac{1}{\rho_0} \nabla p' - \frac{\rho'}{\rho_0} \vec{g} + \left(1 + \frac{\rho'}{\rho_0}\right) \nabla^2 \vec{u} \quad (4.11)$$

In the Boussinesq approximation we neglect the term $\rho'/\rho_0$ except where it occurs in combination with $\vec{g}$. This is justified as long as $\rho' \ll \rho_0$, for more details see Spiegel and Veronis [1960]. The final set of equations is given by (4.3), (4.5), (4.6a,b) and (4.11). For the numerical solution method we refer to Winters et al. [2004].

### 4.3 Limitations

Independent of the solution method, numerical simulations always rely on choices of the domain size, grid resolution, dimensions, boundary conditions and initial conditions, which we summarize briefly for the simulations used in A1, A2 and C5 of this thesis.

#### 4.3.1 Grid spacing, dimensionality and domain size

The set of differential equations is solved, in general, for the computational box $0 \leq x \leq L_x$, $0 \leq y \leq L_y$, $0 \leq z \leq L_z$ where $x$, $y$ are the Cartesian coordinates in the horizontal and $z$ in the vertical. Our choices for $(L_x, L_y, L_z)$ vary but non exceeds 1 m for reasons of computational expenses.

In order to fully resolve turbulent motions, the grid spacing $\Delta x$ must be small enough to resolve smallest scales of the slower diffusing scalar $S$, which is described by the Batchelor
length \( L_B = (v^3/\varepsilon)^{1/4}(\tau/\nu)^{1/2} \), where \( \varepsilon \) is the volume-averaged rate of dissipation of kinetic energy, \( \tau = \kappa_S/\kappa_T \) is the diffusivity ratio and \( \text{Pr} = \nu/\kappa_T \) is the Prandtl number. For all our simulations, the condition \( \Delta v/L_B < 2 \) is satisfied, which is expected to be sufficient for our purpose (for a detailed discussion see Smyth and Moum [2000] and Smyth et al. [2001]).

Three-dimensional simulations were chosen in A2, but in A1 and C5 we use the computationally less expensive 2-D simulations. Two-dimensionality is either achieved by making \( L_y \) small compared to \( L_x \) and \( L_z \) (A1) or omitting the third dimension (C5), which requires modification to the original code.

### 4.3.2 Initial conditions

The simulations are initiated by horizontally uniform \( T \) and \( S \) profiles representing interfaces of initial thickness \( h_0 \)

\[
\rho_T(z) = -\frac{\Delta \rho_T}{2} \tanh \left[ \frac{2(z - L_z/2)}{h_0} \right] \tag{4.12a}
\]

\[
\rho_S(z) = \frac{\Delta \rho_S}{2} \tanh \left[ \frac{2(z - L_z/2)}{h_0} \right] \tag{4.12b}
\]

and two adjacent mixed layers. Random noise is added to the vertical velocity field to seed instabilities that develop near the interface [Carpenter et al., 2012b].

### 4.3.3 Boundary conditions:

All simulations have periodic boundary conditions in the horizontal directions; that is,

\[
f(x + L_x, y, z, t) = f(x, y, z, t) = f(x, y + L_y, z, t) \tag{4.13}
\]

where \( f \) represents any field variable of the final set of equations. This means that fluid leaving the computational domain at the right (in the back) is automatically reentering at the left (in the front).

The conditions for the upper and lower boundaries vary for the 3-D and the 2-D simulations. For 3-D simulations, rigid-lid and free-slip boundary conditions are used representing laboratory experiments with insulated boundaries, except that friction is neglected at the vertical boundaries. For 2-D, we use periodic boundary conditions in the vertical except that \( \Delta \rho_T \) and \( -\Delta \rho_S \) are added to \( \rho_T \) and \( \rho_S \) of fluid leaving the domain at the lower and reentering at the upper wall (and vice versa) to ensure continuity of the density steps in the vertical. The repetition
of an individual step represents an infinite staircase and periodic boundary conditions may thus be more representative for natural staircases.

In the following chapter 5 we show, that interface thicknesses and fluxes measured in Lake Kivu are well reproduced by 2-D DNS with periodic boundary conditions on all side walls.
5 Representativeness of Direct Numerical Simulations for double diffusion in natural systems

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5.1 Abstract

Oceanic double-diffusion transforms uniform background gradients of temperature and salinity into “staircases” of homogeneous mixed layers that are separated by high-gradient interfaces. Direct Numerical Simulations (DNS) and microstructure measurements are two independent methods of predicting double-diffusive fluxes. By performing DNS under similar conditions as found in our measurements in Lake Kivu, we are able to compare results from both methods for the first time. We find that (i) the DNS reproduces the measured interface thicknesses of in-situ microstructure profiles, (ii) molecular heat fluxes through interfaces capture the total vertical heat fluxes for density ratios larger than three and (iii) a commonly-used heat flux parameterization underestimates the total fluxes by a factor of 1.3 to 2.2.
5.2 Introduction

The diffusive type of double diffusion occurs in oceans and lakes where both temperature and salinity increase with depth, creating staircase-like structures with nearly homogeneous mixed layers separated by thin high-gradient interfaces [Schmitt, 1994; Kelley et al., 2003; Ruddick and Gargett, 2003]. Quantifying the vertical fluxes through such staircases is important, in particular in the Arctic Ocean, where double-diffusive heat transport contributes to the melting of the overlying ice [Turner, 2010].

With increasing computation power, Direct Numerical Simulations (DNS) are becoming more attractive to study complex fluid behavior such as double diffusion [Noguchi and Niino, 2010a, 2010b; Carpenter et al., 2012a; Flanagan et al., 2013]. However DNS are still limited by the size and dimensions of the computational domain at sufficient grid resolution and rely on choices of the boundary conditions that may not be representative of natural staircases. Given all the sources of variability and the presence of other processes that may be acting to alter fluxes across interfaces (e.g. mean shear as found in CSALT salt finger interfaces [Gregg and Sanford, 1987]), comparing in-situ measurements to DNS is an extremely valuable technique for understanding both the ability of DNS to reproduce the natural dynamics and the signals found in the in-situ measurements.

In this work we compare high resolution microstructure profiles of temperature and conductivity measured in Lake Kivu to two-dimensional DNS (Fig. 5.1). In addition to a qualitative explanation of common interface and mixed layer structures, we compare interface thicknesses and the related molecular fluxes through the interfaces in both systems. The molecular fluxes are then compared to the total vertical fluxes in the DNS and to the commonly applied flux parameterization by Kelley [1990]. Notation and definitions are summarized in Table 5.1.
Table 5.1. Notation and definitions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Description</th>
<th>Calculation method / Values used</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>K$^{-1}$</td>
<td>thermal expansion coefficient</td>
<td>(243 to 278) x 10$^{-6}$, not needed</td>
</tr>
<tr>
<td>$\beta$</td>
<td>kg g$^{-1}$</td>
<td>haline contraction coefficient</td>
<td>(0.89 to 1.02) x 10$^{-3}$ (includes contribution of dissolved gases), not needed</td>
</tr>
<tr>
<td>$\rho_0$</td>
<td>kg m$^{-3}$</td>
<td>reference density</td>
<td>1000 (mean density for below 100 m depth), 997</td>
</tr>
<tr>
<td>$T$</td>
<td>kg m$^{-3}$</td>
<td>density contribution of temperature</td>
<td>$-\rho_0 \alpha$ times in-situ temperature (K), direct</td>
</tr>
<tr>
<td>$S$</td>
<td>kg m$^{-3}$</td>
<td>density contribution of salt (and dissolved gases for Lake Kivu)</td>
<td>$\rho_0 \beta$ times in-situ salinity (g kg$^{-1}$), direct</td>
</tr>
<tr>
<td>$\rho$</td>
<td>kg m$^{-3}$</td>
<td>density</td>
<td>$\rho_0 + T + S$, as Kivu</td>
</tr>
<tr>
<td>$c_p$</td>
<td>J kg$^{-1}$ K$^{-1}$</td>
<td>specific heat capacity of water</td>
<td>4168 to 4177, 4170</td>
</tr>
</tbody>
</table>

**Dimensional control parameters**

| $\Delta T, \Delta S$ | kg m$^{-3}$ | $T$ and $S$ step across interface (Fig. 5.1c) | Difference of the means of $T$ and $S$ in the central 50% of the mixed layers above and below an interface (Fig. 5.2a) | $\Delta T = 12 \times 10^{-4}$ (equiv. to 5 mK) (Fig. 5.2a), $\Delta S = R_\rho \Delta T$ |
| $\kappa_T, \kappa_S$ | m$^2$ s$^{-1}$ | molecular diffusivity of temperature and salt | 1.4 x 10$^{-7}$, 1.43 x 10$^{-9}$, 1.44 x 10$^{-7}$, 1.44 x 10$^{-9}$ |
| $\nu$       | m$^2$ s$^{-1}$ | kinematic viscosity | (8.8 to 9.4) x 10$^{-7}$, 9 x 10$^{-7}$ |
| $H$        | m | layer height | Interface thickness + mean thickness of the adjacent mixed layers (Fig. 5.2b), domain height, 0.33 |

**Dimensionless control parameters**

| $R_\rho$ | - | density ratio $\Delta S/\Delta T$ | Fig. 5.2c, 2, 3, 4, 5, 6 (Fig. 5.2c) |
| Ra        | - | Rayleigh number $g \Delta T H^3/(\rho_0 \nu \kappa_T)$ | Fig. 5.2d, 3.3 x 10$^6$ (Fig. 5.2d) |
| Pr        | - | Prandtl number $\nu/\kappa_T$ | 6.41, 6.25 |
| $\tau$   | - | diffusivity ratio $\kappa_S/\kappa_T$ | 0.01, 0.01 |
5.3 Methods

5.3.1 Lake Kivu data

During two field campaigns to Lake Kivu (East Africa, surface area of 2300 km$^2$, maximum depth of 485 m and volume of 550 km$^3$) [Descy et al., 2012] in 2010 and 2011, we measured 225 microstructure profiles of temperature and conductivity with a Vertical Microstructure Profiler manufactured by Rockland Scientific International, covering a total profiling length of ~55 km [Sommer et al., 2013]. Double diffusive staircases are found below ~100 m depth containing up to 300 interfaces and mixed layers [Newman, 1976; Schmid et al., 2010]. An algorithm was used to extract the $T$ and $S$ properties of 9,401 interfaces and adjacent mixed layers from the temperature and conductivity profiles based on criteria relating small scale gradients to background gradients and requesting approximate linearity in the interface core. For a detailed description of the data set, the evaluation algorithm, the sensor specifications, the density calculation and the method for including dissolved gases in salinity, we refer to Schmid et al. [2010] and Sommer et al. [2013].

5.3.2 DNS

For the DNS we use the code by Winters et al. [2004] to simulate a two-dimensional (2-D) incompressible Boussinesq fluid assuming a linear equation of state (Table 1). The domain size of the simulation is 66 cm (horizontal) x 33 cm (vertical) with an evenly spaced grid of 2048 x 1024 for $R_\rho = 2, 3$ and 1024 x 512 for $R_\rho = 4, 5, 6$ corresponding to a grid spacing of 0.32 mm and 0.64 mm, respectively. At simulation start an interface with two adjacent mixed layers is constructed by horizontally uniform hyperbolic tangent profiles with initial interface thicknesses $h_T = h_S = 3$ cm. Periodic boundary conditions are used on all boundaries except that $\Delta T$ and $\Delta S$ are added/subtracted to $T$ and $S$ of fluid crossing the vertical boundaries to ensure continuity in the vertical (i.e. constructing an infinite staircase). Random noise is added to the vertical velocity field to seed instabilities that develop near the interface [Carpenter et al., 2012b]. For each of the five simulations, we evaluate a time interval of 13 h after a quasi-steady state has been reached. Every 12.5 min, vertical $T$ and $S$ profiles are extracted from the simulated $T/S$ field at horizontal intervals of 1 cm. Each profile is evaluated in the same way as the profiles measured in Lake Kivu.
5.3.3 Comparison

For the direct comparison of interface thicknesses and fluxes for DNS and Lake Kivu we match the parameters \( \Delta T \), \( H \) and \( R \rho \) in both systems. This is done by sorting the Lake Kivu data into bins of \( \Delta T \), \( H \) and \( R \rho \) that correspond to the approximately fixed values of the DNS (Fig. 5.2). The values of \( R \rho \) used in the five simulations span the range observed in Lake Kivu. Due to computational considerations, \( \Delta T \) (5 mK) and \( H \) (0.33 m) are chosen a factor of ~2 smaller than
the average values in Lake Kivu. For $R_\rho = (2, 3, 4, 5, 6)$, the Lake Kivu and DNS bins contain (297, 409, 260, 124, 66) and (4895, 4737, 11798, 18715, 20860) interfaces and mixed layers, respectively. The reason for the varying number of interfaces in the DNS bins is the rejection criteria, which rejects (74, 77, 44, 13, 2) % of the interfaces. For Lake Kivu those percentages are (70, 61, 50, 33, 19), showing that for low $R_\rho$ much more interfaces are rejected than for large $R_\rho$. The elevated percentage at large $R_\rho$ for Lake Kivu is due to electronic noise in the conductivity signal.
5.4 Results

5.4.1 Phenomenological description of DNS and Lake Kivu profiles

We begin with a qualitative description of the $T/S$ structures observed in the DNS and relate these to structures observed in the Lake Kivu staircase. In Fig. 5.1 we show examples of the simulated density fields for $R_p \approx 2$ (at $t = 29 \text{ h}$) and $R_p \approx 6$ (at $t = 61 \text{ h}$). Below each density field, three profiles of $T$ and $S$ are shown (Figs. 5.1c to 5.1h) which are taken along the white vertical lines in 5.1a,b. For each DNS profile a corresponding Lake Kivu profile example is presented (Figs. 5.1i to 5n).

For $R_p \approx 2$, $S$ interfaces are either extremely thin ($h_S = 4 \text{ mm}$ and $2.3 \text{ mm}$ in Figs 5.1d,j, respectively) or they contain very thin mixed regions (Figs. 5.1e,k). Only thin interfaces (Figs. 5.1d,j) that are “undisturbed” are analyzed, whereas the interfaces in Figs. 5.1c,e,i,k are discarded. The DNS suggests that mixed layer fluctuations are signals of distinct plumes (Figs. 5.1c,d,e) rather than turbulence acting on a background gradient as is the case for stratified turbulence [Thorpe, 2007]. A plume usually consists of an $S$-dominated core (yellow color in the lower mixed layer in Fig. 5.1a) driven by a $T$-dominated envelope (Fig. 5.1d at $z \approx 25 \text{ cm}$). Once the $T$ envelope has vanished by diffusion, the $S$ core tends to move back toward the interface while it is advected by mixed layer eddies ($S$ signal in Fig. 5.1c at $z \approx 26 \text{ cm}$).

For $R_p \approx 6$, interfaces are thicker than for $R_p \approx 2$ and they are dominated by a diffusive core (green band in Fig. 5.1b) which contains linear gradients in $T$ and $S$. Plumes do not penetrate into the diffusive core and plume signatures are barely visible in the mixed layers of the $T$ and $S$ profiles.

5.4.2 Comparison of interface thicknesses

We continue by comparing distributions and arithmetic means of interface thicknesses for the DNS and Lake Kivu, which are needed to calculate molecular fluxes through interfaces. The interface thickness of $T$ (and analogously for $S$) is defined by

$$h_T = |\Delta T(dT/dz)^{-1}|$$

(5.1)

where, $dT/dz$ is the vertical gradient $T$ in the central 50% of the interface. Two corrections are applied to $h_T$ to account for the sensor responses and for underestimating the maximum gradient by the linear fit [Sommer et al., 2013].
Distributions of $h_T$ and $h_S$ (Figs. 5.3a,b) for $R_\rho \approx 3$ are in excellent agreement between DNS and Lake Kivu and the bimodal distribution of $h_S$ is successfully reproduced by the DNS.

The $R_\rho \approx 3$ regime can be understood qualitatively as an intermediate regime between small and large $R_\rho$ and the double-peak thus as a combination of the interface thicknesses shown in Fig. 5.1. Extremely thin interfaces are seen in Figs. 5.1d,j forming the left peak. Intermediately-thick interfaces are disturbed as in Figs. 5.1e,k. Such interfaces are rejected by the algorithm and are thus missing in Figs. 5.3a,b, creating the gap between the two peaks. Thick interfaces are as in Figs. 5.1f,g,h,l,m,n and form the right peak. For $R_\rho \approx 3$, however, such thick interfaces are only found in profiles taken close to or within plumes.

In double diffusion laboratory experiments of the salt-sugar type, Stamp et al. [1998] observed small mixed regions within the interface, which traveled along the interface. Such a traveling behavior could not be observed in the DNS, possibly because the interface is continuously under deformation by close-by plumes. It is well possible that interfacial waves would be observed if the horizontal domain size was increased.

The arithmetic means of $h_T$ in the DNS and Lake Kivu (Fig. 5.3c) agree well within the confidence intervals of the Lake Kivu estimates, except at $R_\rho = 2$, where the 2-D limitation of the DNS is thought to be important [Flanagan et al., 2013]. The means of $h_S$ are almost identical at $R_\rho = 3$ but at $R_\rho = 2$ the 2-D limitation might again cause the observed discrepancy. At large $R_\rho$, $h_S$ in Lake Kivu is ~20% larger than in the DNS, but the reason for this is not yet understood.

### 5.4.3 Comparison of heat and salt fluxes and density flux ratios

We use the interface thicknesses of the previous section to calculate molecular fluxes through interfaces, which we then compare to the total vertical fluxes in the DNS and to the flux parameterization by Kelley [1990]. The three different methods used to calculate heat fluxes $F_H$ (W m$^{-2}$), S fluxes $F_S$ (in density units of kg m$^{-2}$ s$^{-1}$) and density flux ratios $R_F = (c_p F_S)/(\alpha F_H)$ (-) are introduced in the following.

(i) Molecular flux through the interface: By definition of $h_T$ and $h_S$

$$F_{H,\text{mol}} = \frac{c_p}{\alpha} \kappa_T \frac{\Delta T}{h_T} \quad \text{(W m}^{-2}\text{)} \quad \text{(5.2a)}$$

$$F_{S,\text{mol}} = \kappa_S \frac{\Delta S}{h_S} \quad \text{(kg m}^{-2}\text{ s}^{-1}) \quad \text{(5.2b)}$$
(ii) Total vertical fluxes (only applicable for the DNS) given by the molecular transport across the central isotherm \( \sigma \) satisfying \( T = 0 \) (for details see Winters and D’Asaro [1996], Carpenter et al., [2012a], Carpenter and Timmermans [2013]):

\[
F_{H,\text{tot}} = \frac{c_p}{\alpha A} \int_\sigma \kappa_T |\nabla T| d\sigma \quad \text{(W m}^{-2})
\]  

Fig. 5.3. Comparison of \( T \) and \( S \) interface thicknesses for DNS and Lake Kivu observations. In (a,b) the probability density functions (pdf) labeled “Kivu (\( R_\rho \approx 3 \))” (n = 409) and “DNS (\( R_\rho \approx 3 \))” (n = 4734) correspond to the sub-data set with \( R_\rho \approx 3 \). For completeness the entire Kivu data set (labeled “Kivu,all”, n = 9,401) is shown. Note the logarithmic scales in (a,b). (c) Arithmetic means of \( h_T \) and \( h_S \) as a function of \( R_\rho \) with shadings representing bootstrapped 95% confidence intervals of the Lake Kivu data set. For DNS, the confidence intervals are thinner and close to the width of the dashed lines (not shown).
where $A$ is the plane cross-sectional area (definition of $F_{S,\text{tot}}$ analogously). If $\sigma$ is a flat isotherm then $F_{H,\text{tot}}$ is identical to horizontally averaged estimates of $F_{H,\text{mol}}$. For $R_\rho \approx 2$ and in particular for $S$, interfacial fluid was entrained into the mixed layers forming additional isothermal “islands” in the mixed layers. In that case $F_{H,\text{tot}}$ was calculated by the sum of the integrals. We compared $F_{H,\text{tot}}$ to the advective flux through the mixed layer calculated by $F_{H,\text{adv}} = -c_p/\alpha <wT>_{A}$ where $w$ is the vertical velocity, and $<>$ indicates a spatial average over a plane area, $A$, that is taken in the center of the mixed layer. Both methods agree within 2% and 15% for $T$ and $S$, respectively. We found that $F_{H,\text{adv}}$ is much more variable than $F_{H,\text{tot}}$ and we therefore use $F_{H,\text{tot}}$ to estimate the total vertical fluxes.

(iii) Fluxes calculated using the parameterization of Kelley [1990], based on laboratory data, dimensional analysis and assuming that $F_H$ is independent of $H$: 

Fig. 5.4. Comparison of (a) heat fluxes $F_H$ and (b) density flux ratios $R_F$ for DNS, Lake Kivu observations and the parameterizations of Kelley [1990]. The subscripts “mol” and “tot” denote molecular fluxes through interfaces and the total vertical fluxes, respectively. See text for details. The grey shadings visually group the Lake Kivu and the DNS estimates.
\[ F_{H,\text{Kel}} = 0.0032 \exp \left( \frac{4.8}{R_{p}^{0.72}} \right) c_{p} \rho_{0} \left( \frac{\kappa^{2} g \alpha}{\nu} \right)^{1/3} \left( \frac{\Delta T}{\rho_{0} \alpha} \right)^{4/3} \text{ (W m}^{-2} \right) \]  

(5.4a)

\[ R_{F,\text{Kel}}(R_{p}) = \frac{R_{p} + 1.4(R_{p} - 1)^{3/2}}{1 + 14(R_{p} - 1)^{3/2}} \text{ (-)} \]  

(5.4b)

In Fig. 5.4a,b we show arithmetic means of \( F_{H} \) and \( R_{F} \) as function of \( R_{p} \), calculated from methods (i) and (ii) (grouped by the gray shading) and additionally the Kelley [1990] estimate of method (iii).

In the DNS, \( F_{H,\text{mol}} \) underestimates \( F_{H,\text{tot}} \) by less than 10\% for \( R_{p} \geq 3 \), in agreement with the three-dimensional (3-D) simulations of Carpenter et al. [2012a]. This means that for \( R_{p} \geq 3 \) the total fluxes are well represented by molecular fluxes through the interfaces. For \( R_{p} < 3 \), \( F_{H,\text{mol}} \) strongly depends on the rejection criterion for disturbed interfaces, which can lead to overestimates (as here, by 29\%) as well as underestimates (without rejecting, 20\%) of \( F_{H,\text{tot}} \). We note that Flanagan et al. [2013] showed that at \( R_{p} = 2 \), 2-D simulations result in a factor of 1.5 smaller heat fluxes than the corresponding 3-D simulations. This questions, in general, the validity of the 2-D DNS in accurately capturing fluxes at small \( R_{p} \). For \( R_{p} \geq 3 \), however, 3-D fluxes were found to agree well with the 2-D simulations. Molecular heat fluxes through interfaces in Lake Kivu agree within 24\% and 38\% to \( F_{H,\text{tot}} \) and \( F_{H,\text{mol}} \) of the DNS, respectively, for the entire range of \( R_{p} \).

The Kelley [1990] parameterization can be seen to underestimate \( F_{H,\text{tot}} \) by a factor of 1.3 to 2.2. Sommer et al. [2013] suggest a correction factor for the Kelley [1990] estimates based on a different choice of the exponent in the scaling of Nusselt number \( Nu \) to \( Ra \), where \( Nu \) is \( F_{H} \) divided by the diffusive heat flux \( c_{p} \kappa T \Delta T / \alpha H \) (W m\(^{-2} \)). The suggested correction factor is \( (Ra/Ra_{\text{int}})^{0.2 - 1/3} = 1.6 \) with \( Ra = 3.3 \times 10^{6} \) and \( Ra_{\text{int}} = 10^{8} \) being the Rayleigh number of the DNS and a typical Rayleigh number of laboratory experiments, respectively. A correction factor of 1.6 compensates for most of the observed difference and thus supports the scaling suggested by Sommer et al. [2013].

The density flux ratio \( R_{F} \) agrees well between all estimates for large \( R_{p} \) and approaches \( R_{F} = 0.15 \) at \( R_{p} \approx 6 \), which is the constant value found in the first double diffusion experiments by Turner [1965] for \( 2 < R_{p} < 7 \). At small \( R_{p} \), however, the methods (i) to (iii) deviate from each other and do not follow the increase of \( R_{F,\text{Kel}} \) at small \( R_{p} \) usually explained by increasingly turbulent interfaces. However, laboratory data [Fig. 2 in Kelley, 1990] show an extremely sharp
transition between approximately constant $R_F$ at large $R_\rho$ and the rapid increase for $1 < R_\rho < 2$. This transition is not captured accurately by the fit function and as a result $R_{F,Kel}$ overestimates laboratory data (as well as our measurements) by ~25% at $R_\rho \approx 2$. 
5.5 Conclusions

The diffusive-type of double diffusion was studied by comparing Direct Numerical Simulations (DNS) to microstructure profiles from Lake Kivu. We showed that two-dimensional DNS is a valuable tool for interpreting microstructure signals measured in natural environments and that the interface thicknesses measured in Lake Kivu are successfully reproduced by DNS. For the DNS we found that molecular heat fluxes through interfaces capture the total fluxes for \( R_p \geq 3 \) within 10% and that the DNS heat flux estimates agree well with the Lake Kivu estimate. This suggests that in Lake Kivu double-diffusion is the main contributor to the vertical “diffusive” flux (which excludes upwelling) and external turbulence by shear or internal wave breaking is of minor effect. In both the DNS and Lake Kivu, heat fluxes were found larger than predicted by the parameterization of Kelley [1990]. Applying the correction factor suggested by Sommer et al. [2013], which accounts for a different exponent in the Rayleigh/Nusselt number scaling, compensates for most of the difference.

The results are promising and motivate further comparison studies including a quantitative analysis of the mixed layer structure for variable Rayleigh numbers and domain sizes. Such studies might answer the question of whether turbulent flux methods [Osborn and Cox, 1972; Osborn, 1980] can be used as independent estimates for vertical fluxes in addition to molecular fluxes through interfaces and flux parameterizations.

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6 Conclusion

Double diffusion in Lake Kivu has been studied using in-situ microstructure profiles of temperature and conductivity. During two field campaigns in 2010 and 2011, 225 profiles were collected in the Rwandese part of Lake Kivu with a total profiling length of ~55 km. The characteristics of 9,401 interfaces and adjacent mixed layers have been evaluated and compared to existing theories and laboratory experiments (chapters 2 and 3). Direct Numerical Simulations (DNS) were introduced to resolve the temporal dynamics of double-diffusive convection in two and three dimensions (chapter 4, appendices I and II) and the results of the DNS have been validated by the Lake Kivu measurements (chapter 5). The major findings of this dissertation are as follows:

(i) Double-diffusive staircases can be used to determine microstructure sensor responses by measuring the thickness of double-diffusive interfaces at different profiling speeds. The SBE-7 conductivity sensor was shown to be extremely, but not “infinitely” fast, as previously assumed. The derived time constants of the FP07 temperature and SBE-7 conductivity sensors are 10 ms and 2.2 ms, respectively, assuming double-pole frequency responses. The sensor response corrections were found to be important for estimating molecular fluxes through thin double-diffusive interfaces (chapter 2).

(ii) Temperature interfaces of double-diffusive staircases are usually thicker than salinity interfaces resulting in boundary layers adjacent to the interface. The detachment of those boundary layers from the interface is a time-dependent process which is influenced by the adjacent mixed layer motions and thus cannot be predicted by linear stability analysis. The amount of buoyancy stored in the boundary layers was quantified using a critical boundary layer Rayleigh number which, on average, was found $O(10^2)$ with maximum values of $O(10^4)$ in both, the Lake Kivu measurements and the DNS. For simplified models which assume detachment at a critical boundary layer Rayleigh number, a value of $O(10^3)$ is a reasonable choice (chapter 3). However future models should also incorporate the motions within the mixed layers. The DNS showed that mean horizontal velocity is close zero in the mixed layer center and increases toward the boundary layers. A functional approximation of this increase was used to predict the scaling of the ratio of the interface thicknesses with the ratio of the molecular diffusivities ($h_T/h_S \sim (\kappa_S/\kappa_T)^{1/5}$) (appendix I).
(iii) Heat flux parameterizations, which assume an exponent of 1/3 in the scaling Rayleigh to Nusselt number (Ra ~ Nu^{1/3}), should be corrected, because both, Direct Numerical Simulations and the Lake Kivu data provide strong evidence for a smaller exponent of ~0.2. Estimating the heat flux through double-diffusive staircases in the Arctic is of particular interest, because of its contribution to the melting of the overlying ice. Our suggested correction reduces previous heat flux estimates for the Arctic Ocean and at the same time decreases the variation found in those estimates (chapters 3 and 5).

(iv) Fluxes through the core of double-diffusive interfaces depend on the density ratio $R_p$. For $R_p > 3$, molecular fluxes through interfaces were shown to agree with the total fluxes within 10%. For $R_p \leq 3$ interfaces are affected by the adjacent mixed layer motions resulting in distorted interfaces, small mixed regions within the interface and extremely sharp interfaces. Density flux ratios were observed in the range of 0.09 to 0.2 for $2 < R_p < 8$ in both, the Lake Kivu measurements and the DNS. This finding agrees with previous laboratory experiments. However, we found strong evidence that the flux ratio increases with $R_p$ when $R_p$ exceeds approximately four (chapters 2, 5 and appendix II). This has been predicted by Newell [1984], but disagrees with the most commonly used parameterization of Kelley [1990].

(v) Two-dimensional DNS is a promising way to study double diffusion. Interface thicknesses and vertical heat fluxes are accurately reproduced by the DNS (chapter 5).

(vi) Mixed layer fluctuations were identified as signatures of distinct plumes rather than isotropic, homogenous turbulence acting on a background gradient. The validity of turbulent flux methods in the mixed layers is thus questionable and more studies are needed to determine the conditions for their applicability (chapter 5).
7 Outlook

In this thesis I have extensively explored the vertical structure of double-diffusive staircases with a focus on double-diffusive interfaces, which are important for estimating vertical fluxes. For the future I see three major challenges: (i) The resolution of the mixed layer structure for estimating turbulent fluxes, (ii) understanding the staircase dynamics at different time scales and (iii) understanding the interaction of double-diffusion and the water body. I will outline the major ideas and the restrictions in the following.

7.1 Mixed layer structure

Molecular fluxes through interfaces capture only the total fluxes for density ratios \( R_\rho \geq 3 \) (chapter 5). For smaller \( R_\rho \), vertical fluxes can be obtained from the microstructure in the mixed layers [Osborn and Cox, 1972; Osborn, 1980]. Those methods assume homogenous, isotropic and steady turbulence. In our comparison study of DNS and in-situ measurements (chapter 5), we found that mixed layer structures are dominated by distinct plumes rather than turbulence acting on a background stratification. The criteria of steadiness, isotropy and homogeneity are thus questionable. For systems with larger buoyancy fluxes [Sánchez and Roget, 2007; Polyakov et al., 2012], these assumptions might be justified, but a quantitative study is still missing. I recommend a combined approach of Direct Numerical Simulations (DNS) and in-situ measurements similar as described in chapter 5.

For the DNS, preliminary analysis suggests that the horizontal domain size has an effect on the mixed layer structure and should thus be varied. With increasing computation power, the approximations used in the DNS (chapter 4) should continuously approach more realistic conditions. This includes extending the vertical domain size in addition to the horizontal one, switching from periodic to rigid-lid boundary conditions and performing simulations in three instead of two dimensions.

The in-situ measurements face a number of challenges. Turbulent flux methods rely on the resolution of the mixed layer fluctuations of temperature \( T \), salinity \( S \) and velocity and on accurate estimates of the mixed layer gradients of \( T \) and \( S \). Flux estimates are extremely sensitive to the mixed layer gradients, because they are usually close to zero and appear in the dominator of the flux equations.
**Fluctuations:** In our measurements only the $T$ fluctuations could be resolved. For conductivity and shear the signal was dominated by noise and for those sensors the signal-to-noise ratio should be increased in the future to retrieve turbulence information.

**Horizontal measurements:** The horizontal microstructure of the mixed layer is essential for verifying the isotropy and homogeneity assumption for turbulent flux methods, but has not been studied so far. Information about the horizontal structure could potentially be obtained from autonomous underwater vehicles (AUVs) that follow individual mixed layers and take measurements along their path.

**Vertical mixed layer gradients:** Whereas the conductivity gradients in the mixed layers were measured accurately in this work, the $T$ microstructure sensors often measured unrealistic inverse gradients (temperature decreasing with depth). This is most likely caused by a temperature-dependent component of the internal electronics that is responsible for the amplification of the signal derivative [Mudge and Lueck, 1994]. In Powell Lake ($T$ between 4 °C and 9 °C) this effect was found larger than in Lake Kivu ($T$ between 23 °C and 26 °C), because the instrument was calibrated at room temperature. However, for accurately measuring the mixed layer gradients in the future, the responsible component must be replaced by a less temperature-dependent component.

### 7.2 Staircase dynamics

**In-situ** measurements of staircase dynamics are extremely challenging. So far measurements of staircase dynamics have been either based on closely-spaced thermistor chains [Timmermans et al., 2007] or moored vertical profilers [Polyakov et al., 2012] deployed in the staircase region. In this approach, however, changes in the staircase structures over time cannot be separated from spatial heterogeneities that are advected across the thermistor chain by currents. In Lake Kivu horizontal currents are expected to be $< 1$ cm s$^{-1}$, but even at such small flows, a distinction is not possible because layer merging and splitting occurs over time scales of weeks. In the future, acoustic detection techniques might be used to study staircase dynamics. They detect density changes in the water column and provide instantaneous two-dimensional snap-shots of the double-diffusive layering. A time series of such snap-shots would be the ideal tool to study staircase dynamics. Unfortunately, the current detection limit inhibits the resolution of the small density jumps across double-diffusive interfaces [Ross and Lavery, 2010]. Considering the limitations of the in-situ observations, DNS offers an alternative for studying staircase dynamics,
but only if computational restrictions are overcome and domain sizes in two or preferably three dimensions are increases sufficiently.

### 7.3 Interaction between the water body and double-diffusion

Double-diffusion is often considered a phenomenon that is “riding” passively on the background gradients of $T$ and $S$. Rarely is questioned whether double-diffusion is able to actively change the background structure of a water body, horizontally as well as vertically. Observations in Lake Powell motivate this idea. There, double diffusive staircases are embedded in a larger-scale step structure whose origin is unknown (Fig. 7.1). Is it possible that double diffusion plays a role in the formation of those large-scale structures? If yes, this would also be important for Lake Kivu, where the background gradients of $T$ and $S$ are assumed to be created by the discharge of sub-aquatic springs only. If double-diffusion played a role in creating the background gradients, then the discharge rates of the sub-aquatic sources estimated by Schmid et al. [2005] might be questionable.

A different large-scale phenomenon that might be affected by double diffusion is that of internal waves. Internal waves are periodic oscillations in stratified water, usually induced by wind stress on the water body. The strong variation of the density within double-diffusive staircases is an interesting scenario for studying internal wave behavior. It is not clear whether internal waves are reflected at the double-diffusive interfaces or whether they penetrate into the staircase region causing stretching and squeezing of the mixed layers. It is also not understood where the internal wave energy is dissipated in a double-diffusive system and whether internal waves increase the vertical fluxes through the staircases. From preliminary analysis of thermistor data in Lake Kivu we expect similar dissipation rates of turbulent kinetic energy from internal waves as well as double diffusion and both are close to the detection limit of microstructure sensors. Distinguishing between turbulence caused by double diffusion and internal waves will thus be challenging. For mapping internal waves in a water body, acoustic detection techniques would again be the favorable technique, but as long as technology is limited, a network of thermistor chains may be used to measure internal wave amplitudes simultaneously at discrete locations.
Next steps

During the next year, we will focus on the transformation of staircases, horizontal structures and interaction with internal waves based on available vertical profiles and data from moored thermistors and current meters.

The following studies will benefit from an extended data set that includes measurements from Powell Lake (Canada, British Columbia, 19 – 21 June, 2013) and an additional campaign to Lake Kivu, which will also include the Congolese part of the lake (in November/December
Four publications are planned, of which two are in collaboration with the University of British Columbia (UBC), Canada.

In the following we briefly introduce Powell Lake and outline the research questions of the planned manuscripts (M1 to M4), which focus on the description of double-diffusion in Powell Lake (M1), the lateral structure of double-diffusion in Powell Lake and Lake Kivu (M2), the interaction of internal waves and double-diffusion (M3) and a synthesis on double-diffusion in Lake Kivu (M4).

### 7.4.1 Powell Lake

Powell Lake is an ex-fjord (max. depth 360 m) on the south-west coast of British Columbia that became isolated from the sea 10,000 – 13,000 years ago due to the uplift of the bedrock sill after the last glaciation. It consists of six basins (Fig. 7.2), of which only the South and East Basins still contain sea water in the deep [Williams et al., 1961; Sanderson et al., 1986]. The salty water is warmer than the overlying fresh water because of geothermal heating, creating conditions favorable for double-diffusion of the diffusive type. Vertical profiles of temperature and salinity in the South Basin are shown in Fig. 7.1a with a close-up of the staircase structure in Fig 7.1c. Lake Kivu profiles are also presented for comparison (Figs. 7.1b,d). In contrast to Lake Kivu, where double-diffusive steps are distributed over almost the entire water column, the steps in Powell Lake are only found below 294 m and are most prominent between 324 m and maximum depth (~360 m).

A major advantage of Powell Lake is the availability of an independent estimate of the vertical heat flux through the double-diffusive staircase. This heat flux is expected to be $27 \pm 8$ mW m$^{-2}$, given by the sediment heat flux [Hyndman, 1976] and the molecular flux through the gradient between 310 m and 323 m [Scheifele, 2013]. In Lake Kivu, the discharge of subaqueous springs at various depths cause the heat flux to be vertically variable over large vertical scales and thus difficult to estimate [Schmid et al., 2005]. The gradients at 180, 250, 315 and 365 m in Lake Kivu (Fig. 7.1b) are a consequence of those springs. In Powell Lake, similar gradient structures are observed at 284, 293 and 300 m (Fig. 7.1a), but their origin is a mystery, because no subaqueous springs have been discovered so far in Powell Lake.
We plan two publications that involve the Powell Lake data set. In the first one, we provide a detailed description of the double-diffusive structures in Powell Lake using two independent evaluation methods (M1). In the second one we compare Powell Lake to Lake Kivu with a focus on the lateral structure of the double-diffusive staircases (M2).

7.4.2 M1. Double-diffusion in Powell Lake

The data set comprises 39 high resolution CTD profiles of temperature and conductivity in the South Basin (UBC). We contribute additional 42 microstructure profiles with an approximately ten times finer vertical resolution than the CTD casts.

By measuring double-diffusion in the same system with two independent instruments and different evaluation methods, we are able to study the effect of the methodology on the statistics
of staircase parameters and on heat flux estimates. The known steady-state heat flux will serve to validate the different methods.

7.4.3 M2: Lateral structure of double-diffusion in Lake Kivu and Powell Lake

Lake Kivu and Powell Lake water bodies are very different in terms of geographical location, evolution, size, temperatures and salinities. Furthermore, the vertical heat flux at Powell Lake (~27 mW m$^{-2}$) is on average about four time less than in Lake Kivu (~100 mW m$^{-2}$). Despite those differences, the double-diffusive structures in both systems are surprisingly similar with average layer thicknesses (mixed layer plus interface) of ~1 m (Figs. 7.1c,d) and laterally coherent staircases over several kilometers.

In this publication we will compare the double-diffusive structures in the two systems Lake Kivu and Powell Lake (M1, chapter 3). The emphasis, however, will be on the lateral structure of double-diffusive staircases. In both systems the lateral density ratio of temperature and salinity along coherent mixed layers is surprisingly close to the vertical density flux ratio. Examining this relationship will be one goal of this comparison. The starting point will be the theory of McDougall [1991], who assumes that the lateral advective fluxes along mixed layers are balanced by the vertical divergences of the fluxes.
7.4.4 M3: Interaction of internal waves and double-diffusion

Internal waves are periodic oscillations in a stratified water body. In this publication we will use those oscillations to study the evolution of double-diffusive staircases and the effect of internal waves on the presence of double-diffusive staircases.

By deploying closely-spaced thermistor chains within a double-diffusive staircase, the vertical oscillations of internal waves are used to examine staircase dynamics such as layer merging and splitting. An exemplary time series of 24 thermistors is shown in Fig. 7.3.

From the same data set, internal wave amplitudes (and thus their energy) can be estimated from the observed temperature variations and the vertical temperature gradients. Internal wave energy is usually dissipated at the boundaries [Wüest and Lorke, 2003], where we also observe the double-diffusive structures to vanish. Using energy arguments we plan to predict the distance from the shore, where double-diffusive staircases are destroyed by turbulence caused by internal waves.

Fig. 7.3. A five days thermistor time series of 24 thermistors deployed in Lake Kivu between 264.5 and 275.5 m depth with a vertical spacing of 0.5 m. The horizontal lines (created by the superposition of various thermistor signals) correspond to mixed layers with nearly constant temperature. The differences between those lines represent temperature steps across interfaces. Between 1 May and 2 May 2010 and 24.94 °C and 24.95 °C (right upper corner), three mixed layer evolve into about five layers.
wave breaking.

7.4.5 M4: The role of double diffusion for Lake Kivu

The goal of this study is to understand the feedback mechanisms between double diffusion and the Lake Kivu water body.

We will summarize and link the previous studies on double diffusion, which discuss the vertical and horizontal structure of double-diffusive staircases [Schmid et al., 2010, chapter 3], vertical and horizontal fluxes (chapter 3, M2) as well as staircase transformation and the influence of internal waves (M3). The temporal variation of all aspects will play a major role. Measurements are available from 2002 [Lorke et al., 2004, background profiles only], 2004 [Schmid et al., 2010, temperature microstructure only], 2010, 2011 and 2014.

One specific research question will be: Is double diffusion “riding” passively on the vertical background gradients or does it actively modify the stratification? If the second one was true, then double diffusion could possibly explain the mysterious large-scale gradients in Powell Lake (Fig. 7.1a)

7.5 Concluding remark

More than four years of studying double diffusion and evaluating staircase structures seems a long time. I feel, however, that only now the individual mosaics are starting to form a coherent picture. Including DNS in the analysis was a major step in interpreting measured profiles. Another important step will be the comparison of two double-diffusive systems – Lake Kivu and Powell Lake - with different geothermal forcing. I am confident that in the close future, we will have a better understanding of the feedback mechanisms between double-diffusion and the vertical and horizontal large-scale structure of the lake. Extrapolating those findings to much more complex and unexplored environments such as the ocean or even stars will be the ultimate challenge
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Appendix I. Stability of a double-diffusive interface in the diffusive convection regime

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Stability of a Double-Diffusive Interface in the Diffusive Convection Regime

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ABSTRACT

In this paper, the authors explore the conditions under which a double-diffusive interface may become unstable. Focus is placed on the case of a cold, freshwater layer above a warm, salty layer [i.e., the diffusive convection (DC) regime]. The “diffusive interface” between these layers will develop gravitationally unstable boundary layers due to the more rapid diffusion of heat (the destabilizing component) relative to salt. Previous studies have assumed that a purely convective-type instability of these boundary layers is what drives convection in this system and that this may be parameterized by a boundary layer Rayleigh number. The authors test this theory by conducting both a linear stability analysis and direct numerical simulations of a diffusive interface. Their linear stability analysis reveals that the transition to instability always occurs as an oscillating diffusive convection mode and at boundary layer Rayleigh numbers much smaller than previously thought. However, these findings are based on making a quasi-steady assumption for the growth of the interfaces by molecular diffusion. When diffusing interfaces are modeled (using direct numerical simulations), the authors observe that the time dependence is significant in determining the instability of the boundary layers and that the breakdown is due to a purely convective-type instability. Their findings therefore demonstrate that the relevant instability in a DC staircase is purely convective.

1. Introduction

A fundamental result in the study of ocean mixing is that certain configurations of temperature $T$ and salinity $S$ are unstable to small perturbations, despite the fact that the water column is gravitationally stable. This instability is due to the differing rates of diffusion of $T$ and $S$, and has come to be known as double-diffusive (DD) instability. The first stability analysis to demonstrate the basic mechanism of DD was performed by Stern (1960) using linear profiles of $T$ and $S$, bounded above and below (see Fig. 1a, where $T$ and $S$ are plotted in density units). This analysis was subsequently extended by Veronis (1965), Nield (1967), and Baines and Gill (1969), keeping the same linear profiles. These studies found that unstable motions may develop from small perturbations of the $T$–$S$ profiles, as long as at least one component is in a gravitationally unstable configuration, thus providing the energy source required to drive the instability. Two different cases exist depending on whether $T$ (the faster diffusing component) or $S$ is destabilizing: (i) the salt-finger case where warm, salty water overlies cool, fresh water or (ii) the diffusive convection (DC) case with cool, fresh water over warm, salty water (Fig. 1).

Conditions favoring DD are found over vast areas of the oceans (You 2002; Kelley et al. 2003), as well as in lakes (Hoare 1966; Schmid et al. 2004; Sánchez and Roget 2007; Boehrner et al. 2009; Schmid et al. 2010), and are often accompanied by a thermohaline staircase structure in the $T$ and $S$ fields. These staircases consist of a sequence of sharp, high-gradient interfaces of $T$ and $S$ surrounded by nearly homogeneous mixed layers. In this study, we shall focus on the stability properties of the “diffusive interface”: that is, with cool, fresh water...
overlying warm, salty water, as shown in Fig. 1b (for a recent examination of the salt-finger interface, see Smyth and Kimura 2007). We show that the presence of the staircase considerably modifies the linear stability properties of the water column from the linear representation. Whereas the stability analysis of the linear $T$--$S$ profiles has been crucial in our understanding of the basic mechanism of instability, and recently in the process of staircase formation (Noguchi and Niino 2010), the stability analysis of the diffusive interface constitutes an important step in understanding the processes governing staircase evolution and maintenance. To our knowledge, the linear stability properties of the diffusive interface have not been studied previously.

Despite the clear mechanism of instability that has developed from analysis of the linear profiles, which consists of an exponentially growing oscillation of the water column, a different mechanism is often invoked for assessing the stability of a diffusive interface (Linden and Shirtcliffe 1978; Newell 1984; Padman and Dillon 1987, 1989; Worster 2004). In this case, the basic instability mechanism is thought to result from the formation of gravitationally unstable layers on either side of the interface (Fig. 1b). Because the $T$ interface diffuses more rapidly than the $S$ interface, molecular diffusion will tend to produce a relatively thicker $T$ interface (i.e., $h_T > h_S$; Fig. 1b). Because the $T$ profile is gravitationally unstable, this leads to a density profile that exhibits regions of gravitationally unstable fluid, which we will refer to as the diffusive boundary layer. It is the convective-type (nonoscillatory) instability of this boundary layer that is thought to be responsible for the maintenance of turbulence and enhanced mixing that occurs within the mixed layers of a thermohaline staircase. In keeping with the purely convective-type breakdown of the boundary layer, it has been assumed that a critical Rayleigh number that is characteristic of the boundary layer, of the order of $10^3$, must be exceeded for the boundary layers to break away from the interface (Linden and Shirtcliffe 1978).

The stability properties of the diffusive interface, as opposed to the linear profiles, are fundamental to understanding the enhanced fluxes of heat and salt present in thermohaline staircases. The microstructure profiles of $T$ and $S$ taken in the thermohaline staircase of Lake Kivu by T. Sommer et al. (2012, unpublished manuscript) clearly illustrate the presence of diffusive boundary layers (an example is shown in Fig. 2). The present study is largely motivated by these observations and the need to provide a more relevant theoretical understanding of the conditions limiting the growth of the boundary layer. The results of this study provide a basis for developing simple phenomenological models for DC (Linden and Shirtcliffe 1978; Newell 1984; Fernando 1989; Kelley 1990; Worster 2004), as well as in the interpretation of laboratory (Shirtcliffe 1973; Marmorino and Caldwell 1976; Newell 1984; Fernando 1989) and field measurements of the diffusive interface and its stability (Padman and Dillon 1987, 1989; Sánchez and Roget 2007; T. Sommer et al. 2012, unpublished manuscript).

After formulating the basic linear stability problem and its solution in section 2, we present the results of the stability analysis (section 3). These results shed light on the assumption of a purely convective-type instability of the boundary layer. In particular, we find that the first mode to become unstable is oscillatory and is more akin to the DC modes found in linear gradients than to a
purely convective mode. However, the assumption of steady \( T \) and \( S \) profiles that is used in the linear analysis is then tested in section 4 using direct numerical simulations (DNS) of the interface breakdown. The results of the DNS show that time-dependent effects are important for the type of unstable mode that develops (i.e., DC or convective), and the conditions under which the nonlinear breakdown of the interface takes place can exceed the linear predictions. By accounting for this diffusive growth of the interface in time, we propose that the dominant mode of instability for the diffusive interface is in fact of the convective type and is concentrated in the boundary layers. In section 5, we examine the applicability of a critical boundary layer Rayleigh number to describe the onset of instability and breakdown. Conclusions are stated in the final section.

2. Formulation and solution of the linear stability problem

a. Formulation

In this section, we derive the equations that govern the evolution of small (linear) perturbations to the background profiles (indicated with an overbar) of temperature \( \overline{T}(z) \) and salinity \( \overline{S}(z) \). We choose to represent \( T \) and \( S \) in density units so that the resulting density can be approximated by the following linear equation of state:

\[
\rho = \rho_0 + T + S, \tag{1}
\]

where \( \rho_0 \) is a reference density.

Our starting point is the two-dimensional incompressible Boussinesq equations of motion for a density-stratified fluid,

\[
\begin{align*}
    u_t + uu_x + wu_z &= -\rho \rho_0 / \rho_0 + \nu \nabla^2 u, \\
    w_t + uw_x + ww_z &= -\rho \rho_0 / \rho_0 - g \rho / \rho_0 + \nu \nabla^2 w,
\end{align*}
\]

and we combine these with advection–diffusion equations for \( T \) and \( S \),

\[
\begin{align*}
    T_t + uT_x + wT_z &= \kappa_T \nabla^2 T \quad \text{and} \\
    S_t + uS_x + wS_z &= \kappa_S \nabla^2 S, \tag{3a}
\end{align*}
\]

and the equation of state (1). In the above equations we have represented partial derivatives by subscripts, where time is given by \( t \); the horizontal and vertical coordinates are given by \( (x, z) \) with velocity components of \( (u, w) \), respectively; \( \rho \) is the pressure; \( \nu \) is the kinematic viscosity; and \( \kappa_T \) and \( \kappa_S \) the molecular diffusivities of \( T \) and \( S \), respectively. Now consider perturbations about a background state of no motion (i.e., \( \overline{u} = \overline{w} = 0 \)). We can write

\[
\begin{align*}
    T &= \overline{T} + \tilde{T}, \quad S = \overline{S} + \tilde{S}, \quad \rho = \overline{\rho} + \tilde{\rho}, \quad u = \tilde{u}, \\
    w &= \tilde{w}, \quad \text{and} \quad p = \overline{p} + \tilde{p}, \tag{4}
\end{align*}
\]

where the tilde indicates perturbations from the background profiles, with the background pressure defined by hydrostatic balance. The background density profile is \( \overline{\rho}(z) = \rho_0 + \overline{T}(z) + \overline{S}(z) \).

We proceed to linearize the equations by substituting the decomposition in (4) and neglecting the products of the perturbation quantities, which is justified as long as they are small quantities. Solutions are then taken to be of the normal mode form with

\[
\{ \tilde{\omega}, \tilde{T}, \tilde{S} \} = \{ \tilde{\omega}(z), \tilde{T}(z), \tilde{S}(z) \} e^{i(kx + \alpha t)} \tag{5}
\]

and similar expressions governing the other perturbation quantities. Here, \( k \) is a horizontal wavenumber, which we take to be real; \( \alpha = \sigma - i \omega \) is a complex number, which is composed of a growth rate \( \sigma \) and a frequency \( \omega \); and the hat denotes the vertical structure of the perturbation quantity. Choosing the normal mode form in (5) allows us to separate the \( x \) and \( t \) dependence and produces a set of ordinary differential equations in
where \( \{ \hat{w}_n, \hat{T}_n, \hat{S}_n \} \) are coefficients and \( f_n(\zeta) \) is chosen to satisfy the boundary conditions in each case. For those listed above, this corresponds to

\[
f_n(\zeta) = \sin \left( \frac{n \pi (\zeta + H/2)}{H} \right),
\]

and the series is a truncated Fourier representation of the eigenfunctions. Similar to the standard procedure for determining the Fourier coefficients of a function, we multiply each equation in (7) by \( f_m(\zeta) \) and take the inner product, defined by

\[
\langle \beta(\zeta) \rangle = \frac{2}{H} \int_0^H \beta(\zeta) \, d\zeta,
\]

where \( \beta(\zeta) \) is some arbitrary function. Using the identity \( \langle f_n(\zeta)f_m(\zeta) \rangle = \delta_{nm} \), where \( \delta_{nm} \) is the Kronecker delta, we can write the system of equations as

\[
\sigma \alpha_n^2 \hat{w}_n = -\text{Ra} \text{Pr} \alpha_n^2 \langle \hat{T}_n \rangle - \text{Pr} \alpha_n^4 \hat{w}_n,
\]

\[
\sigma \hat{T}_m = -\sum_{n=1}^{N} \hat{w}_n \langle \hat{T}(\zeta)f_n(\zeta)f_m(\zeta) \rangle - \alpha_m^2 \hat{T}_m, \quad \text{and}
\]

\[
\sigma \hat{S}_m = -\sum_{n=1}^{N} \hat{w}_n \langle \hat{S}(\zeta)f_n(\zeta)f_m(\zeta) \rangle - \alpha_m^2 \hat{S}_m,
\]

where we define \( \alpha_m^2 = (n \pi/H)^2 + \alpha^2 \) for a more compact notation. The equations in (11) have the form of a matrix eigenvalue problem \( AX = \lambda X \), with \( X \) a vector of size \( 3N \) that is formed by concatenating all of the Fourier coefficients \( \{ \hat{w}_n, \hat{T}_n, \hat{S}_n \} \) together into a single vector. This form facilitates the solution of the problem using standard matrix eigenvalue software (in our case, the R software package was used).

3. Linear stability properties

In this section, we present the results of the stability analysis that was formulated in the previous section. Before discussing new results for the diffusive interface, we shall briefly review some important results from the analysis of the linear profiles.

a. Linear profiles

Following the previous work of Stern (1960), Veronis (1965), Nield (1967), and Baines and Gill (1969) (see also Turner 1973; Linden 2000), we take linear background profiles for \( \hat{T} \) and \( \hat{S} \),

\[
\hat{T}(\zeta) = \zeta \quad \text{and} \quad \hat{S}(\zeta) = -\zeta,
\]

on the domain \(-\frac{H}{2} \leq \zeta \leq \frac{H}{2}\). This is equivalent to choosing the domain height \( L_z \) as the length scale to nondimensionalize by (the only available extrinsic length scale). The dimensionless domain height is unity, and the appropriate Rayleigh number is

\[
\text{Ra}_H = \frac{g \Delta T L_z^2}{\rho \nu k T}.
\]

The linear profiles in (12) considerably simplify the system of equations in (7), and an analytical solution is possible. The dispersion relation governing the eigenvalues can be found in Baines and Gill (1969), and the reader is referred to this work as well as Turner (1973) and Linden (2000) for further details.

The results of the stability analysis are most conveniently displayed on what we shall refer to as a stability diagram, which is shown in Fig. 3. It contours the \( \text{Ra}_H - \text{Ra}_n \) plane with the positive unstable growth rates \( \sigma \), in thin contours and color filling and the frequency of oscillation \( \sigma \) in thick contours. At each point in the unstable region (i.e., for a fixed \( \text{Ra}_H \) and \( \text{Ra}_n \), there is generally a continuous band of unstable wavenumbers present. However, we plot only the mode with the largest growth rate, because it is this “most unstable mode” that is expected to dominate the initial linear growth phase and possibly the nonlinear transition to turbulent convection.

Three different regions of the diagram in Fig. 3 may be identified:

(i) A stable region exists for either sufficiently low \( \text{Ra}_H \) or sufficiently high \( \text{Ra}_n \). The lowest \( \text{Ra}_H \) that may be
unstable occurs for $R_p = 0$, in which no gravitationally stabilizing $S$ stratification is present, and we recover the classical case of pure thermal convection in a linear gradient (Linden 2000; Kundu et al. 2004). This has the well-known solution that instability is triggered once a critical $Ra_{Heff} = 27\pi^{3/4} = 658$ is exceeded (though this value depends on the form of the boundary conditions). The resulting unstable modes are of the convective type and form the second region of the diagram.

(ii) In the large $Ra_H$, small $R_p$ portion of the diagram, instability is due to a convective-type instability; the unstable modes are nonoscillatory with $\sigma_l = 0$. The physical mechanism of growth for this convective type of instability is straightforward: the perturbations are able to extract the potential energy available in the gravitationally unstable (top heavy) density field to directly increase their amplitude over time, once the stabilizing effects of viscosity and diffusion are overcome. These convective-type unstable modes exist only when the density field is gravitationally unstable and so are limited to the region $0 \leq R_p < 1$, assuming that $Ra_H$ is sufficiently large.

(iii) The third portion of the diagram consists of DC-type unstable modes that have an oscillating growth with $\sigma_l > 0$ (region of thick dark contour lines in Fig. 3). These DC-type modes are the first to become unstable as $Ra_H$ is increased and are the only type of instability that is possible when the density stratification is gravitationally stable (i.e., $R_p > 1$). The physical mechanism of instability can be understood as follows: After any small displacement from its equilibrium level, a fluid parcel will find itself in a different $T$-$S$ state than it originated from. Because of the differing rates of molecular diffusion, the parcel exchanges $T$ more rapidly than $S$ with its surrounding environment. Because $S$ is stably stratified, the parcel either sinks or rises back to its original level, but it overshoots, because it carries with it a density anomaly. The density anomaly grows because the parcel is now exchanging $T$ in more or less buoyant surroundings. The oscillation can therefore grow in time. However, the DC instability is very restricted in that it cannot operate if $R_p$ is too large, and the flow is found to be stable for $R_p > (Pr + 1)/(Pr + \gamma) \approx 1 + Pr^{-1} \approx 1.16$. Also, the transition between the DC-type modes and the convective-type modes occurs at $R_p \to 1$ as $Ra_H \to \infty$.

Because most geophysical observations of DC unstable profiles have a mean $R_p > 1.16$ (Padman and Dillon 1987; Kelley et al. 2003; Schmid et al. 2004; Timmermans et al. 2008; Schmid et al. 2010), it is unlikely that the instability of the linear profiles plays a role in these systems. Therefore, in order to assess DC processes in thermohaline staircases, we now turn to the stability of the diffusive interface.

b. The diffusive interface

When considering the stability of a diffusive interface, it is necessary to introduce two additional length scales into the problem (in addition to the vertical domain size $L_z$). These are the thicknesses of both the $\overline{T}$ and $\overline{S}$ interfaces, which will be denoted by $h_T$ and $h_S$, respectively (Fig. 1b). Each interface thickness is defined by the dimensional relation

$$h_l = \Delta \phi / \left( \dfrac{\partial \phi}{\partial \xi} \right)_{\phi_0},$$

(14)

where $\phi$ represents either $T$ or $S$ and the $\phi_0$ subscript indicates that the derivative is evaluated on the $T$-$S$ scalar value at the interface center. In the case of the simulations, we calculate the gradient by averaging over $-\Delta \phi/8 < \phi_0 < \Delta \phi/8$.

In our analysis of the diffusive interface we shall choose $L = h_T$ as the length scale in the nondimensionalization. Two different model profiles will be considered, (i) the “erf” interface model with

$$\overline{T}(z) = \text{erf}(\sqrt{\pi}z)/2 \quad \text{and} \quad \overline{S}(z) = -\text{erf}(\sqrt{\pi}z)/2,$$

and (ii) the “tanh” interface model with

$$\overline{T}(z) = \text{tanh}(2z)/2 \quad \text{and} \quad \overline{S}(z) = -\text{tanh}(2z)/2,$$

which are both nondimensional. Note that the $\sqrt{\pi}$ factor and the factor of 2 appear in the arguments in order to satisfy (14). In Fig. 1b, the difference between the erf and the tanh profiles would be virtually indistinguishable. However, these two different profiles are used to assess the sensitivity of the results; the erf interface is a solution to the diffusion equation, whereas the tanh interface is an analytically convenient form.

With the introduction of the $h_T$ and $h_S$ scales, come two additional dimensionless numbers,

$$r = h_T/h_S \quad \text{and} \quad H = L_z/h_T,$$

(15)

the interfacial thickness ratio and the dimensionless domain height, respectively. When examining the diffusive interface, $H$ measures the relative thickness of the interface to the mixed layers above and below. Within thermohaline staircases, the interfaces are generally found
to be much thinner than the mixed layers on either side (Neal et al. 1969; Turner 1973; Padman and Dillon 1989; Schmid et al. 2010), and so we shall generally restrict ourselves to $5 \leq H \leq 40$. In addition, we will treat $r$ as an independent variable in the analysis that follows; however, it is likely that it is controlled by the physics of diffusive convection. If it is pure molecular diffusion that is acting within the interfaces, then an upper bound is found to be $r \approx r^{-1/2} \approx 10$, whereas a reasonable lower bound would be $r = 1$. We shall therefore restrict ourselves to this range $1 \leq r \leq 10$, which is also the range that has been reported in the laboratory experiments of Marmorino and Caldwell (1976).

It is also more appropriate, when examining the stability of the diffusive interface, to use an interfacial length scale in defining the Rayleigh number, and so we shall use

$$Ra_I = \frac{g \Delta T \rho I^3}{\rho \nu \kappa T}$$

as the “interfacial Rayleigh number.”

Stability diagrams using the tanh interface model are shown in Fig. 4 for various $r$. Beginning with $r = 1$ (Fig. 4a), the profiles of $T$ and $S$ have the same interface thicknesses. In this case, no boundary layers exist, and for $R_p > 1$ the background density field is gravitationally stable for all $\zeta$. We should intuitively expect that the stability diagram show similar behavior to the linear gradient results in Fig. 3. This is because approximately linear gradients are present within the interfaces and only the length scale has changed, along with the proximity of the vertical boundaries. In comparing Figs. 4a and 3, this is indeed what is observed. In both cases, there is a stable region at low $Ra$, and the cutoff in $R_p$ occurs at the same value of 1.16, above which the profiles are stable.

As $r$ is increased from unity, diffusive boundary layers develop above and below the gravitationally stable interface center (Fig. 1b). These boundary layers can be seen to modify the stability properties by destabilizing the profiles at larger $R_p$ values. As is to be expected, the larger $r$ becomes—and therefore the thicker and more gravitationally unstable the boundary layers become—the lower is the $Ra_I$ required to achieve instability.
is restricted only to three-dimensional rectangular domains. We therefore choose a relatively small scale for the third dimension $L_y$—compared to the horizontal $L_x$ and vertical $L_z$—scales in testing the two-dimensional linear predictions. All of the parameters chosen in the DNS are summarized in Table 1.

Of the five simulations that were performed, four are used to directly test the linear predictions by “turning off” the molecular diffusion of the background $T$-$S$ profiles (simulations I–IV in Table 1). In each of these cases, which will be referred to as “stationary,” there is a well-defined $\sigma$ and $\alpha_{\text{max}}$ that can be compared with the linear predictions. It is also of interest to observe the finite-amplitude motions of these instabilities before proceeding to the time-dependent nonstationary case where molecular diffusion is acting on the background profiles.

Each simulation is initialized with background $\overline{T}$ and $\overline{S}$ profiles, where the corresponding dimensionless parameters $Ra_f$, $Re$, $r$, $Pr$, $\tau$, and $H$ are chosen. In the stationary cases, these parameters do not change in time; however, in the nonstationary case, $Ra_f$, $r$, and $H$ are all functions of $t$. All simulations are also initialized by random noise in the velocity field that is centered on the interface level. This random perturbation is a seed for the instability to grow from. The boundary conditions are periodic in the horizontal directions $(x, y)$ and correspond to a free-slip, rigid-lid condition on the velocity field and a no-flux condition in the $T$-$S$ fields on the vertical boundaries. Although the linear stability analysis used a constant $T$-$S$ condition on the vertical boundaries, it is not expected to significantly affect the results, and this will be confirmed in the following.

b. Testing the linear predictions: The stationary interface

As an initial test of the linear analysis, we have chosen four simulations (I–IV in Table 1) that are predicted to produce a stable mode (I), a DC-type unstable boundary layer mode (II), a convective-type unstable boundary layer mode (III), and a DC-type unstable interface mode (IV).

The growth of the perturbations in time is best seen by plotting the volume-averaged kinetic energy. In the case of simulation I, the kinetic energy simply decayed in time (not shown). The other simulations, II–IV, are shown in Figs. 8a–c, respectively. Because the vertical axis is a logarithmic scale, a strictly exponentially growing perturbation will appear as a straight line, as is predicted by the linear theory. This growth rate prediction (dashed lines) is found to be in agreement with the DNS results, despite the fact that the growth rates each differ by nearly an order of magnitude in each case. Oscillations in the kinetic energy are observed only in the DC-type unstable modes (simulations II and IV in Figs. 8a,c), and the predicted period of oscillation, given by the scale indicated by the arrows, is also in agreement with the simulations.

It is also possible to test the linear predictions of whether the instability will be centered in the boundary layers or the interface. This can be seen in Figs. 9a,b, where contours of the $T$ field are shown for simulations III and IV once the instability has developed a finite amplitude. In the case of Fig. 9a, the central core of the interface is left virtually undisturbed, and the dislocations are focused in the boundary layers at the interface.
TABLE 1. Values of various important parameters for the simulations performed. The gridpoint resolution listed for the simulations \( \{N_x, N_y, N_z\} \) is that of the S field. The \( T \), velocity, and pressure fields are resolved on a grid with half this resolution. In the case of the nonstationary simulation (V), the dimensionless parameters listed are evaluated using the initial conditions. In all cases, \( Pr = 6 \), \( r = 0.01 \), and \( L_x/h_x = 0.66 \). Also included is the total number of waves (in the horizontal \( x \) direction) predicted in the domain. Here, \( L_x \) and \( N_x \) have been doubled for simulation II to ensure two wavelengths of the most unstable mode are possible. Note that the value of \( H \) in these simulations is different from that of Fig. 4, and they cannot be directly compared.

<table>
<thead>
<tr>
<th>Simulation</th>
<th>( {N_x, N_y, N_z} )</th>
<th>( Ra_T )</th>
<th>( Ra_p )</th>
<th>( r )</th>
<th>( H )</th>
<th>( n )</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>( {360, 16, 180} )</td>
<td>( 10^3 )</td>
<td>3</td>
<td>1.5</td>
<td>8</td>
<td>—</td>
</tr>
<tr>
<td>II</td>
<td>( {720, 16, 180} )</td>
<td>( 1.5 \times 10^3 )</td>
<td>3</td>
<td>1.5</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>III</td>
<td>( {360, 16, 180} )</td>
<td>( 10^3 )</td>
<td>3</td>
<td>1.5</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>IV</td>
<td>( {360, 16, 180} )</td>
<td>( 2 \times 10^3 )</td>
<td>1.1</td>
<td>1</td>
<td>8</td>
<td>13</td>
</tr>
<tr>
<td>V</td>
<td>( {800, 32, 400} )</td>
<td>( 10^3 )</td>
<td>3</td>
<td>1</td>
<td>15</td>
<td>—</td>
</tr>
</tbody>
</table>

edges. In contrast, the predicted DC interface-centered instability of Fig. 9b shows displacements that are focused within the interface itself. In this case, the interface performs exponentially growing standing oscillations.

Because it is necessary to choose a finite horizontal domain size \( L_x \) in the DNS, it is not possible to represent a continuous range of \( \alpha \). Instead, the periodic boundary conditions allow only discrete values of \( \alpha = 2\pi nh_x/L_x \), where \( n = 1, 2, \ldots \) is the number of waves in the domain. The wavenumber that is expected to emerge from the DNS is that with the largest growth rate, and this is not necessarily the wavenumber of maximum growth \( \sigma_{\text{max}} \). In Table 1, the total number of waves \( n \) predicted by the linear theory is listed. For each of the \( T \) fields plotted in Figs. 9a,b, the linear predictions agree with the number of waves observed. The wavelengths predicted by the linear theory, once corrected for the periodic boundary conditions, correspond to the length of the scales shown in Figs. 9a,b.

c. Breakdown of the time-dependent diffusive interface

In the nonstationary case, the simulation (V) is begun with \( T \) and \( S \) interfaces that have an equal thickness \( r = 1 \) and are allowed to diffuse in time. The initial \( Ra_T, Ra_p \) and \( H \) are chosen such that the profiles are stable at all wavenumbers. Each interface will then grow in time due to molecular diffusion, according to

\[
h_o(t) = 2[\pi \kappa_o (t+t_o)]^{1/2}
\]

in the case of the \( erf \) interface. Here, \( \sigma \) represents \( T \) and \( S \), and the \( t_o \) time shift is chosen to satisfy the initial interface thicknesses. The evolution of the linear stability properties of the diffusive interface may then be followed in the \( r-Ra_T \) plane, as shown in Fig. 10.

At the initial time \( t = 0 \), the interface has a position on the diagram corresponding to the initial values of \( r \) and \( Ra_T \) and is located in the stable region (Fig. 10). The position of this boundary, however, is changing in time because of its dependence on \( H(t) \). At a later time, both \( r \) and \( Ra_T \) have increased. The location of the interface therefore moves upward and rightward on the trajectory shown in Fig. 10, whereas the position of the stability boundary moves away as \( H \) decreases. During the simulation the interface crosses into the unstable portion of the diagram, thus initiating instability. A complete breakdown of the boundary layers occurs at the final position shown in Fig. 10.
The growth and eventual breakdown of the instability on the nonstationary interface may be seen by looking at a plot of the time evolution of \( h_T(t) \). This is shown in Fig. 11a, where we have normalized by the initial thickness \( h_0 = h_T(0) \). As the instability develops, a range of different \( h_T \) are present in the domain at a given \( t \) [note that \( h_T \) is measured using Eq. (14) at each \( x \) and \( y \) in the domain]. We therefore plot the mean, as well as the 10th and 90th percentiles of \( h_T \), given by the gray shading. At early times, these curves all fall on one another as \( h_T \) grows by molecular diffusion, in accordance with (17). The interface enters the unstable region predicted by the linear theory soon after the simulation begins, indicated by the vertical gray strip denoting the time spent inside the DC unstable region. The interface does not experience a growth in the kinetic energy during this time, which can only be seen well after the interface enters the convective unstable region of the diagram (right of the vertical gray strip in Fig. 11b). In other words, the kinetic energy only starts to grow in the convective-type region. The increase in kinetic energy indicates an increasing growth rate over time and eventually saturates after the boundary layers have broken away. The time of the interface breakdown \( t_b \) is defined as the time of the greatest mean \( h_T \), which is indicated by the vertical dashed line at \( t = t_b \).

The delay in the growth of the instability when the interfaces are also growing in time may be understood by considering the relative growth rates of these two competing processes. The growth rate of the \( T \) interface can be defined in dimensional units as

\[
\frac{1}{h_T} \frac{dh_T}{dt} = \frac{2\pi \sigma_T}{h_T^2},
\]

where the equality follows from the molecular diffusion of an erf interface expressed in (17). In order for the linear instability to dominate over the growth of the interface, we require \( \sigma_T \) from linear theory to exceed this interface growth rate. This can be expressed in dimensionless units as the simple relation

\[
\sigma_T > 2\pi.
\]

Therefore, any instability growing on an interface that is diffusing in time likely requires a (dimensionless) \( \sigma_T \) in excess of \( 2\pi \) to emerge. Because the \( \sigma_T \) of the DC-type modes are generally less than \( 2\pi \), we should instead expect convective-type instabilities in the boundary layers, as is observed. The time at which \( \sigma_T = 2\pi \) is shown by the solid vertical line in Figs. 11a–c.

The instability can be seen in the \( T \) field at the time of breakdown \( (t = t_b) \), where a series of plumes have formed in the boundary layers and are in the process of detaching from the interface to be mixed in the upper and lower layers (Fig. 12). Note that the central core of the interface is left undisturbed, because the instability is centered in the boundary layers, as expected.

The results of the nonstationary simulation show that the time-dependent growth of the interface is significant in determining the development of the instability. In the
Fig. 11. Time evolution of parameters in the nonstationary simulation (V) as a function of time. The vertical gray strip indicates the time interval of DC instability with stability at earlier times and convective instability at later times. The time at which $\sigma_t = 2\pi$ (i.e., when the instability growth rate equals the growth rate of the $T$ interface) is indicated by the vertical solid line. (a) The $T$ interface thickness $h_T$, normalized by its initial value $h_{T0}$ with the upper and lower lines with gray shading indicating the 90th and 10th percentiles found within the domain and the central line indicating the mean. (b) Volume-averaged kinetic energy. (c) $Ra_{bl}$ In (a)-(c), the time axis has been nondimensionalized by $10^9 \varepsilon_T L_x^2 h_T$, and the vertical dashed line indicates the time of peak $h_T$, which is denoted $t = t_0 = 2$.

In the case of simulation V, the interface moves rapidly through the DC-type unstable region composing the stability boundary, which does not contribute to the eventual mode of interface breakdown. We can understand this behavior by requiring that the instability growth rate exceed that of the interface. This predicts that the breakdown is of the convective type and is concentrated in the boundary layers, in agreement with the interpretation of previous investigators (Linden and Shirtcliffe 1978; Newell 1984; Worster 2004). We next investigate whether the transition to instability in the boundary layers can be described by an appropriately defined boundary layer Rayleigh number.

5. Critical boundary layer Rayleigh number

As discussed in the introduction, numerous investigators assumed that the nonlinear breakdown of the diffusive interface is governed by a convective-type instability of the unstable boundary layers. In analogy with single-component convection, the criterion for breakdown was taken to be determined by a critical Rayleigh number that is appropriate for the boundary layers, $Ra_{bl} = O(10^3)$ (Linden and Shirtcliffe 1978). Furthermore, comparisons with field measurements based on this model have also been attempted (Padman and Dillon 1989; Sánchez and Roget 2007). In this section, we test the use of $Ra_{bl}$ in describing the linear stability properties, as well as the nonlinear state of the diffusive interface once convection has begun.

Following Linden and Shirtcliffe (1978), the boundary layer Rayleigh number is defined as

$$Ra_{bl} = \frac{g \delta \rho b^3}{\rho_0 \beta_x},$$

where $b$ is a representative length scale of the boundary layer (see Fig. 1b), given by

$$b = (h_T - h_\delta)/2 = h_T(1 - r^{-1})/2,$$

and $\delta \rho$ is a representative boundary layer density scale defined by

$$\delta \rho = \int_{z_{bl}}^{L_x/2} [\rho'/2 - \bar{\rho}(z) - \rho_0] dz,$$

where $\Delta \rho = \Delta \bar{S} - \Delta T$ and $z_{bl}$ is determined from $|\bar{\rho}(z_{bl}) - \rho_0| = \Delta \rho/2$ and ensures that the integration in (22) is over the total gravitationally unstable density anomaly in the upper boundary layer. In other words, $z_{bl}$ is chosen such that all the fluid in the upper boundary layer that is lighter than the mixed layer above, for example, is included in the integration. We can now substitute the dimensional erf profiles, say, of $\bar{T}$ and $\bar{\delta}$, into (22) to get

$$\delta \rho = \frac{h_f \Delta T}{2} \int_{z_{bl}}^{H/2} [\text{erf}(\sqrt{\pi} \zeta) - R_\rho \text{erf}(\sqrt{\pi} \zeta) + R_\rho - 1] d\zeta,$$

where $R_\rho$ is

$$R_\rho = \frac{h_f \Delta T}{2} \int_{z_{bl}}^{H/2} [\text{erf}(\sqrt{\pi} \zeta) - R_\rho \text{erf}(\sqrt{\pi} \zeta) + R_\rho - 1] d\zeta.$$
where ζ_{hl} can be found from solution of the equation

\[ \text{erf}(\sqrt{\pi} \zeta_{hl}) - R_p \text{erf}(\sqrt{\pi} r \zeta_{hl}) + R_p - 1 = 0. \]  \hspace{1cm} (24)

It is now possible to express Ra_{hl} in terms of the large-scale parameters Ra_p, R_p, and r used in the stability analysis. The link between them can be written in the form

\[ Ra_{hl} = Ra_{f}(R_p, r), \]  \hspace{1cm} (25)

where

\[ F(R_p, r) = \frac{1}{8}(1 - r^{-1})^2 \int_{\zeta_{hl}}^{H/2} \text{erf}(\sqrt{\pi} \zeta) - R_p \text{erf}(\sqrt{\pi} r \zeta) + R_p - 1 \, d\zeta. \]  \hspace{1cm} (26)

and recall that Ra_f is the interface Rayleigh number (16). It is important to note that a dependence of (25) on H has been neglected. This is justified only if H \approx 4 because below this value the boundary layers have reached the domain boundaries and influence the integration.

We are now in a position to ask the question, how applicable is Ra_{hl} for describing the onset of instability at a diffusive interface? This question is addressed in Fig. 13, where we have plotted the location of the stability boundary in the r–Ra_p plane from the linear stability analysis for different values of the domain height H, at a representative value of R_p = 3. Two cases are examined: (i) where the transition to the DC-type unstable modes occurs at σ_r = 0 (Fig. 13a) and (ii) where the linear instability growth rate exceeds the growth rate due to diffusion of the interface at σ_r = 2\pi (Fig. 13b). In the case of (i), Fig. 13a shows that, by varying H, there are substantial shifts in the stability boundary, even at values of H as large as 40. It is interesting that this is not so for the convective-type modes that compose the boundary in Fig. 13b, whose curves all collapse.

In each case, it is possible to compare these stability boundaries with contours of Ra_{hl} to assess the appropriate critical Ra_{hl}. (We will restrict ourselves to H \geq 5 in order to avoid the dependence of F on H.) It can be seen in both cases that the Ra_{hl} values that represent the stability boundaries most closely are generally more than two orders of magnitude smaller than the value of O(10^5) previously suggested for the nonlinear breakdown. Furthermore, a single Ra_{hl} value is not able to adequately capture the behavior of the stability boundary for the range of r shown and may change by an order of magnitude over 1 < r < 3, as can be seen in Figs. 13a, b. We can therefore conclude that a critical Ra_{hl} \approx 10^3 does not accurately describe the linear stability boundary in the boundary layers of a diffusive interface.

That the Ra_{hl} required for instability is much less than 10^5 can also be seen in the time-dependent simulation.
shown in Fig. 11c. The instability growth, seen in the kinetic energy plot of Fig. 11b, is initiated at a \( R_{\text{sh}} \ll 10^3 \). It is interesting, however, that the \( R_{\text{sh}} \) at the point of the initial breakdown (\( \tau \approx 2 \)) is on the order of \( 10^3 \), which is what has previously been assumed. At later times (\( \tau > 3 \)) during active convection, the interface appears to reach a quasi-steady state where \( R_{\text{sh}} \approx 50 \). The linear stability threshold for time-dependent background profiles, given by \( \sigma_r = 2\pi \), is \( R_{\text{sh}} \approx 5 \).

6. Conclusions

In this study, we have utilized linear stability analysis and direct numerical simulations (DNS) to examine the conditions under which a diffusive interface will become unstable to small perturbations. It may be thought of as an extension of the classic work on linear profiles of \( T \) and \( S \) to include the geophysically relevant case of a diffusive interface. Similarity between the linear profile results and the diffusive interface is found when \( T \) and \( S \) have the same interface thicknesses (\( \tau = 1 \)). In this case, the instability is centered within the interface and has similar stability properties to the linear profiles.

It has been found, however, that the \( T \) interface has a greater thickness than \( S \) (\( \tau > 1 \)), because of the higher \( T \) molecular diffusivity (Turner 1973; Marmorino and Caldwell 1976; Linden and Shirtcliffe 1978; Fernando 1989), and this has recently been found in the observations of T. Sommer et al. (2012, unpublished manuscript), as shown in Fig. 2. When this is the case, we have shown that the instability will take place within the diffusive boundary layers on either side of the gravitationally stable interface core, and instability is then possible at the large \( R_{\text{sh}} \) values typically observed in the staircases of oceans and lakes (i.e., \( 2 < R_{\text{sh}} < 6 \), with \( R_{\text{sh}} = 1.5 \) typically the lowest observed: Padman and Dillon 1987; Timmermans et al. 2008; Schmid et al. 2010).

The stability analysis revealed that, within the gravitationally unstable boundary layers, it is possible for instability to take place as either an oscillating DC-type unstable mode or a convective-type unstable mode. The marginally unstable modes that compose the instability boundary are always of DC type. However, the DNS show that the time-dependent growth of the interface is significant in altering the position of the stability boundary. If these time-dependent effects are accounted for by requiring that the instability growth rate exceed that of the interface, then we find that the instability of the boundary layers is of convective type. This finding adds theoretical support to this idea, which has often been assumed.

The boundary layer Rayleigh number \( R_{\text{sh}} \) is not found to be a useful parameterization of the stability criterion but may be a good description of the time-dependent conditions under which the breakdown of the interface takes place. Further analysis is required to assess this possibility, and a series of fully three-dimensional DNS have been conducted to examine this issue (Carpenter et al. 2012, manuscript submitted to J. Fluid Mech.). The time dependence of the instability shows that it is not a simple matter to directly apply the stability conditions found here to geophysical observations. However, the findings provide insight into the instability mechanisms, as well as lead to bounds on the parameters governing interface stability.

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REFERENCES


Appendix II.  Simulations of a double-diffusive interface in the diffusive convection regime

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Simulations of a double-diffusive interface in the diffusive convection regime

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Three-dimensional direct numerical simulations are performed that give us an in-depth account of the evolution and structure of the double-diffusive interface. We examine the diffusive convection regime, which, in the oceanographically relevant case, consists of relatively cold fresh water above warm salty water. A ‘double-boundary-layer’ structure is found in all of the simulations, in which the temperature (\(T\)) interface has a greater thickness than the salinity (\(S\)) interface. Therefore, thin gravitationally unstable boundary layers are maintained at the edges of the diffusive interface. The \(TS\)-interface thickness ratio is found to scale with the diffusivity ratio in a consistent manner once the shear across the boundary layers is accounted for. The turbulence present in the mixed layers is not able to penetrate the stable stratification of the interface core, and the \(TS\)-fluxes through the core are given by their molecular diffusion values. Interface growth in time is found to be determined by molecular diffusion of the \(S\)-interface, in agreement with a previous theory. The stability of the boundary layers is also considered, where we find boundary layer Rayleigh numbers that are an order of magnitude lower than previously assumed.

**Key words:** double diffusive convection, ocean processes, stratified flows

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1. Introduction

It has been more than 50 years now since Stern (1960) demonstrated that certain configurations of temperature and salinity may develop double-diffusive (DD) instability. The DD instability is known to generate a local convective mixing of the water column, despite the overall density stratification being gravitationally stable. The conditions required for the DD instability to develop have since been generalized (e.g. Veronis 1965; Baines & Gill 1969), showing that only two density-contributing scalars with different molecular diffusivities are required, provided that one exhibits a gravitationally unstable stratification, thus providing the energy source for the instability. Two fundamentally different regimes exist depending on whether \(T\), which we shall take as the faster diffusing scalar (not necessarily temperature), or \(S\), slower

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diffusing, is in a gravitationally unstable configuration. Here we shall focus on the diffusive convection regime where $T$ is gravitationally unstable.

Numerous investigations have identified diffusive convection in the oceans (Neal, Neshyba & Denner 1969; Kelley et al. 2003; Timmermans et al. 2008) and lakes (Hoare 1966; Schmid et al. 2004; Schmid, Busbridge & Wüst 2010), as well as in geological processes (Huppert & Sparks 1984). In these observations the vertical $T$- and $S$-profiles are found to form thermohaline staircase structures composed of sharp high-gradient interfaces sandwiched between nearly homogeneous and turbulent mixed layers. In efforts to understand the transport mechanisms, and $TS$-fluxes, through these thermohaline staircases, a number of laboratory and theoretical studies chose to focus on the simpler configuration of a single interface separated by mixed layers above and below (e.g. Turner 1965; Shirtcliffe 1973; Crapper 1975; Marmorino & Caldwell 1976; Linden & Shirtcliffe 1978; Newell 1984; Fernando 1989; Kelley 1990). Despite the success of these studies in developing various 'laws' that parameterize the interfacial $TS$-fluxes, a basic knowledge regarding the transport mechanisms, and interface structure, is still lacking.

In the present paper we perform a series of three-dimensional direct numerical simulations (DNS) of a 'diffusive interface' in order to further elucidate the processes controlling the fluxes of $T$ and $S$. The simulations are motivated by previous laboratory experiments that have been influential in our current understanding of the diffusive interface, as well as recent high-resolution microstructure observations taken in the thermohaline staircase of Lake Kivu (Schmid et al. 2010; Sommer et al. 2013). DNS has a number of advantages over both laboratory experiments and field observation, such as a precise description of the velocity and scalar fields, the possibility to evaluate exact $TS$-fluxes, and controlled boundary conditions. To our knowledge, this is one of the first series of fully three-dimensional DNS to be performed for the diffusive convection regime (Caro 2009), although two-dimensional DNS have been carried out previously (Molemaker & Dijkstra 1997; Noguchi & Niino 2010a,b; Carpenter, Sommer & Wüst 2012). The DNS of the present paper give us an in-depth look at the diffusive interface that has never before been attained, and allows us to test the assumptions of a number of previous theories.

The paper is organized as follows. After a description of the simulations and their relation to geophysical observations in §2, we provide an overview of the time evolution of the flow (§3). The interface structure, and the large-scale circulations present, are described in §4. The implications for the fluxes of $T$ and $S$, as well as the ratio of these fluxes is discussed in §5. A theory describing the boundary layer stability is then tested in §6, with conclusions presented in the final section (§7).

2. Simulations and methods

2.1. Simulations

The DNS are carried out with a version of the spectral code originally described by Winters, MacKinnon & Mills (2004), which has been modified by Smyth, Nash & Mourn (2005) to carry a second scalar ($S$) at a resolution that is twice that of the other fields (e.g. velocity, pressure, $T$). The code is therefore especially suited to performing DNS of oceanic DD convection, where the molecular diffusivities of $T$ and $S$, denoted by $\kappa_T$ and $\kappa_S$, can vary by two orders of magnitude (Kimura & Smyth 2007). These scalars both satisfy advection–diffusion equations and are related to the fluid density $\rho$, by a linear equation of state given by

$$\rho = \rho_0 + T + S.$$  \hspace{1cm} (2.1)
where $\rho_0$ is a constant reference density, and $T$ and $S$ are henceforth given in density units. A representative example of the $T$, $S$, and $\rho$-fields is shown in figure 1. It is possible to see that the lower $\kappa_S$ leads to the development of finer-scale features and a thinner interface in $S$ than in the much faster diffusing $T$ (figure 1b,c).

The simulations solve the equations of motion for an incompressible Boussinesq fluid (Turner 1973) on a rectangular domain of size $\{L_x, L_y, L_z\}$ with an even spacing.
between grid points in each of the three Cartesian coordinates; \( x, y \) in the horizontal, and \( z \) in the vertical (positive upwards). Initial conditions consist of specifying profiles of \( T \) and \( S \) given by

\[
T(z) = \frac{\Delta T}{2} \tanh \left( \frac{2(z - L_z/2)}{h_0} \right) \quad \text{and} \quad S(z) = -\frac{\Delta S}{2} \tanh \left( \frac{2(z - L_z/2)}{h_0} \right),
\]

where \( \Delta T \) and \( \Delta S \) represent the absolute change in \( T \) and \( S \) across the interface, \( h_0 \) is the initial thickness of the \( T \)- and \( S \)-interfaces, and \( L_z \) is the vertical domain height. In addition to the \( TS \)-profiles, the velocity field is perturbed with random noise at the initial time step in each of the three components \((u, v, w)\). The noise is centred about the interface level, and serves as an initial seed for the instabilities which will eventually develop in the vicinity of the interface.

The boundary conditions chosen for the simulations are periodic in the horizontal (i.e. at \( x = 0, L_x \) and \( y = 0, L_y \)), with a free-slip condition for the velocity field, and no-flux conditions for the scalar fields on the top and bottom boundaries (i.e. at \( z = 0, L_z \)). These boundary conditions mean that no heat or salt is able to escape the domain, and the \( T \) and \( S \) differences across the diffusive interface gradually decrease in time. This ‘run-down’ scenario is similar to a number of previous laboratory experiments that have been carried out in containers that are either insulated against the escape of heat (Newell 1984), or that have been conducted with a scalar other than heat, for example a salt–sugar system (Turner, Shirecliffe & Brewer 1970; Shircliff 1973; Stamp et al. 1998).

2.2. Scales and dimensionless parameters

Of central importance in the study of the diffusive interface are the \( T \)- and \( S \)-interface thicknesses. In accordance with numerous other studies, we shall define the interface thickness by

\[
h_\varphi \equiv \Delta \varphi \left/ \left( \frac{\partial \varphi}{\partial z} \right)_{\varphi_0} \right. \quad (2.3)
\]

Here, and throughout the rest of the paper, \( \varphi \) represents both \( T \) and \( S \), and the \( \varphi_0 \) subscript indicates that the derivative is taken at the location of the isoscalar (i.e. \( \varphi = \text{const.} \)) surface of the interface. In practice, we compute the gradient by fitting a line over the region of the interface where \(-\Delta \varphi/8 < \varphi < \Delta \varphi/8\) at each \((x, y)\) location. Assuming an error-function form of the interface, this averaging underestimates the true gradient by only 1.1\%. In addition, \( \Delta \varphi \) is computed by the absolute difference between the average value of \( \varphi \) for the upper and lower quarters of the domain.

Given the scales defined above, it is possible to form the following independent dimensionless numbers which are characteristic of the diffusive interface:

\[
Ra_l \equiv \frac{g \Delta T h_l^3}{\rho_0 \nu \kappa T}, \quad R_s \equiv \frac{\Delta S}{\Delta T}, \quad Pr \equiv \frac{\nu}{\kappa T}, \quad \tau \equiv \frac{\kappa S}{\kappa T} \quad \text{and} \quad r \equiv \frac{h_T}{h_S},
\]

where \( g \) is gravitational acceleration, and \( \nu \) is the kinematic viscosity. These dimensionless parameters correspond to a thermal interfacial Rayleigh number, the stability ratio, Prandtl number, diffusivity ratio, and interface thickness ratio, respectively. For a given simulation, both \( Pr \) and \( \tau \) remain constant since they are properties of the fluid and the scalars. However, all three of \( Ra_l \), \( R_s \), and \( r \) are changing in time due to the changing of \( \Delta T \), \( \Delta S \), \( h_T \), and \( h_S \). In addition to the
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<table>
<thead>
<tr>
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<th>Dimensionless parameters</th>
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<td>$\Delta T$ (kg m$^{-3} \times 10^3$)</td>
<td>$Ra_t \times 10^{-3}$</td>
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Table 1. The range of parameters and scales used in the simulations, and those measured in the thermo-haline staircase of Lake Kivu by Sommer et al. (2013). The ranges shown for Lake Kivu correspond to the 10th and 90th percentiles. For the simulations we use $\rho_0 = 997$ kg m$^{-3}$ and $v = 9.0 \times 10^{-7}$ m$^2$ s$^{-1}$.

<table>
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<th>Simulation</th>
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<th>$[L_x, L_y, L_c]$ (cm)</th>
<th>$[N_x, N_y, N_z]$ (--)</th>
<th>$h_0$ (cm)</th>
<th>$R_p$ (--)</th>
<th>$\tau$ (--)</th>
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Table 2. Listing of all the simulations performed. Each simulation is referred to by a Roman numeral, shown in the left column. For each simulation we also list the values of the number of dimensions, domain sizes, number of grid points in the S-field, initial interface thicknesses ($h_0$), range of $R_p$ simulated, and $\tau$. All simulations are initialized with equal interface thicknesses for $T$ and $S$.

dimensionless parameters above, it is also possible to define dimensionless domain sizes $[L_x, L_y, L_c]/h_T$.

2.3. Comparison with geophysical observations and laboratory experiments

The choice of dimensional scales used in the simulations is motivated by recent measurements that have been made in the thermo-haline staircase of Lake Kivu by Schmid et al. (2010) and Sommer et al. (2013), as well as by limitations in computational resources. The range of these parameters and scales is given in table 1, showing that the DNS lies well within the range of that found in Lake Kivu.

A total of eleven simulations have been performed, and are summarized in table 2. In keeping with the analogy with run-down laboratory experiments of previous investigations that have used heat, salt, and other soluble components with various diffusivities (e.g. Turner et al. 1970; Shipteliffe 1973; Newell 1984; Stamp et al. 1998), we have chosen four simulations in which $\tau$ is varied (simulations I–IV). The range of $\tau$ chosen is from the heat–salt value of 0.01 to the salt–sugar value of 0.33. By
varying \( \tau \) we are able to gain insight into the processes that control the structure of the diffusive interface. In addition, we also take \( \tau = 0.07 \), and investigate the dependence of the results on the vertical and horizontal size of the domain (simulations V and VI), perform a simulation with two interfaces (simulation VII), and test the dependence on the initial interface thicknesses in a series of two-dimensional simulations at the heat–salt value of \( \tau = 0.01 \) (simulations VIII–XI).

2.4. Capturing scalar mixing at low diffusivities

In the classical Kolmogorov theory of turbulence, the length of the smallest eddies scales with the Kolmogorov length \( L_K = (\nu^3/\epsilon)^{1/4} \), where \( \epsilon \) is the volume-averaged rate of dissipation of kinetic energy. In the spectral-method-based DNS of homogeneous flows, grid resolutions that are of the order of \( L_K \) are usually required for adequately capturing the dissipation of kinetic energy – though simulations using grid spacings up to \( 14L_K \) have been found sufficient (Moin & Mahesh 1998). However, when simulating scalar fields with molecular diffusivities that are smaller than \( \nu \) (i.e., for \( Pr > 1 \) and \( \tau < 1 \)) it is the scalar field with the smallest diffusivity that produces the smallest scales. In the simulations performed in this study, it is therefore the \( S \)-field that requires the greatest numerical resolution. According to the theory of scalar turbulence put forward by Batchelor (1959), the smallest scales are now determined by the Batchelor length \( L_B = L_K (\nu/Pr)^{1/2} \), in the case of the \( S \)-field. It is important to keep in mind that \( L_B \) only denotes a single length within a continuous spectrum of turbulent length scales in which diffusion is acting to damp scalar gradients, and does not necessarily need to be resolved in DNS. Indeed, well-resolved DNS of stably stratified mixing layers have utilized grid spacings of \( 2.5L_B \) (Smyth & Moun 2000; Smyth, Moun & Caldwell 2001). In the present simulations, the resolution of the \( S \)-field had an even grid spacing, \( \Delta x \), in each of the three dimensions, that always satisfied \( \Delta x/L_B < 2 \). The largest \( \Delta x/L_B \approx 2 \) ratio occurred in the three-dimensional \( \tau = 0.01 \) simulation (I) during the initial instability of the interface (discussed in § 3).

In addition to the \( \Delta x/L_B \) ratio, we also monitor the background potential energy \( P_b \) of the scalar fields, defined by

\[
P_b \equiv \frac{g}{L_z} \int_0^{L_z} \varphi_b z_b \, dz_b,
\]

where \( \varphi_b(z_b) \) is the background scalar field obtained by re-sorting all the \( \varphi(x, y, z) \) elements in the domain into a single (monotonic) one-dimensional profile. The \( z_b \) grid of \( \varphi_b \) has the length \( L_z \), but with a total number of elements equal to that of the full three-dimensional domain (see Winters et al. 1995, for further details). Since the boundary conditions do not permit the flux of \( \varphi \) across them, \( P_b \) must be a monotonic function of \( t \), expressing the fact that scalar mixing is an irreversible process. Our experience has shown that this is the most stringent criterion for adequately resolving turbulent scalar mixing with DNS. By monitoring \( dP_b/dt \) we found that the resolution of the \( S \)-field in simulation I, with the oceanic heat–salt value of \( \tau = 0.01 \), was not sufficient at early times (i.e., \( dP_b/dt \) was found to change sign). For this reason, the results of this simulation must be treated with caution, and we shall generally focus our study on the low-\( \tau \) simulation II. However, results from all simulations will be used when discussing the dependence on \( \tau \), and in this case our conclusions from simulation I are supported by the higher-resolution two-dimensional simulations (VIII–XI) at \( \tau = 0.01 \).
Simulations of a double-diffusive interface

Figure 2. The time-dependent run-down of various quantities for simulation II ($\tau = 0.035$). (a) The decrease in the mixed-layer $TS$ differences $\Delta T$ and $\Delta S$ (dashed and dash-dot lines, respectively), normalized by their initial values at $t = 0$, denoted by $\Delta \varphi_0$, as well as the ratio $R_p$. (b–d) The evolution of the interface thicknesses $h_T$, $h_S$, and the ratio $r$, respectively: the thick solid line represents the mean with the grey shading showing the 10th and 90th percentiles within the domain; the dashed line shows the hypothetical interface growth due to only molecular diffusion. The slope of the grey line in (c) indicates the rate of growth of the salinity interface by molecular diffusion at a thickness of 6 cm.

In simulation VIII, the initial breakdown of the thin interface at $\tau = 0.01$ resulted in very sharp $S$-gradients, and we were required to use an especially fine resolution in this case.

3. Time evolution

3.1. General description

It is beneficial to begin with an initial description of the time evolution of the diffusive interface. This is shown in figure 2 where the run-down of both the mixed-layer $TS$ differences, as well as the interface thicknesses, are plotted together with the dimensionless ratios $R_p$ and $r$, for simulation II ($\tau = 0.035$). In figure 2, and throughout this paper, we shall often use dimensional units (e.g. hours and cm). The reason for this is that since the dimensional parameters of the simulations are comparable to those found in relevant geophysical staircases, we believe that using dimensional values – as opposed to a time scale of $(\kappa_T/g^2)^{1/3}$, say – gives one more insight into these systems.

In all simulations, the $TS$-profiles are initiated, at $t = 0$ h, with the same interfacial thicknesses ($r = 1$), and $R_p = 2$. The linear stability analysis of Carpenter et al. (2012) has shown (for $\tau = 0.01$ and $Pr = 6$) that this corresponds to a stable configuration of $T$ and $S$. However, as time increases, both interfaces grow in thickness by molecular diffusion at a rate that is proportional to $\kappa_\psi^{1/2}$. Since $\kappa_T > \kappa_S$ the $T$-interface becomes thicker than the $S$-interface, and $r$ increases (figure 2b–d). Owing to the gravitationally unstable configuration of $T$, this mismatch of interface thicknesses when $r > 1$ has the effect of producing regions of gravitationally unstable density stratification above and below the gravitationally stable central core (figure 3). The gravitationally unstable layers are generally referred to as the ‘diffusive boundary layers’, and when $r > 1$ the interface is said to display a ‘double-boundary-layer’ structure (Fernando 1989). The diffusive boundary layer, and how it is coupled to both the stable core of the interface
and the mixed layers, is a common basis for a number of phenomenological models of the fluxes across the diffusive interface (e.g. Linden & Shirtcliffe 1978; Newell 1984; Fernando 1989; Kelley 1990; Worster 2004).

Convection begins at $t \approx 2$ h when the gravitationally unstable boundary layers break away from the stable interface core. At this time $h_T$ and $h_S$ depart from growth by pure molecular diffusion (dashed curves in figure 2b,c), and experience a rapid thinning. There is a sharp increase in $R_p$ as the boundary layer fluid is mixed into the upper and lower mixed layers (figure 2a). This time period, after the initial breakdown of the boundary layers, is the most energetic phase of the turbulence in the mixed layers. It displays elevated levels of the kinetic energy dissipation rate, and is therefore also the most difficult period to resolve numerically.

After the period of high turbulence following the initial breakdown of the boundary layers, the interfaces appear to slowly adjust to a preferred thickness ratio ($r \approx 2$ for simulation II). Figure 2 shows that while $h_T$ is continuously increasing in $t$, $h_S$ is initially eroded by the convective motions until $r \approx 2$ is reached. This apparent adjustment to a preferred value of $r$ was observed in nearly all of the simulations performed, and can be seen in figure 4 for simulations I–IV. In each case, however, after the initial adjustment, $r$ is still changing slowly in time. In § 6, we shall provide a possible explanation in terms of the interface stability.

### 3.2. Dependence on initial conditions

Worster (2004) has formulated an extension of the Linden & Shirtcliffe (1978) model of the diffusive interface that includes time dependence. The application of this model to laboratory experiments has found good agreement, and shows that the evolution of the diffusive interface is often dependent on the initial conditions. To test this dependence of the DNS we analyse a series of two-dimensional simulations (VIII–XI) at $\tau = 0.01$. Each simulation is initialized with a different interface thickness $h_0 = h_0(t = 0)$, where we fix $h_T = h_S$ (i.e. $r = 1$) at $t = 0$. The evolution of $h_T$, $h_S$, 

---

**Figure 3.** (Colour online) Illustration of the development of diffusive boundary layers due to the relatively thicker $T$-interface. The grey shaded regions highlight the location of the boundary layers and have a vertical height of $b = (h_T - h_S)/2$, which is to be used as a characteristic boundary layer length scale in § 6. Recall that both $T$ and $S$ are plotted in density units.
Figure 4. Time evolution of $r$ for simulations I–IV at different $\tau$. The grey colour of the $\tau = 0.01$ curve indicates the time over which the $S$-field was not completely well-resolved.

Figure 5. Time evolution of interface thicknesses (a) $h_T$, (b) $h_S$, and (c) their ratio $r$, for the sequence of two-dimensional simulations (VIII–XI) at $\tau = 0.01$ for various initial thicknesses $h_0$. The grey line in (b) indicates the rate of growth of $h_S$ by molecular diffusion at a thickness of 5 cm.

and $r$ in time is shown in figure 5. The evolution of $h_S(t)$ is in general similar to that shown in figures 2 and 4. In each case, once convection begins $h_S$ decreases as the salinity interface is initially eroded. This period of erosion becomes longer for each increase in the initial $h_S$ value. For the largest initial $h_S = 7.5$ cm, the period of $h_S$ growth has not yet begun by the end of the simulation. As in figure 4, each of the simulations in figure 5(c) appears to approach a relatively constant value of the interface thickness ratio. For the two simulations with $h_0 = 2.5$ and 5 cm (VIII,
9), the final value of \( r \approx 2.6 \) is nearly identical with the value found from the three-dimensional simulation (1). However, the simulations at the thickest initial values of \( h_0 = 6.5 \) and 7.5 cm have not yet reached this approximately steady value of \( r \).

A consistent run-down of the diffusive interface appears to be attained once the relatively constant value of \( r \) is reached. This is seen to be the case in each of the simulations (I–IV) in figure 4, as well as the \( h_0 = 2.5 \) and 5 cm simulations (VIII, IX) of figure 5. The run-down evolution of the diffusive interface once this state is reached may be understood by referring to the basic assumptions behind the model of Newell (1984), which can also be recovered from the more general formulation of Worster (2004). Initially formulated for the large-\( R_p \) region, with \( R_p > \tau^{-1/2} \), Newell (1984) was able to predict reasonable estimates of interface thicknesses and fluxes based largely on the assumption that the S-interface growth is controlled by molecular diffusion. This has been found to be a good approximation to the time evolution of \( h_S \) for late times, once a constant \( r \) is reached. The expected rate of growth of \( h_S \) by molecular diffusion alone is indicated by the slope of the grey lines in figures 5(b) and 2(c), and is found to agree closely with the observed \( h_S \) increase. Since molecular diffusion causes smaller interfaces to grow faster than thicker interfaces, the \( h_S(t) \) curves in figure 5(b) should all collapse onto a single curve at late times. This is seen to be nearly the case for three of the four simulations. Details of the Newell (1984) model and its implications for the heat fluxes will be discussed further in § 5.

4. Interface and boundary layer structure

4.1. Phenomenological description

In the previous section we showed that a persistent double-boundary-layer structure is present in all of the simulations. This can be seen in figure 1, and results in gravitationally unstable boundary layers above and below the stable interface core. This boundary layer is ultimately responsible for producing turbulence and mixing in the mixed layers, and a number of previous studies have proposed mechanisms to describe the coupling between the boundary layer and the mixed layer (Linden & Shirtcliffe 1978, Fernando 1989; Kelley 1990).

Kelley (1990) describes a model that is based on a large-scale circulation within the mixed layers. This circulation causes a highly sheared horizontal flow within the boundary layer, which forms thin sheet-like plumes that transport the boundary layer fluid vertically into the mixed layers. This description appears to be in good qualitative agreement with the simulations. Relatively thin plumes can be seen in figure 1, as well as in the density field plotted in figure 6(c), to be responsible for transporting boundary layer fluid into the mixed layers. To highlight the locations of the plumes in time we plot a scaled \( 2T/\Delta T(t) \) field taken at the vertical level \( z = h_R(t) + L_c/2 \), at the locations \( y = 0 \) and \( x = 0 \) in figures 6(a) and 6(b) respectively. This shows that the plumes are quasi-steady features with generally one plume being present in each layer. Note that although the plumes are persistent in time, there are always fluctuations in the size (inferred from the \( T \) anomaly present). These fluctuations appear to arise from the formation of new unstable plumes breaking away from the boundary layer, which are subsequently swept into the established plume sites by a large-scale circulation. This causes oscillations of the strength of the established plumes seen in figure 6(a,b). In addition to the fluctuations in plume strength, there are a number of shifts in the plume location.

The large-scale circulation can be seen from the two representative streamline patterns taken at different times and in different planes in figure 7, superimposed
Simulations of a double-diffusive interface

Figure 6. (a) Plot of $2T(x,t)/\Delta T$ for $y = 0$ cm and $z = h_T + L_c/2$ in simulation II showing the location of the plumes at low $2T/\Delta T$ values (recall that $T$ is in density units) as a function of $t$. (b) As in (a) but in the plane $x = 0$ cm. In both (a) and (b) two domains have been included in the spatial dimension for clarity, with the true domain size indicated by the dashed line. The location of the arrow in (b) indicates the time at which the density field $\rho - \rho_0$ at $t = 16$ h and $x = 0$ cm, shown in (c) is taken. Representative examples of $T$-, $S$-, and $\rho - \rho_0$-profiles are shown in (d) from $y = 30$ cm (indicated by the arrow in c), $x = 0$ cm and $t = 16$ h.

on shaded plots of the vertical $T$-gradient. The streamlines show the presence of large-scale circulations in the mixed layers, with very little small-scale turbulent motions. The structure of the velocity field in the same two-dimensional slice as that shown in figure 1(b,c), is plotted in figure 7(b). At this time, a new plume is in the process of forming and breaking away from the lower boundary layer near $x \approx 28$ cm.

In contrast to the Kelley (1990) model of steady large-scale circulations driven by plumes from the boundary layers, Linden & Shirkcliffe (1978) present a model that is based on the growth of the boundary layer by diffusion, then a sudden
breaking away of this unstable layer through a convective instability. The present simulations display elements of both theories, with a persistent unstable boundary layer present (figure 6c,d) that feeds quasi-steady plumes in support of the Kelley (1990) description, as well as periodically fluctuating flow and plume strength due to the formation of instabilities in the boundary layer also leading to shifts in the large-scale circulation in support of Linden & Shircliff (1978). It should be noted that since the convection usually consists of only a single cell the small domain size is likely to be exerting an influence on the flow. However, no significant changes were found in simulations V and VI where the domain size was increased.

4.2. Vertical structure of the interface and boundary layers
Despite the fluctuations and shifts of the large-scale circulation, we may obtain a meaningful picture of the mean velocity structure in the vicinity of the interface if we scale the vertical $z$ coordinate by the half-width of the $T$-interface thickness, i.e. by defining the dimensionless vertical coordinate

$$\xi(t) = \frac{2(z - L_z/2)}{h_T(t)}.$$  \hspace{1cm} (4.1)

Once plotted as a function of $\xi$, and normalized by the volume average to remove the time-dependent amplitude, the root-mean-squared (r.m.s.) vertical velocity field shows
Simulations of a double-diffusive interface

Figure 8. Profiles of (a) $\hat{w}_{\text{rms}}(\xi)$ and (b) $\hat{S}_U(\xi)$ every 0.5 h from $t = 5.8$ h to the end of the simulation at $t = 32$ h ($2.5 < R_\rho < 6.1$). The grey dashed line in (b) shows an $\hat{S}_U \propto \xi^2$ dependence for comparison.

reasonable collapse to a similar form for small $\xi$ (Figure 8a). Mathematically, this can be written as

$$\hat{w}_{\text{rms}}(\xi, t) = \sqrt{\frac{\langle w^2 \rangle_{xy}}{\langle w^2 \rangle_{xyz}}},$$

where we use angled brackets to denote averaging over the variable $X$ as $\langle \rangle_X$. This averaging reduces the (spatial) variability between profiles at various $t$. The averaged profiles are plotted every half-hour in Figure 8, from $t = 5.8$ to 32 h and $R_\rho = 2.5$ to 6.1, after the initial phase of intense turbulence. It can be seen that the vertical velocity vanishes within the interface, indicating that mixed-layer turbulence is not able to penetrate the stable stratification of the core. This has significant implications for the fluxes of $T$ and $S$ that will be discussed in the following section.

Also, shown in Figure 8(b) is the scaled mean horizontal shear defined by

$$\hat{S}_U(\xi, t) = \frac{\langle S_U \rangle_{xy}}{\langle S_U \rangle_{xyz}}, \quad \text{with} \quad S_U = \sqrt{\left(\frac{\partial U}{\partial z}\right)^2 + \left(\frac{\partial V}{\partial z}\right)^2}. $$

An elevated shear can be seen within the boundary layers, which diminishes as the stable core of the interface is approached. In keeping with our phenomenological
Figure 9. Scaling of $r$ with $\tau$ for three-dimensional simulations (I–VI) and the two-dimensional simulations (VIII, IX), together with the slopes of the $\tau^{-1/2}$, $\tau^{-1/3}$, and $\tau^{-1/5}$ models for comparison. The values of $r$ were determined by averaging the last 10 h of the mean $r(t)$ for each simulation.

description, the source for the elevated shear in the boundary layers appears to result from the boundary layer fluid being drawn horizontally towards the plume sites. This observation provides some support for the Kelley (1990) model, which assumes that all of the kinetic energy dissipation occurs in the horizontally sheared boundary layers. However, we also observe significant shear (and hence dissipation) to be present in the mixed layers.

4.3. Scaling of the interface thickness ratio

Although the simulations do appear to adjust to a state in which $r$ is slowly changing in time, it is nonetheless instructive to compare the approximate scaling of $r$ with $\tau$ to gain further insight into the double-boundary-layer structure. Figure 9 shows a log–log plot comparing the four simulations with different $\tau$, along with the two $\tau = 0.07$ simulations (V and VI) where the domain size was varied, and the two-dimensional simulations (VIII and IX) with $\tau = 0.01$. The $r$ values plotted were obtained by averaging over the final 10 h of each simulation (see figure 4 for an indication of this averaging time). A definite dependence of $r$ on $\tau$ is observed. As one would expect intuitively, smaller values of $\tau$ – and therefore a greater difference in the $T$ and $S$ molecular diffusion ‘speeds’ – lead to larger values of $r$, i.e. greater differences between the relative interface thicknesses.

It is interesting to compare the observed scaling of $r$ with $\tau$ to two simple models of the diffusive interface. In each model we assume that interfaces grow by molecular diffusion according to

$$h_y \propto (\kappa_m t)^{1/2}.$$  \hspace{1cm} (4.4)

In the first model we take the time scale, $t_*$, over which the convection process removes the boundary layer fluid to be equal for both $T$ and $S$. Substituting $t = t_*$ into (4.4) the ratio of interface thicknesses then gives the scaling $r \sim \tau^{-1/2}$ (figure 9).
This scaling was suggested previously by Fernando (1989). Note that this scaling also assumes that sufficient time has elapsed between entrainment events of the boundary layer fluid.

The second model builds on the interpretation of Kelley (1990), which was qualitatively found to match our observations, as discussed above. Since the boundary layer fluid is acted on by a large-scale circulation that sweeps it towards the plumes, and because we find that a shear is present across the boundary layers, we should expect that the time scale for diffusion of the $T$- and $S$-interfaces is different. The shear enhances the lateral transport of $T$ relative to $S$, since the thicker $T$-interface finds itself in regions of larger velocity. The time scale for growth of each interface can then be expressed as $t_{\text{eq}} \sim \ell / S_U \nu$, where $\ell$ is the distance between plumes, and $S_U$ is a measure of the velocity shear. In the case of a constant shear, we substitute $t_{\text{eq}}$ into (4.4), taking the ratio, and solving for $r$ yields a $r \sim \tau^{-1/3}$ scaling. This scaling has been proposed to describe the relative thicknesses of the velocity and thermal boundary layers in thermal convection close to a solid no-slip boundary (Grossman & Lohse 2000).

Although taking account of the shear across the interfaces leads to an estimate that is closer to the observations in figure 9, the profiles in figure 8(b) show that the shear across the interface region (from $-1 < \zeta < 1$) is not constant. We therefore propose a more general time scale that accounts for a depth dependence of shear given by

$$t_s = \frac{\ell}{\int_0^1 S_U(\zeta) \, d\zeta}$$

with the denominator representing an effective velocity scale for the advection of the interfaces (by symmetry only the upper half need be considered). Choosing a form that is more representative for the shear $S_U \propto \zeta^3$, as shown in figure 8(b), leads to a scaling that is closer to the observations of $r \sim \tau^{-1/3}$. Note that any power-law relationship could be used, i.e. $S_U \propto \zeta^n$, and would lead to a scaling of $r \sim \tau^{-1/(n+3)}$. However, despite the obvious improvements when a variable shear profile is used, we do not have an adequate number of simulations to accurately test for the best scaling.

It should also be noted that as $\tau \to 1$ the interface thicknesses should be increasingly dominated by molecular diffusion, rather than the DD convection process, and we must have $r \to 1$, as appears to be the case. The value of $r$ is also found to vary weakly with the domain sizes $L_x$ and $L_z$, indicating that the domain size may exert an influence on the properties of the boundary layers. Simulations in larger domains with many large-scale convection cells may reduce this scatter.

5. Heat and salt fluxes

5.1. Are the fluxes through the interface molecular?

Of primary importance in the study of DD convection are the fluxes, denoted by $F_{\phi}$, of $T$ and $S$ across the interface. Furthermore, it is possible to compute these quantities very precisely from DNS. The method that we use is based on the framework of Winters et al. (1995) and Winters & D’Asaro (1996). Every grid point in the domain from the $\phi$ scalar field is assembled and sorted to form a single monotonic background profile $\phi(z_0)$, where $z_0(\phi_0)$ denotes the background level of the $\phi_0$ scalar value. Since the boundary conditions permit no flux of $\phi$ across them, the total “$\phi$-mass” within the
domain must be constant, i.e.

$$\int_V \varphi(x, y, z, t) \, dV = \int_0^{t_e} \varphi(z_b) \, dz_b = \text{const.}$$

(5.1)

where $V$ is the domain volume. The $\varphi$-flux, $F_\varphi$, through the $\varphi_0$-surface, is then easily computed by the total change in storage below (or above, depending on the sorting procedure) the level $z_b(\varphi_0)$, given by

$$F_\varphi = \frac{d}{dt} \int_0^{z_b(\varphi_0)} \varphi(z_b) \, dz_b.$$  

(5.2)

Choosing $\varphi_0$ to be the central $T$ and $S$ scalar values within the interface (i.e. $T_0 = \Delta T/2$ and $S_0 = \Delta S/2$) leads to the determination of the interfacial $TS$-fluxes. These are plotted as a time series for simulation II ($\tau = 0.035$) with the thick solid lines in figure 10.

In addition to the total flux $F_\varphi$ across the diffusive interface, we also plot what we will refer to as the ‘molecular’ flux, $F_\varphi^{\text{mol}}$. This is defined mathematically by

$$F_\varphi^{\text{mol}} \equiv \kappa_\varphi \frac{\partial \varphi}{\partial z} \bigg|_{\varphi_0} = \kappa_\varphi \frac{\Delta \varphi}{h_\varphi},$$

(5.3)

where the $\varphi_0$ subscript indicates that the derivative is evaluated at the $z$ where $\varphi = \varphi_0$, and the second equality follows from the definition of $h_\varphi$ in (2.3). Physically, $F_\varphi^{\text{mol}}$ is the vertical $\varphi$-flux at each horizontal location of the interface, assuming that the flux is purely molecular. In general, $F_\varphi^{\text{mol}}$ need not be a single-valued function of $(x, y)$ since the $\varphi_0$-surface could fold over itself; however, this was not found to be the case for any of the simulations. Both the average value of $F_\varphi^{\text{mol}}$, as well as the 10th and 90th percentiles found within the domain, are plotted in figure 10. This figure shows that, in general, the $T$- and $S$-fluxes are equal to their molecular values. An exception is the phase of intense turbulence from $t = 2$ to $4$ h where $F_S$ is in excess of $F_S^{\text{mol}}$ by 10\%. A
similar spike occurs in \( F_T \) at \( t \approx 2 \) h, but is of very limited duration. For the remainder of the simulation \( F_T = F_T^{\text{mol}} \) to within 5\%. It should be noted that a correction has been applied to \( F_T^{\text{mol}} \) of 1.1\% in order to account for the averaging procedure when calculating the gradients in the interface (see §2.2).

In general, the enhanced transport of scalar quantities that is associated with turbulent mixing (across some isoscalar surface) is accomplished by: (i) a sharpening of gradients; and (ii) an increased area of the isoscalar surface. The close agreement of \( F_T^{\text{mol}} \) shows that the enhanced transport of \( T \) and \( S \) at a diffusive interface is caused almost entirely by (i). This can be seen by noting that the total flux across any \( \psi \)-surface for a turbulent flow is given at each point on the surface by the normal component of the diffusive flux, i.e. \( \kappa_\psi \nabla \psi \cdot \hat{n} \), where \( \hat{n} \) is the unit normal vector to the surface (Winters & D’Asaro 1996). Therefore, for a completely flat and horizontal \( \psi \)-surface, the total flux is given entirely by its vertical component \( \kappa_\psi \nabla \psi \cdot \hat{n} = \kappa_\psi \frac{\partial \psi}{\partial z} \). This was found to be the case in all of the simulations performed, and is in agreement with the vanishing of the r.m.s. vertical velocity within the interface (figure 7b).

The formulation of many phenomenological models of the diffusive interface from previous studies has been based on the assumption of molecular fluxes through the interface core (Linden & Shirtcliffe 1978; Newell 1984; Kelley 1990). Furthermore, the field observations of Padman & Dillon (1987) and Timmermans et al. (2008) have shown a close agreement between \( F_T^{\text{mol}} \) and the \( F_T \) predicted by different laboratory-based flux laws. However, we are not aware of any study that has definitively shown the fluxes to be molecular, with the exception of the experiments of Shirtcliffe (1973) using a salt–sugar interface (\( \tau \approx 0.33 \)).

### 5.2. Comparison with flux laws

The ability to calculate precise fluxes in the DNS allows a comparison with flux laws suggested by previous researchers. Figure 11(a) shows \( F_T \) plotted as a function of \( R_p \) for simulations I–IV. It has become customary to normalize \( F_T \) by the standard 4/3 flux law that is used in the case of single-component convection through a solid plane boundary (e.g. Turner 1973; Linden 2000), which is given in units of kg m\(^{-2}\) s\(^{-1}\) by

\[
F_T^{\text{SP}} = \lambda^{\text{SP}} \kappa_T \left( \frac{g}{\rho_0 \kappa_T} \right)^{1/3} (\Delta T)^{4/3},
\]

where \( \lambda^{\text{SP}} \) is a coefficient taken as 0.085. In this dimensionless form, a horizontal line on figure 11 would indicate that \( F_T \) is given by a 4/3 flux law with \( F_T \propto \Delta T^{4/3} \). This form for the \( T \)-flux was first suggested by Turner (1965); however, he found that \( F_T \) was dependent on \( R_p \), showing decreasing \( F_T \) (and \( F_T/F_T^{\text{SP}} \)) as \( R_p \) increases. In the case of the \( \tau = 0.01 \) simulation (I) we observe no strong dependence on \( R_p \) (figure 11). In all other simulations a decreasing \( F_T \) is observed with increasing \( R_p \).

The flux laws of Kelley (1990) and Linden & Shirtcliffe (1978) generally show lower predicted fluxes than that observed in the simulations, with a stronger dependence on \( R_p \). Note that the Kelley (1990) parameterization is only valid for oceanic values of \( \tau \approx 0.01 \) and \( Pr \approx 7 \), whereas the Linden & Shirtcliffe (1978) parameterization is valid for a range of \( \tau \) and \( Pr \), as long as the condition \( 2 < R_p < \tau^{-1/2} \) is met. We may therefore compare the Linden & Shirtcliffe (1978) predictions to all but the \( \tau = 0.33 \) simulation.

The behaviour of \( F_T \) once the \( r \approx \) constant run-down state is reached can be understood by appealing to the model proposed by Newell (1984). This model is based on the following four assumptions describing the run-down of the interface.
Figure 11. The dimensionless $T$-flux $F_T/F_T^{SP}$ as a function of $R_p$ for (a) simulations I–IV, and (b) the two-dimensional simulations (VIII–XI). Also shown in (a) are the predictions of the flux laws developed by Kelley (1990) for $\tau = 0.01$, and Linden & Shirkcliffe (1978) for $\tau = 0.01, 0.035, 0.07$. The grey region of the $\tau = 0.01$ curve indicates the period over which the $S$-field is not completely well-resolved.

(i) The fluxes through the interface are molecular, giving

$$F_T = \kappa_T \Delta T/h_T. \quad (5.5)$$

(ii) The $S$-interface evolution is determined by molecular diffusion, which, assuming an error function profile is given by

$$h_S(t) = 2[\pi \kappa_S (t + t_0)]^{1/2}, \quad (5.6)$$

where $t_0$ is a time shift used to recover an initial $h_S$ condition.

(iii) The $F_T$ through the interface is used entirely to heat the mixed layer, or in other words, the heat required to increase $h_T$ is negligible. A heat balance then leads to
the relationship

\[
\frac{\mathrm{d}\Delta T}{\mathrm{d}t} = -\frac{4}{I_c} F_T. \tag{5.7}
\]

Note that we have assumed that the mixed layer is a constant thickness of \(L_c/2\) rather than expressing it as a function of \(h_T\).

(iv) A final assumption that is made by Newell (1984) based on measurements taken from laboratory experiments is that the \(T\)- and \(S\)-interfaces have the same thickness, i.e. \(r = 1\). Our simulations show that the thickness ratio is a function of \(\tau\), and so we shall modify Newell’s model with the fourth condition

\[
\frac{\mathrm{d}h_T}{\mathrm{d}t} = r_0 \frac{\mathrm{d}h_S}{\mathrm{d}t}, \tag{5.8}
\]

where \(r_0\) is the approximately constant observed value of \(r\).

Equations (5.5)–(5.8) describe an initial-value problem for a first-order ordinary differential equation that we can solve for \(F_T(t)\), as well as other parameters such as \(\Delta T(t)\) and \(h_T(t)\). The resulting predictions for the \(T\)-flux are shown for simulations I–IV in figure 12, and are found to provide a good prediction of \(F_T\) once a constant \(r\) is reached. This modified Newell (1984) prediction is also shown in the \(F_T/F_T^{37}\) versus \(R_p\) plot in figure 11(b), and predicts only a very gradual decrease in the normalized \(F_T\) as is observed in the simulations.

The results discussed above suggest the following interpretation of the run-down evolution of the diffusive interface. Turbulent motions within the mixed layers are unable to penetrate the strong stratification of the interface, and the resulting fluxes of \(T\) and \(S\) are described by a molecular flux law through the interface core. Owing to this lack of entrainment from the core, the increase of the \(S\)-interface thickness is determined by molecular diffusion. The shear that occurs within the boundary layers,
Figure 13. (Colour online) The flux ratio, $R_F$, plotted against $R_p$ for simulations I–IV in which $\tau$ is varied: (a) $\tau = 0.01$; (b) 0.035; (c) 0.07; (d) 0.33. A comparison is made in each case with the slope predicted by the Newell (1984) and Fernando (1989) models. The Linden & Shirtcliffe (1978) prediction is for a constant $R_F = \tau^{1/2}$ for $R_p < \tau^{-1/2}$, and is therefore only shown in this region.

that is set up by the large-scale circulation, is then responsible for determining the $T$-interface thickness, and hence the $T$-flux. Owing to the slow growth of the $\delta$-interface in the low-$\tau$ simulations, we should expect the $T$-flux to follow a $\Delta T^{4/3}$ dependence, as seen by the weak $R_p$ dependence of the curves in figure 11. This can be explained physically by the fact that a slowly diffusing and stable $\delta$-interface without significant entrainment acts similarly to a solid conducting plane. In this limiting case we should have an $F_T \sim \Delta T^{4/3}$ scaling, and a purely horizontal trajectory in figure 11.

5.3. Coupled TS-fluxes: the flux ratio

The observation of molecular fluxes through the interface has implications for the coupled transports of $T$ and $S$. This is expressed by the flux ratio, defined as

$$R_F = F_{\delta}/F_T.$$  

(5.9)

It is customary to consider $R_F$ to be a function of $R_p$ for a given $\tau$ and $Pr$, and we have plotted this for simulations I–IV in figure 13.

In all cases, we observe an overall increasing $R_F$ with $R_p$. The slope of these curves can be easily explained considering that: (i) the fluxes through the interface are molecular; and (ii) a relatively constant interface thickness ratio $r$, is observed. Writing
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<table>
<thead>
<tr>
<th>Study</th>
<th>$R_F$ parameterization</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Turner (1965)</td>
<td>$R_F = 0.15$</td>
<td>Bottom-heated experiments using heat and salt ($\tau^{1/2} = 0.11$)</td>
</tr>
<tr>
<td>Shirtcliffe (1973)</td>
<td>$R_F = \tau^{1/2}$</td>
<td>Run-down experiments using salt and sugar</td>
</tr>
<tr>
<td>Linden &amp; Shirtcliffe (1978)</td>
<td>$R_F = \tau^{1/2}$</td>
<td>Theoretical model</td>
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<tr>
<td>Takao &amp; Narusawa (1980)</td>
<td>$R_F = 0.039\tau^{-1/3}$</td>
<td>Bottom-heated experiments using heat and various salts</td>
</tr>
<tr>
<td>Newell (1984)</td>
<td>$R_F = \tau R_\rho$</td>
<td>Run-down and bottom-heated experiments (heat–salt)</td>
</tr>
<tr>
<td>Fernando (1989)</td>
<td>$R_F = \tau^{1/2}R_\rho$</td>
<td>Bottom-heated experiments (heat–salt)</td>
</tr>
<tr>
<td>Stamp et al. (1998)</td>
<td>$R_F = \tau^{1/2}$</td>
<td>Run-down experiments (salt–sugar)</td>
</tr>
</tbody>
</table>

**Table 3.** Parameterizations suggested or found in previous studies. The vertical boundary conditions for the laboratory experiments are either of the run-down type, with no flux of $T$ or $S$, or bottom-heated with a flux of $T$ at the bottom boundary. In each study the $R_F$ parameterization applies when $R_\rho$ is not too small, which is generally for $R_\rho \gtrsim 2$.

The flux as $F_\varphi = \kappa_\varphi \Delta \varphi / h_\varphi$, and taking the ratio leads to

$$R_F = \tau R_\rho.$$  \hspace{1cm} (5.10)

Therefore, we expect the $R_F$ versus $R_\rho$ curve to be an approximately straight line with slope $\tau \tau$. Using the scaling of $r \sim \tau^{-1/5}$, we predict a slope of $\tau^{4/5}$ for the curves, and this prediction is shown in figure 13.

A number of previous studies have made predictions for the $R_F$ versus $R_\rho$ relationship that we can use as a reference to compare with. These parameterizations and the methods used to develop them are listed in Table 3. Newell (1984) proposed a similar model to that above, in which he took $r = 1$ based on profiles measured from laboratory experiments. However, his experiments were generally carried out in the so-called large-$R_\rho$ regime, where $R_\rho > \tau^{-1/2}$. In another model of the diffusive interface, Fernando (1989) argues that the interface thicknesses are determined by a competition between growth by diffusion, and entrainment by turbulent convective motions. He assumes that the time scale between successive turbulent entrainment events is long enough that $r = \tau^{-1/2}$. The $R_F$ curve should therefore follow a much steeper slope than that of Newell (1984), as shown in figure 13. However, our lack of turbulent motion in the interface (see figures 7b and 10) suggests that the Fernando (1989) model is not valid for our simulations, and this may be due to the different boundary conditions used in the bottom-heated experiments of Fernando (1989). Yet another model of the diffusive interface, due to Linden & Shirtcliffe (1978), supposes that the interfacial fluxes are determined by the periodic breaking away of boundary layer fluid once a critical boundary layer Rayleigh number is reached. By assuming that $T$ and $S$ are diffused into the boundary layer over equivalent time scales, and that the entire boundary layer breaks away from the interface, they predict that $R_F = \tau^{1/2}$, independent of $R_\rho$. The Linden & Shirtcliffe (1978) model result was first found experimentally by Shirtcliffe (1973), in reasonable agreement with the experiments of Turner (1965), and is only expected to apply for the intermediate-$R_\rho$ range of $2 \lesssim R_\rho < \tau^{-1/2}$, as plotted in figure 13.
Figure 13 clearly shows that the simulations are best described by the $R_F = \tau r R_g$ relation in (5.10) when the observed scaling of $r \sim \tau^{-1/5}$ is used. Although this finding is in agreement with the model presented in Newell (1984) when $r$ is parameterized appropriately, it does not agree with the many studies showing a $R_F = \text{constant}$ relationship (see table 3). From our simulations it would seem that the $R_g$ dependence of $R_F$ is a general feature of the run-down configuration; however, we have no satisfactory explanation for the discrepancy with the experiments of Shirtcliffe (1973) and Stamp et al. (1998) showing a constant $R_F$.

6. Boundary layer stability

We have thus far observed that the diffusive interface naturally evolves to a double-boundary-layer structure with $r > 1$. Turbulent motions are suppressed by the stable interface core, and the interfacial fluxes are governed by molecular transport. We see, therefore, that it is natural for the diffusive interface to support a gravitationally unstable boundary layer. The question arises, however, as to just how unstable this layer becomes? We shall now address this question by appealing to the ideas presented in Linden & Shirtcliffe (1978), and to recent results utilizing a linear stability analysis by Carpenter et al. (2012).

Linden & Shirtcliffe (1978) proposed that the diffusive growth of the interfaces in time is limited by the gravitationally unstable boundary layer becoming hydrodynamically unstable, i.e. evolving to a state in which small perturbations will grow continuously in time. In accordance with the study of single-component convection by Howard (1964), they assumed that a breakdown of the boundary layer would be triggered once a critical boundary layer Rayleigh number $Ra_{bl,cr} \approx 10^5$ is exceeded. $Ra_{bl}$ is defined by

$$Ra_{bl} \equiv \frac{g\delta \rho b^3}{\rho_0\nu k_T},$$

(6.1)

where $b$ is a representative length scale of the boundary layer (see figure 3) given by $b = (h_T - h_S)/2$, and $\delta \rho$ is a representative boundary layer density scale, defined through the relation

$$\delta \rho b = \int_{z_{bl}}^{h_T} [\Delta \rho/2 - |\bar{\rho}(z) - \rho_0|] \, dz,$$

(6.2)

where $\Delta \rho = \Delta S - \Delta T$, $\bar{\rho}(z) = \langle \rho \rangle_{z_{bl}}$ is an average density profile, and $z_{bl}$ is determined from $|\bar{\rho}(z_{bl}) - \rho_0| = \Delta \rho/2$. This choice of $z_{bl}$ ensures that the integration in (6.2) is over the total gravitationally unstable density anomaly in the upper boundary layer. In other words, $z_{bl}$ is chosen such that all the fluid in the upper boundary layer that is lighter than the mixed layer above is included in the integration (see Linden & Shirtcliffe 1978). Since a symmetry of the upper and lower boundary layers is assumed, the same reasoning applies below the interface. In practice, we assume an error-function profile for $T$ and $S$ with the same $h_g$ and $\Delta \varphi$ as measured, which allows us to write $Ra_{bl}$ as a function of $R_g$, $r$, and $Ra_t$, as long as $L_e/h_T$ is not too small (see Carpenter et al. 2012, for further details).

The $Ra_{bl}$ condition of Linden & Shirtcliffe (1978) represents a plausible control on the growth of the boundary layer, and has received some tentative support from field observations (Padman & Dillon 1989; Sanchez & Roget 2007), although these observations lack sufficient knowledge of the $S$-field. It is possible to determine $Ra_{bl}(t)$ in the simulations, and this is shown in figure 14. First, it can be seen that much larger
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![Graph](image)

**Figure 14.** $Ra_{bl}$ of the diffusive interface in time for simulations I–IV. The grey portion of the $\tau = 0.01$ curve denotes the period of the simulation that was not well-resolved.

$Ra_{bl}$ are obtained when the diffusive interface grows from the quiet and stable initial condition at early times, than once the convection process has begun. If there was a true $Ra_{bl}$ that represented an upper limit on the growth of the boundary layers, then we should expect to see the curves in figure 14 saturate at some level. Instead, for each simulation we see that there is a time dependence of $Ra_{bl}$. This time dependence is not very strong once a quasi-steady run-down of the interface has begun. Figure 14 does show that for the growing and convecting diffusive interface, an order-of-magnitude estimate of boundary layer conditions can be obtained with $Ra_{bl} = O(10^2)$, an order of magnitude lower than previously assumed.

The relatively constant values of $Ra_{bl}$ attained in the simulations also support our observation that the boundary layer fluid is removed principally by quasi-steady large-scale motions in the mixed layers. If the periodic breakdown and subsequent growth of the boundary layers to an unstable state was occurring, then we should expect to see large fluctuations in the $Ra_{bl}$ curves.

In the recent study of Carpenter et al. (2012), the linear stability of the diffusive interface was examined in detail. For the oceanographically relevant parameters of $\tau = 0.01$ and $Pr = 6$, instability was found to result from a convective-type mode in the gravitationally unstable boundary layers, confirming some of the basic assumptions of Linden & Shirkcliff (1978). The stability analysis relies on the assumption of a frozen-in-time background state, and predicts that instability occurs for $Ra_{bl}$ as low as 10. However, when the predictions of the stability analysis were tested using a two-dimensional DNS of the interface, it was found that the time dependence of the background state (which is diffusing in time) was important in determining the conditions at the point of boundary layer breakdown. The value of $Ra_{bl} \approx 50$ was found for the quasi-steady run-down of the two-dimensional simulation of Carpenter et al. (2012), showing reasonable agreement with the three-dimensional results found here.

7. Summary and conclusions

A series of DNS have been performed to study the diffusive interface within the range of conditions found in geophysical observations, notably the thermohaline staircase of Lake Kivu. The boundary conditions correspond to previous laboratory
studies, which are carried out in a container insulated against the flux of $T$ and $S$. The DNS therefore exhibit a time-dependent ‘run-down’ of the $T$ and $S$ differences across the interface.

The simulations provide the most detailed observations of the diffusive interface to date, and have revealed a number of important features. The $TS$-interfaces are found to evolve naturally to a double-boundary-layer structure where the $T$-interface is thicker than the $S$-interface, i.e. $r = h_T/h_S > 1$. Therefore, two gravitationally unstable boundary layers are supported on each side of the stably stratified central core of the interface. These unstable boundary layers were found to lead to the formation of plumes that feed large-scale convection cells within the mixed layers. This circulation creates a shear across the boundary layers with a reduced shear inside the interface core. By accounting for the shear across the boundary layers, various scaling laws can be obtained to predict the interface thickness ratio $r$ based on the diffusivity ratio $\tau$. Using the observed shear profiles in the boundary layer we find that $r \sim \tau^{-1/5}$ best describes the simulations, and is consistent with our observed scaling.

The turbulence of the mixed layers was not found to penetrate the stable stratification of the core, and the $TS$-fluxes were reduced to molecular levels inside the interface. Once a quasi-steady run-down state was achieved, the evolution of the interface thicknesses, and therefore also the fluxes, were found to be well-predicted by the model of Newell (1984), which assumes that the $S$-interface thickness is governed by pure molecular diffusion of the interface in time. This model is also consistent with the more general formulation of Worster (2004). The flux ratio $R_F = F_S/F_T$ was predicted well by the ratio of $T$ and $S$ molecular fluxes $R_F = rT\tau R_p$, where the density ratio $R_p$ is determined by the run-down of the mixed layers, and $r \sim \tau^{-1/5}$ was found to be approximately constant in time for each simulation.

Finally, we considered the stability of the boundary layers as a function of the boundary layer Rayleigh number $Ra_{bd}$. We found that an order-of-magnitude estimate of $Ra_{bd} = O(10^2)$ can be used to describe the simulations. However, we remark that the boundary layer stability may be inherently time-dependent and may exhibit a dependence on the circulations that develop. In this case, a critical boundary layer Rayleigh number would not apply to all diffusive interfaces (see Carpenter et al. 2012, for further discussion).

Future work could extend the present DNS in several ways. For example, the run-down behaviour of the interface could possibly be removed by including periodic conditions at the top and bottom boundaries, also bringing the simulations closer to conditions found in natural staircases, and this work is currently underway. Also, more simulations could be performed to test the scaling relationship between $r$ and $\tau$. A future study should also investigate the low-$R_p$ regime in which mixed-layer turbulence is expected to penetrate the interface and alter the coupled transports of $T$ and $S$. Finally, a more accurate description of the stability properties of the diffusive interface might be possible by explicitly including the time-dependent interface growth.

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Magdo, milacku, my se mame. Dekuju! Cas na cestovani. Jedeme, tramvaj, jedeme.
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