
Forward and inverse modelling of thermal stratifications in confined spaces

Submitted for the degree of Doctor of Philosophy by

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I hereby declare that the work in this dissertation is my own. Any work or contribution by others is appropriately referenced.

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Abstract

Spatially heterogeneous heating and cooling is common in practical applications, such as in the ventilation and heating or cooling of buildings. However, simple models of the resulting buoyancy field typically account for either localised or distributed heat sources independently, without necessarily incorporating effects arising from their interaction. As a canonical means of investigating the latter, this thesis studies the flow and thermal stratification of a closed domain subjected to different combinations of line and distributed surface heating and cooling in time and space. Our observations of steady and transient states are drawn from a set of direct numerical simulations in which the ratio Γ of the strength of the distributed sources to the localised sources is varied. We show that Γ plays a decisive role in determining the system's statistically steady state, particularly in restricting the emergence of two-layer stratifications to $\Gamma < 1$, and demonstrate the importance of an increasing lateral dependence of the buoyancy field with increasing distributed heating at $\Gamma < 1$. Especially the dynamic of transient states following a step change in $\Gamma < 1$ is crucially determined by lateral heat transport at a finite velocity. Building on existing approaches that typically assume uniform buoyancy within each layer, we develop a steady state model that incorporates a lateral buoyancy gradient and exhibits a better agreement with observations.

Predicting the effects of different heating distributions finds application in inverse problems of estimating boundary heat fluxes from interior temperature measurements and are of particular interest in building design and heating control. We performed a parameter estimation based on a simple two-dimensional model, however, the results show a large standard deviation from the true values. This suggests that compensating for systematic modelling errors, for example via a Bayesian approach, may be necessary to infer heterogeneous boundary conditions from simple stratification models.

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Chapter 1

Introduction

1.1 Motivation

In the current context of anthropogenic climate change, reducing greenhouse gas emissions and, by extension, energy consumption has become a chief concern. Buildings account for a third of the global energy consumption and correspond to an even greater share in some of the nations with the greatest energy demand, such as for 41% in the EU [40]. The first step in attempting to reduce building energy consumption while maintaining comfortable conditions for the occupants is a thorough understanding of the building's ventilation, temperature structure and heat exchange. An appropriate modelling of this thermal system can then be utilised in the context of optimal design and optimal energy management of buildings.

Beyond considerations of sustainability in building design and management, the COVID-19 pandemic has highlighted the important role that indoor temperature structures and local flow patterns play in the transmission of airborne viruses [15]. The prediction of such local effects is extremely challenging, since they take place in the typically complex geometries of indoor environments, depend on heterogeneous boundary conditions imposed by ventilation openings and heating or cooling appliances and are subjected to time-varying forcings resulting from occupancy and use conditions. In this context, a detailed understanding of the impact of heterogeneous forcings and their reconstruction from limited measurements could help to develop mitigating strategies.

The character of indoor air flow and temperature structure is crucially dependent on the spatial distribution of heat sources and sinks. Localised sources of heat give rise to turbulent plumes [73], which are free-shear flows that entrain and mix fluid from their environments. A confined plume typically leads to a stable stratification of the surrounding environment [9], as relatively warm, buoyant fluid accumulates below the ceiling in a deepening layer of increasingly warmer fluid [117]. In a building context, plumes can represent the effect of radiators, air conditioners, electrical appliances, occupants and/or lighting [61–63, 95]. In contrast to the effect of localised heat sources, sources of uniformly distributed heat flux typically result in vigorous turbulence throughout the considered enclosure, which homogenises the density field. Rayleigh-Bénard convection, which occurs when a fluid is uniformly heated from below and uniformly cooled from above, is a canonical flow of this type [1]. In buildings, distributed sources may represent the effect of conductive heat transfer through walls and windows or solar gains.

Physical models of indoor temperature structure commonly account for either localised or distributed sources of heat, corresponding to a stably stratified or homogeneous temperature field, respectively. However, distributed or localised heating or cooling represent only two extremal cases in a wide range of possible heterogeneous buoyancy flux distributions on a domain boundary. In particular, elements in building applications that represent localised or distributed heat sources are more generally found in combination with each other. In the case of a combination of localised and distributed sources of buoyancy, a competition results between the stabilising effect of the localised source, and the destabilising effect of the distributed source [116], which raises the question of how the flows resulting from the different types of forcing interact.

Determining the flow and temperature field from given boundary conditions, or generally, the physical state of a system from its cause, is termed a *forward* problem. To utilise an understanding of the *forward* effect of heterogeneous buoyancy sources in control or design applications typically requires the solution of an *inverse* problem, where one aims to determine the parameters that determined an observed physical state. Inverse problems find application, for example, in energy retrofitting of existing buildings [43], fault detection and diagnosis [120] or to develop predictive control strategies, e.g. based on weather forecasts [81]. In this context, the objective of the inverse problem is to determine unknown parameters of a thermal model of the building that would be expensive or inaccurate to measure directly or cannot be measured, such as internal gains due to occupancy and use conditions.

The subject of this thesis is the effect of combined localised and distributed buoyancy sources and the numerical ‘inversion’ of the temperature structures they produce. In the following, we will first review existing work related to this subject, before specifying the problem that is considered in this thesis.

1.2 Related work

The focus of this thesis is on configurations where combinations of distributed and localised buoyancy sources give rise to a stable stratification in the bulk, i.e., ignoring boundary layers. In the current section, we first consider work on stable stratifications arising from one or multiple localised source(s) in an enclosure. Existing work on combined localised and distributed sources is discussed in the second part of this section and builds upon the understanding of configurations with solely localised sources of buoyancy. Lastly, we give a brief overview of the vast topic of inverse heat transport problems, particular in the context of building applications, and discuss work considering multiple sources of buoyancy.

Confined plumes and stratification

A localised buoyancy source results in a turbulent plume, which entrains and mixes fluid from its ambient [73]. A confined plume thus influences the flow and density field in its environment, which results in a situation where the plume impacts its environment and vice versa. A canonical case of this type is the filling box mechanism first described in detail by Baines and Turner [9, fig. 1.1a]. In an enclosure of homogeneous density that contains a localised source at floor level, buoyant fluid from the resulting plume reaches the ceiling and spreads out below it. Gradually, a deepening, stratified layer is formed above the homogeneous fluid, as the plume entrains fluid from the newly formed buoyant layer and thus fluid in the plume where it reaches the ceiling becomes continually more buoyant.

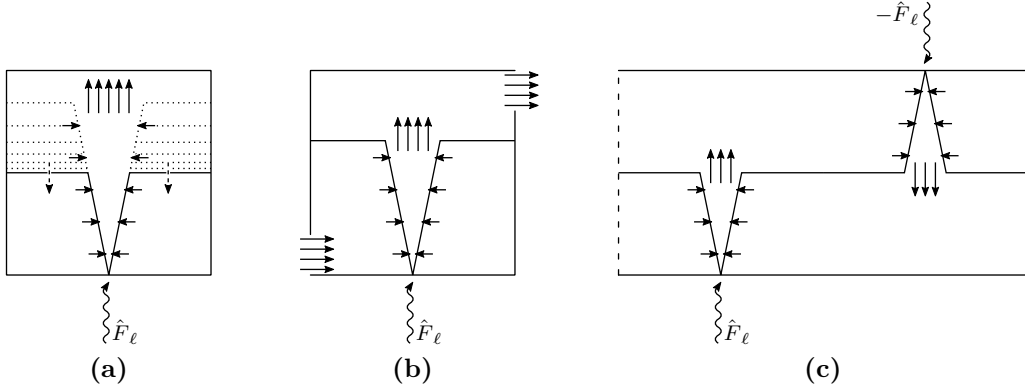


Figure 1.1: Selected cases of confined plumes from localised buoyancy sources ($\hat{F}_\ell$) in the literature ($\hat{F}_\ell > 0$). Depicted are (a) a filling box first described by Baines and Turner [9], (b) an emptying-filling box first described by Linden, Lane-Serff and Smeed [63] and (c) a configuration of ascending and descending plumes from sources of opposite and equal strength, as investigated by Craske and Davies Wykes [29] in a periodic domain (simplified representation).

Baines and Turner [9] modelled the temporal position of the density step between the stratified and the homogeneous density field as well as the asymptotic late-time density gradient by employing the classical plume theory of Morton, Taylor and Turner [73]. Germeles [39] developed a numerical scheme to describe the time-dependent density field of the filling box mechanism and extended the model to include mass and momentum flux at the buoyancy source. Worster and Huppert [117] gave an approximate solution of the temporal density field, assuming that the rate of change of the density field is independent of spatial position.

A system of a plume in an enclosure can attain a steady state, if the net buoyancy flux of the considered domain is zero. Such a configuration was described by Linden, Lane-Serff and Smeed [63, fig. 1.1b], who considered a configuration similar to the filling box with ventilation openings added near the floor and ceiling, allowing a mass exchange between the considered enclosure and a quiescent unstratified exterior. In the steady state, the density field of this emptying-filling box is separated into a lower layer of uniform density, and an upper stratified layer. The outflow of buoyant fluid through the upper ventilation opening is balanced by the entrainment of the plume, which supplies fluid to the upper layer; the lower layer is maintained by an inflow through the lower ventilation opening, driven by the plume's entrainment. Linden, Lane-Serff and Smeed [63] found that, for a pure plume of zero volume and momentum flux at the source, the position of the interface between the upper and lower layer is independent of the strength of the buoyancy source and solely determined by the geometry of the configuration and the entrainment of the plume. However, the strength of the stratification and the volume flux through the ventilation openings depend on the source strength. The emptying-filling box has since been studied extensively, particularly as a model of natural ventilation. Cooper and Linden [28], for example, extended the emptying-filling box to cases of two plumes of generally unequal strength and equal or unequal orientation. In modelling the resulting stratification, Cooper and Linden [28] consider a plume whose ambient density undergoes a step change. Above the density step, the plume is modelled as a forced plume from a virtual point source, where the position of the virtual source is chosen such that the momentum and volume flux of the plume are continuous across the density step. This model is based on the work of Morton [72] on forced plumes.

Another configuration of confined plumes that allows for a steady state is that of two localised

sources of opposite and equal strength in an unventilated enclosure, where the source of negative buoyancy flux is placed at the ceiling, producing a descending plume, and the source of positive buoyancy flux is placed at the floor level, resulting in an ascending plume (cf. fig. 1.1c). Baines and Turner [9] considered this configuration theoretically and predicted a stable stratification of two layers of equal depth and uniform density in the steady state, where each plume entrains fluid from the layer in its ambient and discharges fluid to the respective adjacent layer above or below it. The buoyancy of the layers is considered as equal to the buoyancy of the plume at the height of the interface between both layers, allowing for a prediction of the density difference between the layers, and the plume is predicted to become a constant-momentum jet upon penetrating the interface. Baines and Turner [9] remark that a sharply defined two-layer stratification can only be expected if the plumes are sufficiently far apart to prevent fluid discharged by one plume from being directly entrained into the plume of opposite orientation near its source. Craske and Davies Wykes [29, fig. 1.1c] used direct numerical simulations to examine a related system of periodically arranged ascending and descending axisymmetric plumes for different aspect ratios of the distance between plumes to the domain height. They found that the mean flow driven by the plumes does not solely consist of a global circulation between the plumes, such as predicted by Baines and Turner [9], but generally contains secondary and tertiary circulation cells, whose extent and strength depend on the aspect ratio of the domain. Craske and Davies Wykes [29] use estimates of the entrainment coefficient from observation to check whether the plumes are sufficiently far apart to be modelled using plume theory and found entrainment coefficients exceeding that of an unconfined non-interacting plume. Also, they remark that the flow that replaces the plume upon penetrating the interface is not of uniform density, rendering it different from a true jet of zero buoyancy.

Beyond steady states resulting from confined plumes, several authors have considered transient states arising from an unsteady localised source. Killworth and Turner [51] considered a filling box with a time-varying (sinusoidal) source strength and observed that a plume would gradually penetrate deeper into the stratified layer as its source strength was increased and conversely decrease in height as its source strength was decreased. Modelling this process and comparing their prediction with experiments, Killworth and Turner [51] concluded that fluid from the plume would spread as a layer at the height where it achieved zero buoyancy relative to its ambient, rather than at the height of zero vertical momentum. Kumagai [55] studied a starting plume in an environment which was initially stratified into two distinct layers, such that fluid from the plume would spread between the pre-existing layers. They noted that the plume would impinge on and entrain fluid from the adjacent layer, i.e., the layer which was not penetrated by the plume. Cardoso and Woods [24] considered a case similar to that of Kumagai [55], using an initially linearly stably stratified environment; they describe the overshoot of the plume into the adjacent layer as a fountain and observe considerable entrainment through this process. The lower boundary of the newly formed layer in the experiments of Cardoso and Woods [24] would propagate analogously to the density step in the filling box of Baines and Turner [9].

Kaye and Hunt [50] extended existing work on transient filling boxes to transient emptying-filling box configurations. They studied the transient state resulting from an abruptly activated buoyancy source in a ventilated enclosure of initially homogeneous fluid and observed that the depth of the buoyant layer supplied by the plume may overshoot its steady state value for certain geometry configurations relative to the plume's entrainment coefficient. Bolster, Maillard and Linden [18] considered the transi-

ents between two stratified steady states in an emptying-filling box, where the localised source strength was abruptly increased or decreased. Equivalent to Kaye and Hunt [50], they found that the depth of the buoyant layer would overshoot or undershoot the steady state layer depth after a source strength increase or decrease, respectively. Moreover, Bolster, Maillard and Linden [18] modelled the buoyant layer as either well-mixed or stratified along the lines of the model of Germeles [39] and found that both models showed similar agreement with experimental results, where they observed a buoyant layer that was neither perfectly stably stratified nor perfectly mixed. Bower et al. [20] likewise examined transients in an emptying-filling box resulting from a step increase and decrease of source strength and identified two qualitatively different flows for the respective source dynamic. Under an increase of the source strength, they observed a ‘filling flow’, where the plume penetrates the original upper layer of the preceding steady state and forms a new buoyant layer above it, while the original layer is gradually depleted by entrainment into the plume. If the source strength is decreased, an ‘intruding flow’ results: the fluid in the plume is less buoyant than the original upper layer and spreads out below it, forming a deepening intermediate layer. The original layer is depleted by the outflow through the upper ventilation opening and through penetrative entrainment into the intermediate layer, caused by the plume overshooting into the original layer as described by Killworth and Turner [51], Kumagai [55] and Cardoso and Woods [24]. Modelling the transient states as stratifications of three homogeneous layers, Bower et al. [20] found that the effect of the penetrative entrainment is negligible if the change of the source strength is sufficiently large. The cases of transients in an emptying-filling box were further extended by Bolster and Caulfield [17], who considered a periodically time-varying buoyancy source at different frequencies, and Fitzgerald and Woods [37], who classified different transient flow regimes for an emptying-filling box that is initially filled with a homogeneous fluid buoyant relative to the exterior.

Configurations of combined localised and distributed sources of buoyancy

Whilst localised sources of buoyancy in an enclosure typically lead to a stable stratification of the density field, distributed buoyancy sources promote vertical mixing and thus tend to homogenise the density field. The combination of localised and distributed sources of buoyancy thus results in a competition between the stabilising effect of the localised source(s), and the destabilising effect of the distributed source(s) [116]. Wells, Griffiths and Turner [116, fig. 1.2a, b] studied the effect of competing localised and distributed sources in a configuration equivalent to a filling box with added distributed heating: the localised and distributed source were either of the same sign and positioned on the same horizontal boundary (fig. 1.2a), or of opposite sign and positioned on opposite boundaries (fig. 1.2b). The considered configurations do not generally produce a steady state and, following Baines and Turner [9], Wells, Griffiths and Turner [116] focused on the position of the interface between qualitatively distinct layers and the asymptotic late-time density gradient. They demonstrated that the relative strength $\Gamma = \hat{F}_d/\hat{F}_\ell$ of the distributed to the localised source is a key parameter in determining the system’s state: both configurations result in a partially mixed and partially stably stratified density field if the localised source strength exceeded the distributed one and the latter is finite ($0 < \Gamma < 1$); conversely, the density field becomes fully mixed if the distributed source strength exceeded the localised one ($\Gamma > 1$). In configurations leading to a partially stratified density field, the depth of the mixed layer depends monotonically on Γ , though the relationship is different for the two considered types of configuration.

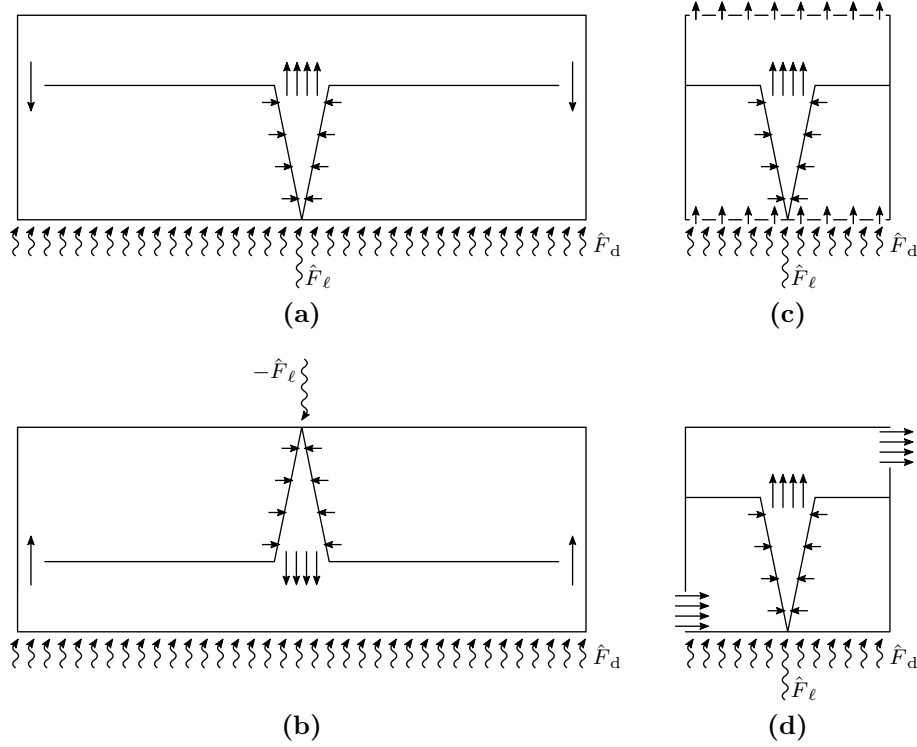


Figure 1.2: Combined localised ($\hat{F}_\ell$) and distributed ($\hat{F}_d$) buoyancy sources investigated in the literature ($\hat{F}_\ell, \hat{F}_d > 0$). Depicted are the configurations for confined volume heating from Wells, Griffiths and Turner [116], using sources on (a) the same and (b) opposite boundaries. Also sketched are the configurations for the heating of a mechanically ventilated domain as considered by (c) Chenvidyakarn and Woods [25] and a naturally ventilated domain considered by (d) Hunt, Holford and Linden [47] and Partridge and Linden [85].

Hunt, Holford and Linden [47, fig. 1.2d] extended the work of Wells, Griffiths and Turner [116] to systems of combined localised and distributed heating that allowed for a steady state, by adding ventilation openings near the floor and ceiling of the enclosure. The configuration investigated by their experiments is equivalent to an emptying-filling box with added distributed heating at the bottom boundary. Analogously to Wells, Griffiths and Turner [116], Hunt, Holford and Linden [47] described the resulting density field in the steady state as determined by the ratio Γ of the distributed to the localised source strength: if the value of the buoyancy flux ratio is less than a critical value of $\Gamma_c \approx 6$, a two-layer stratification is maintained by the plume; if the buoyancy flux ratio exceeds Γ_c , the density field becomes well-mixed. For a stratified density field, an increase of the effective ventilation area or an increase of Γ results in a rise of the interface position between the two layers and in a decrease of their density difference. In addition to the impact of the ventilation area and the buoyancy flux ratio, Hunt, Holford and Linden [47] observed that the flow field also depended on the location of the ventilation openings, noting that the flow showed a strong horizontal inhomogeneity for certain configurations.

Chenvidyakarn and Woods [25, fig. 1.2c] considered steady states in a mechanically ventilated enclosure containing a localised and distributed source of buoyancy at the bottom boundary. Air was supplied at a controlled flow rate at the bottom and extracted at the top of the domain. In contrast to Hunt, Holford and Linden [47], they observe that the critical point between a stably stratified and

a well-mixed density field in the steady state is not solely determined by the relative strength of the distributed to the localised source, but also depends on the ventilation rate: the density field becomes well-mixed at large values of the ventilation volume flux and large values of the buoyancy flux ratio Γ . In modelling the density field, Chenvidyakarn and Woods [25] accounted for penetrative entrainment of fluid from the upper layer into the lower layer, caused by convective currents that rise from the distributed source and impinge on the interface. The corresponding buoyancy flux was modelled as proportional to the distributed source strength with a finite proportionality constant, giving a good agreement between the model predictions and the experiments.

Partridge and Linden [85, fig. 1.2d] re-examined the configuration considered by Hunt, Holford and Linden [47] in more detail. They confirmed the result of Chenvidyakarn and Woods [25] that the critical ratio Γ_c of the distributed to the localised buoyancy flux is not a constant in a ventilated domain, but depends on the ventilation volume flux, which is determined by the effective opening area of the vents in a naturally ventilated enclosure. Instead of a critical buoyancy flux ratio, they proposed a critical Richardson number as marking the breakdown of the two-layer stratification. Partridge and Linden [85] modelled the interfacial entrainment equivalent to Chenvidyakarn and Woods [25], however, in contrast to the latter, they obtained the best agreement between model predictions and experiment if entrainment across the interface was neglected. Partridge and Linden [85] noted that their experiment differed from the one of Chenvidyakarn and Woods [25] in the position of the ventilation openings, which were located at the vertical and horizontal boundaries, respectively, and suspected that penetrative convection into the upper layer was suppressed by the flow from the ventilation opening in the lower layer. For large ventilation flow rates, Partridge and Linden [85] observed an inclination of the interface between the layers which cannot be described by their one-dimensional model of the density field.

The authors of [116], [47], [25] and [85] recognize the key role of the ratio Γ of the buoyancy fluxes of the distributed to the localised sources, however, none of the configurations were investigated by solely changing Γ and preserving the total buoyancy flux into the domain, due to experimental limitations. Hence, any conclusions drawn on the impact of the buoyancy flux ratio crucially rely on the accuracy of the employed model. Both Chenvidyakarn and Woods [25] and Partridge and Linden [85] model the density field as a one-dimensional stratification, however, Hunt, Holford and Linden [47] and Partridge and Linden [85] observe horizontal inhomogeneities of the steady state. All studies investigating steady states from combined localised and distributed heating consider ventilated enclosures, thus adding a variable volume flux as an additional parameter to the system. Moreover, there exist conflicting accounts on the flow and entrainment at the interface between the layers in stably stratified density fields that require clarification [25, 85]. To the best of our knowledge, considerations of unsteady sources, such as exist for systems with an isolated localised buoyancy source, have not been extended to configurations of combined localised and distributed buoyancy sources to-date.

The inverse heat transport problem

An inverse problem is based on a dataset, or measurement, and a model: the problem consists in determining suitable model parameter values such that the model prediction aligns with the given data. Inverse problems are typically ill-posed in the sense of Hadamard [42], which entails that the solution may become unstable due to errors inherent to (measurement) data of the system's state on which the inverse problem is based. Although there exist early attempts of solving inverse heat

transport problems, such as the work of Shumakov [100] and Stolz [102] in the 1950's, inverse heat transfer problems were long considered as impossible to solve, due to their ill-posed nature, and thus regarded as meaningless to practical applications [83]. Advances in the field were made possible by the introduction of different regularisation techniques, most notably, Tikhonov's regularisation method [106–109], the function specification method by Beck [11, 13, 14], iterative regularization techniques by Alifanov [2–5] and the Mollification method by Murio [74, 75]. Generally, the concept of regularisation consists in the approximation of an ill-posed problem by a similar well-posed problem. Since these early attempts, a considerable amount of work has been dedicated to inverse heat transfer problems. Here, we aim to give a brief overview of the range of the subject by highlighting the numerical methods and models used in the context of inverse heat transfer problems in building applications.

A variety of numerical approaches have been developed to solve inverse problems, which can still be computationally challenging even if regularised, e.g. due to non-linear equation systems and/or large parameter spaces [13]. Generally, inverse problems are phrased as optimisation problems, minimizing the difference between a parameter dependent model and (measurement) data, and most of the numerical approaches used in their solution can be divided into gradient-based and stochastic algorithms [64]. Gradient-based algorithms tend to converge faster than stochastic ones, however, they converge to a local optimum which is not guaranteed to be a global optimum in non-convex problems. In contrast, stochastic methods determine a global optimum. A gradient-based algorithm commonly used in inverse heat transfer problems is the conjugate gradient problem [19, 22, 70, 71, 77, 82], since it possesses self-regularising properties [79] such that regularisation can be realised via a suitable stopping criterion [12]. A type of stochastic algorithm that has been applied to inverse heat transfer problems are genetic algorithms [26, 46, 64, 65, 113, 114, 119].

Models used in inverse problem settings can be classified as white-box, black-box or grey-box models; their respective definitions are not consistent in the literature, here, we use these terms as in Li et al. [59]. White-box models are based on physical principles and derived from an analysis of the building structure. They can be constructed with different degrees of complexity, e.g. an entire building can be modelled as a single zone of homogeneous temperature with a single internal heat source and an envelope that may allow for heat and mass exchange, as in Nassiopoulos, Kuate and Bourquin [78]. In contrast, detailed zonal-nodal models, such as in Artiges et al. [7], represent a building as composed of multiple such zones, where a zone may include several rooms or, conversely, a large room may be divided into multiple zones. Black-box models are data-driven models, where the parameters to be determined do not have a physical interpretation, such as artificial neural networks used in Mustafaraj, Lowry and Chen [76] or Auto-Regressive Integrated Moving Average models in Feng and O'Neill [36]. White-box models can have a large number of parameters and can thus be computationally expensive, whereas black-box models are usually computationally efficient but require a vast amount of training data [7]. Low order physical models, so called grey-box models, are intended to strike a balance between white-box and black-box modelling approaches, with parameters that have physical meaning and a simple structure that allows for efficient computation [59]. The most commonly used grey box models are lumped-capacitance or resistance-capacitance (RC) models [54], e.g. Wang and Xu [113], where several physical parameters of a zone are combined to a thermal resistance and thermal capacitance, resulting in a thermal network of zones analogous to an electrical network. A suitable choice of model depends on the details of the considered problem, such as the available data, the intended use of the estimated parameter values, the flexibility required in applying the model to different applications and

the criticality of performance, among others.

In this thesis, we consider a system heated and cooled by localised and distributed sources. Multiple heat sources or different types of heat sources cannot easily be distinguished in an inverse problem setting, since the measured temperature field results from a superposition of the effect of all sources. Moreover, building models used in inverse problem settings often work with simplified settings, such as zones of uniform temperature and flow, which do not allow to establish a causal relationship between spatial details of the fields and the location, number or type of sources. Inverse problems of multiple sources in fluid dynamic systems have been considered, among others, in the context of tracing contaminants, e.g. Wei et al. [115] present an approach to determine the contaminant sources and respective release rates that cause a given concentration measurement from a pool of potential sources with known location. They assume that the flow field is fixed and known, such that there exists a linear relationship between the release rates of the sources and concentration measured at the sensors; the time lag between release and detection is neglected. This approach was adapted by Lei et al. [58] to determine the time-dependent heat flux of three heat sources, where the location of the sources is known, and the sources' temporal heat flux is synchronised. However, this approach requires a detailed simulation of the temperature and flow field at each iteration step (Lei et al. [58] employ a re-normalisation group k - ϵ model), since, in contrast to the passive contaminants considered by Wei et al. [115], the temperature field can generally not be decoupled from the flow field. Indeed, it is questionable whether the approach of Wei et al. [115] can be extended to transport problems of active scalars such as the temperature field, since it implies that the flow remains approximately unchanged over the duration of the considered transport, despite unsteady sources of the active scalar. Lei et al. [58] fail to provide the initial choice of the heat fluxes to be estimated by their optimisation procedure, which is information crucial to evaluate the performance of their algorithm.

Another approach for distinguishing different types of heat sources was taken by Brouns et al. [23]: they characterise different sources by their dynamics, distinguishing between smooth variations of the temperature, assigned to heat diffusion in the building envelope, air leakage or air renewal, and stepwise changes, which are attributed to the use of electrical appliances and occupancy. They adapt an approach from image processing to construct regularisation terms that restrict the two heat fluxes to be estimated to function spaces of either smooth or piecewise constant solutions. This method allows them to reconstruct the heat fluxes from two sources with different dynamics, smooth and piece-wise constant, using a single sensor and assuming a uniform temperature field.

Work in the area of the inverse problem of distinguishing multiple heat sources in a system dominated by convective heat transfer is limited. In particular, the usage of spatial information of the density field to address the inverse problem typically depends on computationally expensive detailed flow models.

1.3 Problem statement

To gain a better understanding of the impact of spatially heterogeneous heating and cooling, we aim to investigate the effect of combined localised and distributed boundary conditions when applied to a confined volume. To this end, we choose a configuration with a distributed source of buoyancy ($\hat{F}_d$) and a localised source of buoyancy ($\hat{F}_\ell$) on both the top and bottom boundary, as sketched in fig. 1.3. This can be understood as a combination of the two cases investigated by Wells, Griffiths and Turner

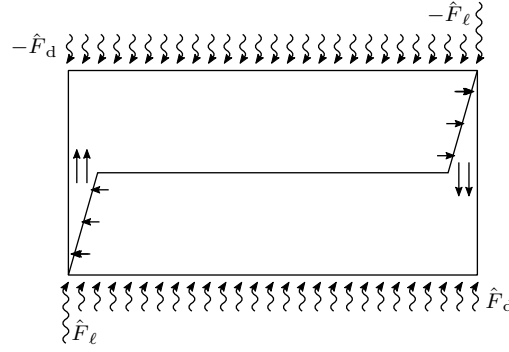


Figure 1.3: Configuration of combined localised ($\hat{F}_\ell$) and distributed ($\hat{F}_d$) buoyancy sources investigated in this thesis.

[116, fig. 1.1a, b]. By complementing the buoyancy sources with equivalent sinks of equal strength on the opposite boundary, we enable steady states without the additional parameter of a volume flux through a ventilation opening. Such a configuration allows us to study heating from a distributed and a localised source on the same boundary in a simple setting, in accordance with the efforts of previous publications illustrated in fig 1.2.

Spatially localised or distributed sources of buoyancy promote different flows and density fields. However, the models commonly employed to solve inverse heat transfer problems in building applications typically assume zones of uniform temperature and flow. Such models cannot easily distinguish between different types of buoyancy sources. Hence, there is potential in utilising the understanding gained about the combined effect of localised and distributed sources in an inverse problem setting that may offer an approach to separate these two types of sources. It is with this in mind that we attempt such a parameter estimation of a simple configuration of combined localised and distributed sources.

1.4 Aim and objectives

The aim of this thesis is to study the effect of spatial boundary buoyancy flux distributions and, with this knowledge, to reconstruct thermal boundary conditions from observations. In particular, we consider configurations that combine a localised line source of buoyancy and a distributed source on the top and bottom boundary, respectively, where the localised and distributed sources on each boundary are of equal strength. From observations of this system, we aim to construct a suitable model to later address the inverse problem of estimating the boundary conditions from measurements of the system's state.

We structure our approach into the following objectives:

1. To investigate the effect of combined localised and distributed sources on steady and transient states via numerical simulations.
2. To model the corresponding mean buoyancy field.
3. To estimate the boundary conditions from observations of a steady state, with observational data obtained from numerical simulations.

1.5 Structure of the thesis

In chapter 2, we investigate the effect of combined localised and distributed sources of buoyancy flux on the buoyancy field and flow, based on direct numerical simulations (DNS). This is the first study to concentrate on horizontal structures arising in such configurations, although their occurrence has been noted before by Hunt, Holford and Linden [47] and Partridge and Linden in ventilated enclosures with combined localised and distributed buoyancy sources. Two models of the buoyancy field are constructed, a one-dimensional model in the tradition of Chenvidyakarn and Woods [25] and Partridge and Linden [85] and a novel two-dimensional model that allows for horizontal heterogeneity and exhibits a better agreement with observations than the traditional model. We pay particular attention to the flow and entrainment at the interface, adding to existing work on the interfacial heat transport in configurations of combined localised and distributed sources, for which conflicting observations have been reported [25, 85]. The work of chapter 2 has been published in [66].

In chapter 3, we examine transient states arising from step changes in the strength of the localised and distributed sources, likewise based on DNS. Such systems represent a first expansion of the transient states resulting from isolated unsteady localised sources in an enclosure of stratified fluid to configurations including additional unsteady distributed sources of buoyancy. We construct two types of one-dimensional model of the transient buoyancy field, based on models of equivalent transient states from unsteady localised sources by Bolster, Maillard and Linden [18] and Bower et al. [20] and compare them to the DNS data.

Chapter 4 complements chapter 2, as we invert the causal relationship considered in the latter and undertake the first estimation of the relative strength of the distributed to the localised sources based on a simple spatially two-dimensional model of the buoyancy field. Samples of the DNS data that we presented in chapter 2 serve as the ‘measurement’ data that is assimilated by the parameter estimation. Although the estimated parameters show a large standard deviation from their respective true values, we consider the causes of error in detail that may inform future work. In chapter 5 we draw conclusions and offer an outlook to further work.

Chapter 2

Steady states

The work of this chapter, excepting §2.8, forms the basis of Mader, Reeuwijk and Craske [66].

2.1 Introduction

In this chapter, we study the steady states that result from a combination of localised and distributed heating and cooling on the boundary of an unventilated enclosure. The flows and buoyancy structures produced by localised sources of heat differ from those produced by distributed sources. Localised sources result in turbulent plumes [73], which entrain and mix fluid from their ambient. In an enclosure, plumes typically produce a stable stratification of their environment [9], as the heated fluid from the plume accumulates below the ceiling and forms a deepening layer of increasingly warmer fluid [117]. If the total heat input to the domain is zero, a statistically steady state can be attained, of which the two-layer stratification created by ‘equal and opposite’ plumes [9, 29, fig. 1.1c] is a canonical example.

Distributed heat sources produce flows and stratifications that are markedly different from those produced by localised heat sources. An example is Rayleigh-Bénard convection [1], which promotes turbulent mixing throughout the domain and thus suppresses the emergence of stably stratified layers (note, however, that the flow can organise into large-scale patterns or ‘wind’ which cause spatial heterogeneity [89]). The combination of localised and distributed sources of heat, and therefore buoyancy, leads to a competition between the stabilising effect of the localised source, and the destabilising effect of the distributed source [116].

Despite their prevalence in realistic settings, cases of combined localised and distributed heating have received relatively little attention. Wells, Griffiths and Turner [116] experimentally investigated a system of a single localised source combined with a distributed source on the same and on opposite boundaries in an unventilated enclosure (fig. 1.2a,b). In this configuration, the density field cannot reach a steady state but approaches a static density gradient at late times. Wells, Griffiths and Turner found that the stable stratification created by the plume breaks down in both cases, when the buoyancy flux from the distributed source $\hat{F}_d$ exceeds that of the plume, $\hat{F}_\ell$. Work by Chenvidyakarn and Woods [25], Partridge and Linden [85] and Hunt, Holford and Linden [47] in this regard focused on steady states attainable in a ventilated domain, considering a mechanically driven inflow and outflow through the bottom and top boundary [25, fig. 1.2c] or natural ventilation through openings in the side walls [47, 85, fig. 1.2d]. In these cases, the volume flux or ventilation is an additional parameter on which the

breakdown of the stratification depends [25, 85] (Hunt, Holford and Linden [47] describe a breakdown that is independent of the ventilation based on a set of preliminary experiments; this concept was improved by Partridge and Linden [85]). In spite of differences in their models' formulation regarding buoyancy transport between the layers, Chenvidyakarn and Woods [25] and Partridge and Linden [85] both report successful predictions of the system.

In this chapter, we study combinations of localised and distributed heating in a closed domain. In contrast to Wells, Griffiths and Turner [116], we focus on configurations involving no net heating or cooling of the domain, which therefore admit statistically steady states, even for different ratios of localised and distributed heating. This choice allows us to obtain statistics from averages with respect to time. The specific case we consider consists of heating and cooling on the bottom and top boundaries, respectively, from a combination of a localised *line* source and a distributed *area* source. The line sources on the top and bottom boundary are of equal strength, as are the area sources. Previous work has studied similar arrangements involving localised *point* sources in the absence of distributed sources [9, 29].

2.2 Problem description

We consider a box of width L_x , depth L_y and height H which is heated at the bottom and cooled at the top by a combination of localised and distributed sources (fig. 2.1). The origin of the coordinates in the corresponding directions, $(\hat{x}, \hat{y}, \hat{z})$, is placed at the centre of the domain. The problem is statistically homogeneous in the $\hat{y}$ direction. At the vertical boundaries of the domain, we impose a free-slip condition on the flow velocity and at the horizontal boundaries we impose a no-slip condition, where all boundaries of the domain represent impenetrable walls (fig. 2.1).

We study the enclosure under different distributions of boundary heating, where the total buoyancy

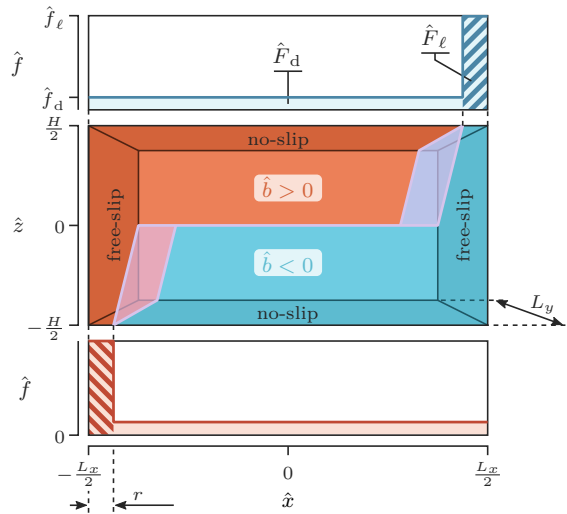


Figure 2.1: Schematic of the investigated configurations. The horizontal boundaries are set to a constant local buoyancy flux $\hat{f}_\ell$ within a strip of width r ; the remainder of each boundary is set to $\hat{f}_d$ (top and bottom graphs). The structure of buoyancy $\hat{b}$ sketched in the middle depicts two plumes in a stable two-layer stratification.

flux $\hat{F}$ per unit width on the top and bottom boundary,

$$\hat{F} \equiv \frac{1}{L_y} \int_{-\frac{L_x}{2}}^{\frac{L_x}{2}} \int_{-\frac{L_y}{2}}^{\frac{L_y}{2}} \hat{f}(\hat{x}, \hat{z}) \Big|_{\hat{z}=\pm \frac{H}{2}} d\hat{x} d\hat{y}, \quad (2.1)$$

is held constant for different heating distributions. The local buoyancy flux $\hat{f}(\hat{x}, \hat{z})$ which we impose on the top and bottom boundary corresponds to a buoyancy gradient, $\hat{f} \Big|_{\hat{z}=\pm \frac{H}{2}} = -\kappa \partial_z \hat{b} \Big|_{\hat{z}=\pm \frac{H}{2}}$, since there is no advective buoyancy transport across the boundaries. The buoyancy field $\hat{b} = g (\rho_0 - \rho) / \rho_0$ accounts for the density ρ of the fluid relative to a reference density ρ_0 , where g is the absolute value of the gravitational acceleration and κ the thermal diffusivity. The buoyancy flux at the side walls is set to zero.

The total buoyancy flux $\hat{F}$ at each of the horizontal boundaries can be decomposed into a buoyancy flux $\hat{F}_\ell$ from a localised source and a buoyancy flux $\hat{F}_d$ from a distributed source:

$$\hat{F} = \hat{F}_\ell + \hat{F}_d, \quad (2.2)$$

where $\hat{F}_\ell > 0$ and $\hat{F}_d > 0$ assume the same values on the top and bottom boundary of the domain (fig. 2.1). The localised sources are line sources, realised as strips of width r , and result in a pair of oppositely oriented planar plumes (fig. 2.1). Distributed heating is included by setting the remaining area of the horizontal boundaries to have the buoyancy flux $\hat{F}_d$. We consider the case of purely localised heating ($\hat{F}_d = 0$) as the base case and investigate the flow and stratification for increasing values of the distributed heat flux $\hat{F}_d > 0$.

The sources corresponding to $\hat{F}_\ell$ and $\hat{F}_d$ are heated or cooled uniformly, such that the respective local buoyancy fluxes $\hat{f}_\ell$ and $\hat{f}_d$ are constants (fig. 2.1). We only consider cases with $\hat{f}_\ell \geq \hat{f}_d$. Noting the planar geometry of the problem, the quantities $\hat{F}$, $\hat{F}_\ell$ and $\hat{F}_d$ are defined as buoyancy fluxes per unit length, which we refer to as buoyancy fluxes for brevity. Equivalent terminology will be applied to the volume and momentum flux.

A combination of localised and distributed heating can result in a stable stratification in two layers [116] at a buoyancy difference $\Delta \hat{b}$ (fig. 2.1). The buoyancy difference is determined by the geometry of the domain, L_x , L_y , H , the strip width r , the buoyancy fluxes $\hat{F}_\ell$ and $\hat{F}_d$ on the boundaries and the fluid's properties, the kinematic viscosity ν and thermal diffusivity κ . Using H and $\hat{F}$ to non-dimensionalise the problem, the dimensionless buoyancy difference $\Delta b = \Delta \hat{b} H \hat{F}^{-\frac{2}{3}}$ becomes a function of six dimensionless characteristic parameters

$$\Delta b = h(\lambda, \Lambda, \Lambda_y, \text{Re}, \text{Pr}, \Gamma), \quad (2.3)$$

where

$$\lambda = \frac{r}{L_x}, \quad \Lambda = \frac{L_x}{H}, \quad \Lambda_y = \frac{L_y}{H}, \quad \text{Re} = \frac{H \hat{F}^{\frac{1}{3}}}{\nu}, \quad \text{Pr} = \frac{\nu}{\kappa}, \quad \Gamma = \frac{\hat{F}_d}{\hat{F}_\ell}. \quad (2.4)$$

The quantities λ , Λ and Λ_y are the aspect ratio of the plume source and the aspect ratios of the domain's width and depth, respectively, and therefore capture the geometry of the domain. Here, an ideal line source of infinitesimal width corresponds to $\lambda = 0$. The Reynolds number Re is defined

independently of the distribution of the buoyancy flux on the boundary and Pr is the Prandtl number. The ratio Γ of the distributed to the localised buoyancy flux measures the distribution of the buoyancy flux on the boundaries. Due to the restrictions placed on $\hat{F}_\ell$ and $\hat{F}_d$, the buoyancy flux ratio in this problem is limited to $\Gamma \geq 0$. The buoyancy flux ratio $\Gamma = 0$ corresponds to the case of localised sources in an insulated boundary, whereas for Rayleigh-Bénard convection its value is $\Gamma = \lambda^{-1} - 1$. If the localised source was a line source of infinitesimal width, the latter value would be independent of the line source width λ and $\Gamma \rightarrow \infty$ for Rayleigh-Bénard convection.

From (2.2) and (2.4), the dimensionless counterparts of $\hat{F}_\ell$ and $\hat{F}_d$ are

$$F_\ell \equiv \frac{\hat{F}_\ell}{\hat{F}} = \frac{1}{1 + \Gamma}, \quad F_d \equiv \frac{\hat{F}_d}{\hat{F}} = \frac{\Gamma}{1 + \Gamma}, \quad (2.5)$$

such that $F_\ell + F_d = 1$. The dimensionless local buoyancy fluxes are termed f_ℓ and f_d .

To maximise the distance between the plumes without introducing the additional complications associated with no-slip boundary conditions, we use free-slip boundary conditions on the vertical walls. However, a plume at such a wall should not be regarded as half of an unconfined plume, because the impenetrable wall limits the scale of cross-stream turbulent motion and reduces entrainment, nor does it represent an experimentally observable wall-bounded plume, due to the lacking wall-shear stress (for details, see appendix A).

2.3 Direct numerical simulations

In this thesis, observations of the states arising from combined localised and distributed buoyancy sources are drawn from direct numerical simulations (DNS), which were performed using the code SPARKLE. SPARKLE is based on a finite-volume discretisation of the incompressible Navier-Stokes equations (see §2.4) with up to two active scalars. It has been previously employed for a range of turbulent flow simulations, such as thermal convection [90], shear-driven turbulence [48] and turbulent jets and plumes [30, 31, 92, among others].

SPARKLE uses a staggered grid to avoid odd-even decoupling: the velocity components are stored on the cell boundaries and the scalars are stored in the cell centre (see fig. 2.2). The spatial derivatives are calculated with the fourth-order symmetry-preserving method of Verstappen and Veldman [111], which intrinsically conserves mass, momentum and energy and is accurate to fourth order. The high-order accuracy of this method is achieved via Richardson extrapolation, which involves combining standard central differences with respect to two nested control volumes (see fig. 2.2). The staggered arrangement of variables on the grid means that interpolations are necessary to calculate the fluxes of a transported quantity. The time-stepping algorithm employed is a third order Adams-Bashford scheme. It is adaptive, such as to always satisfy the Courant-Friedrichs-Lewy (CFL) stability condition

$$N_{\text{CFL}} = \frac{\mathcal{U} \Delta \hat{t}}{\Delta \hat{x}} \leq 1, \quad (2.6)$$

where $\mathcal{U}$ is a characteristic velocity of the flow; $\Delta \hat{t}$ and $\Delta \hat{x}$ denote the time interval and spacing of the grid, respectively.

The simulated domain can be equipped with periodic, Dirichlet and Neuman boundary conditions for both the velocity and the scalar quantities. These conditions are imposed using ghost cells. The

largest stencil of any operator in the discretisation corresponds to the Laplace operator, spanning seven cells in each direction, accordingly, three layers of ghost cells are required. For details on the implementation of the boundary conditions, see [32]. The DNS code is fully parallelized by decomposing the simulated domain along two directions.

A DNS code is designed to fully resolve all dynamically active scales of the flow, hence, care must be taken to choose a sufficiently small grid spacing $\Delta\hat{x}$. Most prominently, from a physical perspective, the grid spacing should not exceed the Kolmogorov length scale $\eta_{\text{Kol}} = \nu^{3/4} \epsilon^{-1/4}$, where ν denotes the kinematic viscosity and ϵ corresponds to the rate of turbulent kinetic energy dissipation. To ensure that the smallest turbulent eddies are fully resolved, the grid spacing $\Delta\hat{x}$ should satisfy [87, p. 221]

$$\Delta\hat{x} \leq \eta_{\text{Kol}} \sim \mathcal{L} \text{Re}^{-3/4}, \quad (2.7)$$

where $\mathcal{L}$ corresponds to a characteristic length scale of the flow and Re denotes the Reynolds number.

The grid spacing is further restricted by the central differencing scheme used in SPARKLE. To avoid computational artefacts, the cell Reynolds numbers $\text{Re}_{\text{cell}} = \mathcal{U} \Delta\hat{x} \nu^{-1}$ and cell Péclet numbers $\text{Pe}_{\text{cell}} = \mathcal{U} \Delta\hat{x} \kappa^{-1}$ should not exceed $\mathcal{O}(1)$. For a discretisation grid of length L , the characteristic velocity can be expressed as $\mathcal{U} = \nu \text{Re} L^{-1}$ and the conditions on the grid spacing can be rewritten as

$$\Delta\hat{x} \lesssim L \text{Re}^{-1}, \quad \Delta\hat{x} \lesssim L \text{Pr}^{-1} \text{Re}^{-1}, \quad (2.8)$$

where $\text{Pr} = \text{Pe}/\text{Re}$ denotes the Prandtl number. For $\text{Pr} < 1$ or $\text{Pr} > 1$, the condition on the left or on the right of (2.8) is more restrictive, respectively. For $\text{Re} < 1$, the limit (2.7) resulting from physical considerations is more restrictive than the limit (2.8) resulting from the numerical method, whereas the reverse holds for $\text{Re} > 1$.

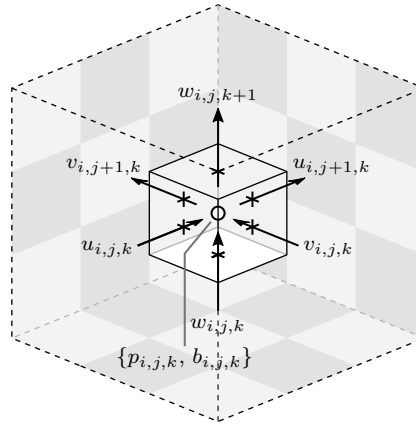


Figure 2.2: Staggered arrangement of variables on a single grid cell used in the DNS. Components of the velocity vector $\mathbf{u} = (u, v, w)$ are stored on the cell boundaries (marked as arrows) and scalars, such as the pressure p and the buoyancy b are stored in the cell centre ('o'-marker). If 'o' denotes a transported quantity, the arrows mark the location of its fluxes. The nested control volumes of 'o' used by the method of Verstappen and Veldman are outlined in straight and dashed lines.

2.4 Simulation details

The configurations introduced in §2.2 were investigated using the DNS code SPARKLE described in §2.3. To study the effect of the heating distribution, all characteristic parameters of the problem were kept constant apart from the buoyancy flux ratio Γ . Simulations were run for different values of the buoyancy flux ratio, ranging from the case of purely localised heating, $\Gamma = 0$, to a configuration for which the distributed contribution to the buoyancy flux on the boundary exceeds the localised one, $\Gamma > 1$.

The non-dimensional governing equations are those of an incompressible fluid under the Boussinesq approximation:

$$\nabla \cdot \mathbf{u} = 0, \quad (2.9a)$$

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \text{Re}^{-1} \Delta \mathbf{u} + b \mathbf{e}_z, \quad (2.9b)$$

$$\partial_t b + \mathbf{u} \cdot \nabla b = \text{Pe}^{-1} \Delta b, \quad (2.9c)$$

where $\mathbf{u}$, p and b correspond to the velocity vector, the kinematic pressure and the buoyancy, respectively, and $\mathbf{e}_z$ denotes the unit vector in the vertical; $\text{Pe} = \text{Pr Re}$ is the Péclet number. The scales used to non-dimensionalise space $\mathbf{x}$, time t , velocity, pressure and buoyancy are H , $H \hat{F}^{-\frac{1}{3}}$, $\hat{F}^{\frac{1}{3}}$, $\hat{F}^{\frac{2}{3}}$ and $H^{-1} \hat{F}^{\frac{2}{3}}$, respectively.

The Prandtl number was chosen as that of air, $\text{Pr} = 0.7$, and the Reynolds number is $\text{Re} = 7.34 \times 10^3$, corresponding to a Rayleigh number $\text{Ra} = \text{Pr Re}^2 = 3.77 \times 10^7$. The buoyancy flux ratio Γ on the boundary takes the values $\Gamma \in \{0, 0.10, 0.23, 0.39, 0.60, 1.29\}$. The governing equations (2.9) were solved on a domain of aspect ratios $\Lambda = 2$ and $\Lambda_y = \frac{3}{2}$, discretised as a staggered equidistant Cartesian grid of $1024 \times 768 \times 512$ cells. The resulting grid spacing, $\Delta x = 2 \times 10^{-3}$, is appropriate for the Kolmogorov length $\eta_{\text{Kol}} \sim \text{Pr}^{\frac{3}{8}} \text{Ra}^{-\frac{3}{8}} = 1.26 \times 10^{-3}$ (cf. (2.7)) and sufficient to avoid computational artefacts (cf. (2.8)). The initial volume integrated buoyancy of the domain is zero.

A free-slip condition is imposed at the vertical boundaries of the domain and a no-slip condition at the horizontal boundaries. A line source of width $\lambda = \frac{1}{16}$ was found to be sufficiently small to produce a planar plume (see appendix A). To initiate turbulent plumes [86], we add 1% of white noise to the vertical velocity on a single horizontal layer of grid points adjoining the source areas.

We define the mean of a field $h(t, x, y, z)$ over the homogeneous y direction and time as

$$\bar{h}(x, z) = \frac{1}{T \Lambda_y} \int_0^T \int_{-\frac{\Lambda_y}{2}}^{\frac{\Lambda_y}{2}} h(t, x, y, z) dy dt \quad (2.10)$$

and $h' = h - \bar{h}$ as the corresponding fluctuation. Statistics are taken at the steady state over $T = 10$ dimensionless turnover times, where the turnover time is one unit of non-dimensional time consistent with (2.9). Due to the symmetry of the boundary conditions, the mean fields of the Reynolds averaged governing equations are (anti-)symmetric to the axis $(x, z) = (0, 0)$ in the steady state. We exploit this property when taking statistics, such that the resulting mean fields obey these symmetries exactly.

Using a Reynolds decomposition and integrating (2.9c) over the width Λ of the domain, we obtain the following relation for F , the mean buoyancy flux over a horizontal slice, in the steady state:

$$\partial_z F \equiv \partial_z \int_{-\frac{\Lambda}{2}}^{\frac{\Lambda}{2}} (\bar{w} \bar{b} + \overline{w' b'}) - \text{Pe}^{-1} \partial_z \bar{b} dx = 0. \quad (2.11)$$

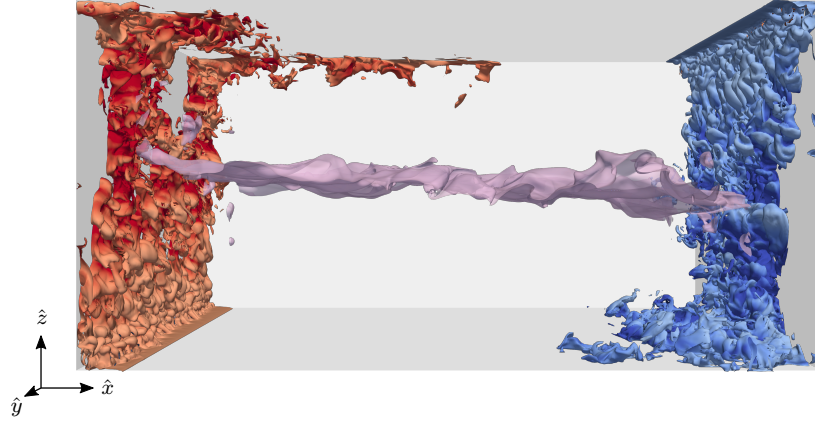


Figure 2.3: Isopycnals of two oppositely oriented plumes, arising from two localised line sources of equal strength ($\Gamma = 0$). Red marks an isosurface at buoyancy $b \approx 5$, blue corresponds to $b \approx -5$; the colour saturation indicates the kinetic energy. The fluid in the bulk of the domain is stably stratified in two layers, which are separated by an interface of zero buoyancy (violet). The displayed isosurface of zero buoyancy is cropped at the boundaries so as not to obscure the plumes.

Thus, the mean buoyancy flux F is conserved in z . This relation is utilised to determine whether the steady state is reached; we consider a state as statistically steady if the standard deviation of the buoyancy flux F , with respect to the unit buoyancy flux at the top or bottom boundary, is less than a given critical standard deviation $\sigma_c = 10^{-2}$.

Depending on the buoyancy flux ratio Γ , one turnover time took between 4.4×10^3 and 7.4×10^3 core hours to compute.

2.5 Results

2.5.1 Buoyancy structure

Heating and cooling the domain via two localised line sources of buoyancy on otherwise insulated boundaries ($\Gamma = 0$) leads to a stable stratification, consisting of two layers of near-uniform buoyancy (fig. 2.3 and 2.5a). The line sources produce two oppositely oriented turbulent planar plumes. Each

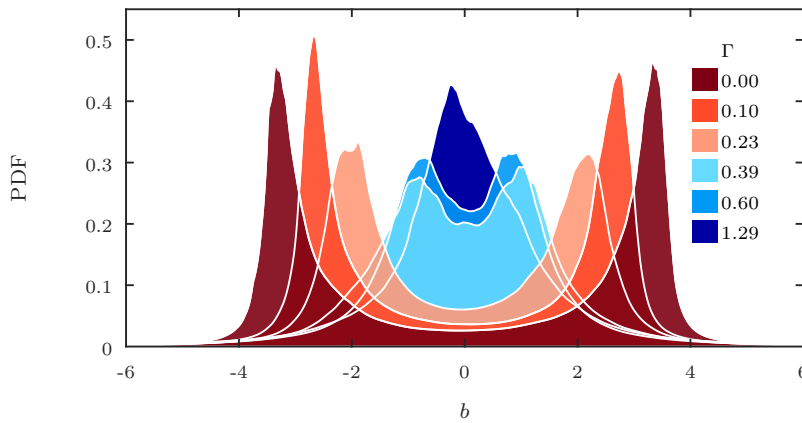


Figure 2.4: Time averaged probability density function of the buoyancy field.

plume supplies one layer of the resulting stable two-layer stratification by entraining fluid from its ambient layer and discharging into the opposite layer. The two layers are separated by an interface which has zero buoyancy, since the buoyancy sources on the top and bottom boundary are of equal strength and the initial volume integrated buoyancy of the domain is zero. The mean buoyancy $\bar{b}(x, z)$ of the domain, shown representatively at $x = 0$ in fig. 2.6, is characterised by a weak stratification in each layer and a thin transitional layer with a high buoyancy gradient at the interface.

The two-layer stratification at $\Gamma = 0$ (fig. 2.5a) manifests as two distinct peaks in the time-averaged probability density function (PDF) of the buoyancy field (fig. 2.4). The approximate uniformity of the buoyancy field in each of the layers is evident from the narrow width of the PDF peaks. The uniformly low value of the PDF between the peaks corresponds to the sharp separation of the two layers, resulting in the distinct interface visible in fig. 2.5a.

When a distributed buoyancy flux is added to the boundary ($\Gamma > 0$), the buoyancy difference between the layers decreases (fig. 2.6), which means that the distance between the peaks of the PDF in fig. 2.4 decreases. This trend continues as the value of Γ increases, until the two-layer stratification breaks down for $0.60 < \Gamma < 1.29$ (fig. 2.5e and 2.5f). The transition is evident from the PDF, as the two peaks of $\Gamma < 1.29$ merge into a single peak at $\Gamma = 1.29$ (fig. 2.4). This behaviour is in agreement with

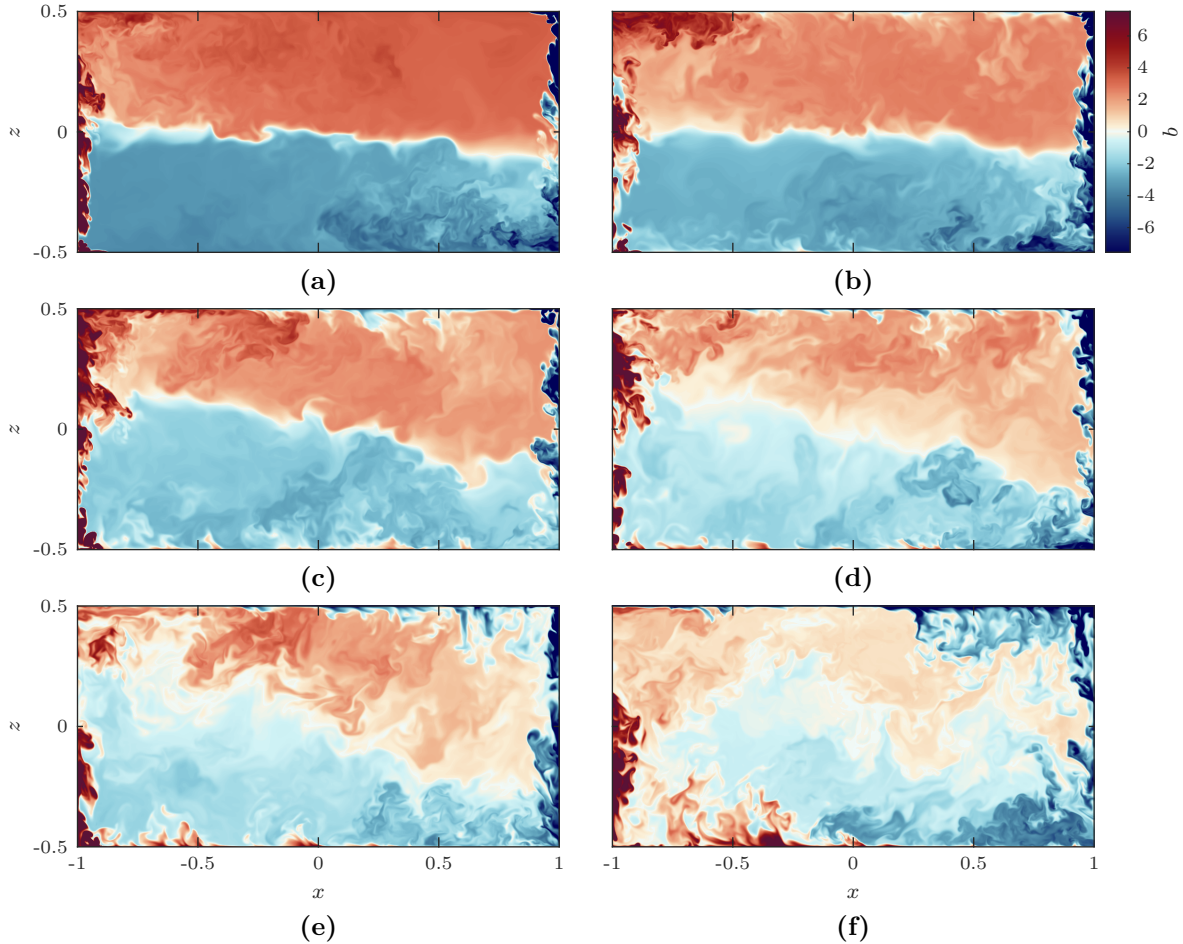


Figure 2.5: Instances of the buoyancy field: the individual figures correspond to (a) $\Gamma = 0$, (b) $\Gamma = 0.10$, (c) $\Gamma = 0.23$, (d) $\Gamma = 0.39$, (e) $\Gamma = 0.60$ and (f) $\Gamma = 1.29$.

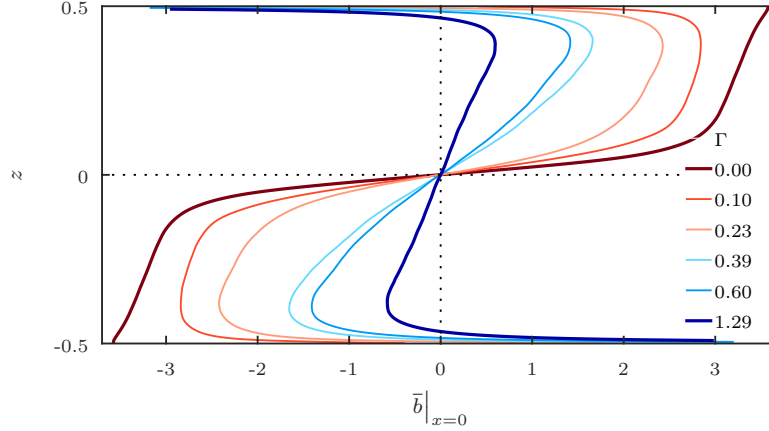


Figure 2.6: Mean buoyancy $\bar{b}$ along a vertical slice in the middle of the domain ($x = 0$). At the chosen position $x = 0$, the interface elevation is $z = 0$ for all configurations.

the breakdown of the stable stratification for $\Gamma > 1$ reported by Wells, Griffiths and Turner [116]. The experimental configurations of Wells, Griffiths and Turner are similar to the ones investigated here, if one localised and one distributed source were removed from the latter (cf. fig. 1.2a,b and fig. 2.1). The correlation with Wells, Griffiths and Turner suggests $\Gamma = 1$ as the critical value for the breakdown of the two-layer stratification in the configurations considered in the present work.

As Γ increases from 0 to 0.60, the buoyancy field of each layer of the stable stratification decreases in homogeneity: the individual peaks in the PDF increase in width and decrease in amplitude (fig. 2.4). The interface between the upper and lower layer of the stratification in fig. 2.5 appears less distinct as Γ increases and the gradient of the mean buoyancy between the layers decreases (fig. 2.6).

Between $\Gamma = 0.23$ and 0.39, the buoyancy difference between the layers decreases abruptly and then shrinks only marginally as Γ increases to 0.60. The abrupt decrease of the buoyancy difference between the layers is accompanied by a marked increase in the heterogeneity of the buoyancy field in each layer, which is reflected in the width of the PDF peaks. The increase in the amplitude of the peaks in the PDFs for $\Gamma \geq 0.39$ results from the growing overlap between the formerly distinct peaks. The vertical gradient of the mean buoyancy in each layer, which is small for $\Gamma \leq 0.23$, is markedly increased for $\Gamma \geq 0.39$ and becomes comparable in magnitude to the mean buoyancy gradient at the interface (fig. 2.6).

2.5.2 Flow structure

We first consider the flow at $\Gamma = 0$. Each of the localised sources produces a turbulent plume, which entrains fluid from its environment, i.e., its adjoining buoyancy layer. Each plume discharges fluid into the layer above (or below), which corresponds to the environment from which the oppositely oriented plume entrains fluid. As a result, a large-scale circulation develops, which transports fluid between the layers via the plumes and spans the width of the domain (fig. 2.7a).

For simplicity of expression, we will now limit our considerations to the left-hand plume and the upper layer. The flow in the plume is driven by the buoyancy of the plume's fluid relative to the local ambient fluid. As the plume penetrates the interface between the two layers of the stratification (solid red line in fig. 2.7), the mean buoyancy difference between the plume and its ambient becomes approximately zero (see appendix A). Since the plume represents the only buoyancy source to the

layer into which it is discharging, the mean buoyancy of the upper layer is approximately equal to the mean buoyancy of the plume where it penetrates the interface [9]. Thus, the plume is replaced in the upper layer by a flow that is akin to a jet in the statistical average (see appendix A for details). The entrainment of fluid into the jet drives a secondary circulation cell, nested into the large-scale circulation, as observed by Craske and Davies Wykes [29], albeit for slightly different boundary conditions. The secondary circulation is confined to the upper layer.

The interface between two layers tilts with increasing Γ in the rotational direction of the global circulation. Consequently, the vertical extent of the jet in the upper layer decreases. The horizontal spread of the jet increases with Γ , since the width of the plume at the interface height increases with Γ . At $\Gamma = 0.39$, the depth of the upper layer on the left-hand side is comparable to the width of the plume where it penetrates the interface and the secondary circulation cells disappear (fig. 2.7d). The collapse of the secondary circulations at $\Gamma = 0.39$ coincides with an abrupt increase of the buoyancy

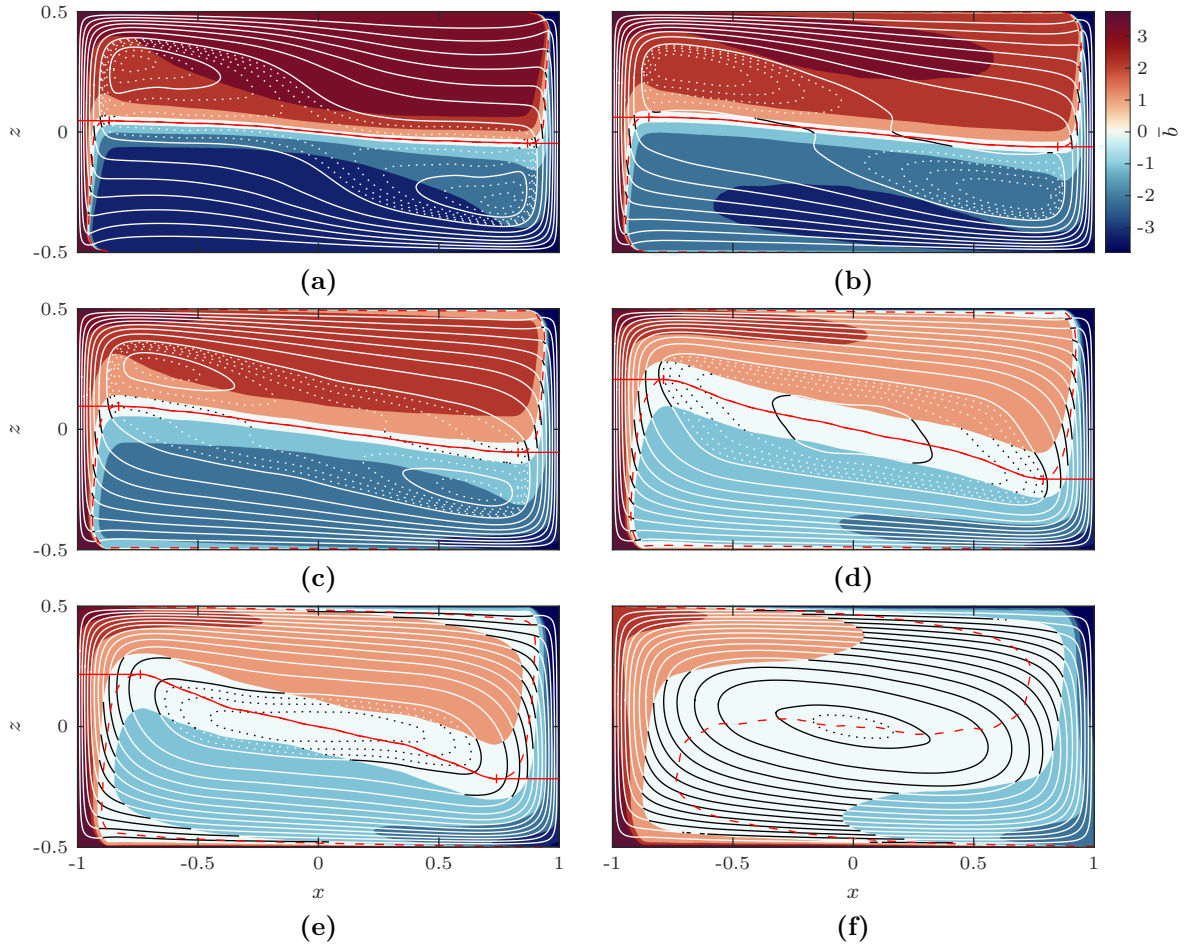


Figure 2.7: Mean buoyancy field $\bar{b}$ and streamlines of the mean flow $\bar{\mathbf{u}}$: the individual figures correspond to (a) $\Gamma = 0$, (b) $\Gamma = 0.10$, (c) $\Gamma = 0.23$, (d) $\Gamma = 0.39$, (e) $\Gamma = 0.60$ and (f) $\Gamma = 1.29$. Dotted streamlines correspond to a finer scaling than solid ones, marking a fifth of the difference between the solid streamlines. The isosurface at buoyancy $b = 0$ is marked by a red dashed line, the interface between the layers and its horizontal continuation to the boundaries is marked by a solid red line. The interface is separated from the continuation by a ‘+’. For definitions of the interface and the ‘+’ markers, see appendix B.

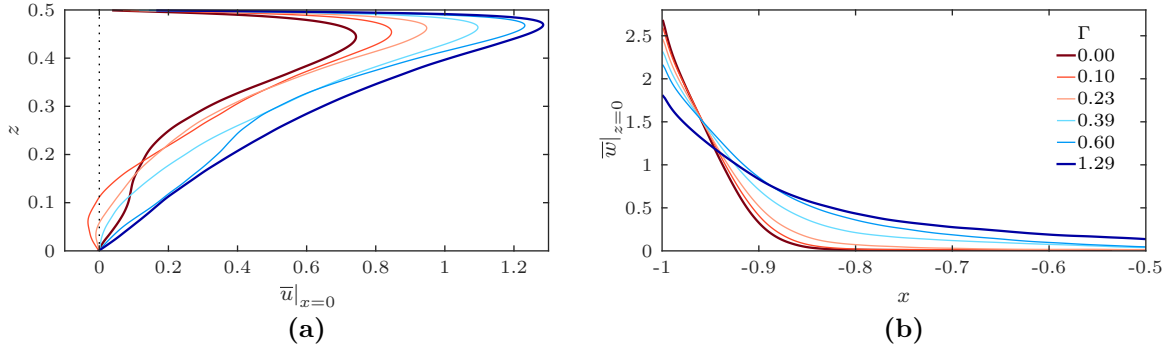


Figure 2.8: Profiles of mean velocities: **(a)** the horizontal velocity $\bar{u}$ along a vertical slice in the middle of the domain ($x = 0$) and **(b)** the mean vertical velocity $\bar{w}$ in the left-hand plume at $z = 0$. At the position $x = 0$ depicted in **(a)**, the interface elevation is $z = 0$ for all configurations and the mean velocity is antisymmetric to $z = 0$, $\bar{u}(0, z) = -\bar{u}(0, -z)$.

field's heterogeneity in each layer (§2.5.1). The observed change in the vertical distribution of the mean buoyancy (§2.5.1) also appears to be connected to the secondary circulations. The mean buoyancy profile, which is characterised by near-uniform values in each layer and a high interfacial gradient in the presence of the secondary circulation cells ($\Gamma \leq 0.23$), takes on an approximately constant vertical buoyancy gradient in the bulk as the secondary circulations disappear ($\Gamma \geq 0.39$, fig. 2.6).

Increasing Γ beyond $\Gamma = 0.39$, the interface tilts further, until the stable stratification breaks down at $\Gamma = 1.29$ (fig. 2.7d) and the isosurface $\bar{b} = 0$ returns to a near-horizontal orientation in the bulk. The flow retains a large-scale circulation, where the direction of rotation is determined by the localised buoyancy sources. If Γ was increased further, we would expect a Rayleigh-Bénard-like flow, where the bias of the flow orientation disappears (at least in an ensemble-averaged manner [89]), although it is potentially susceptible to spontaneous change [104]. We therefore expect the buoyancy distribution in the vertical to continue the trend visible in fig. 2.6 and reach a near-uniform buoyancy value in the bulk.

The slice of the mean buoyancy field in fig. 2.6 was placed at $x = 0$ because at this position the interface is conveniently at a constant elevation $z = 0$ for all Γ . The buoyancy in the layers is, however, not uniform in x . A fluid parcel in the upper layer is gradually cooled by the top boundary's buoyancy flux as it is transported from left to right. Consequently, the distributed heating in conjunction with a large-scale circulation results in a lateral buoyancy gradient within the layer, where the gradient increases with Γ (fig. 2.7). This lateral gradient will be the subject of further analysis in §2.6.

The value of the mean lateral velocity $\bar{u}$ in each layer peaks close to the horizontal boundary and its highest absolute value increases with Γ (fig. 2.8a). Close to the interface ($z = 0$ in fig. 2.8a), the behaviour of $\bar{u}$ appears to be non-monotonic with Γ for small values of Γ . This is a result of the changing width of the secondary circulation cells: at $\Gamma = 0$, the slice $x = 0$ does not intersect the secondary circulation, but does so at $\Gamma \in \{0.10, 0.23\}$, leading to different curves $\bar{u}(0, z)$ close to the interface. Fig. 2.8a implies that the volume flux of the primary circulation increases with Γ , since the horizontal velocity component dominates the mean flow at $x = 0$. Thus, we observe a larger volume flux when the bias of the localised sources on the flow orientation is reduced. However, our observations concern configurations where a two-layer stratification persists; the effect of localised sources on the volume flux for $\Gamma > 1$ might differ.

The value of the mean vertical velocity $\bar{w}$ in the plumes peaks at the side walls, where a free-slip

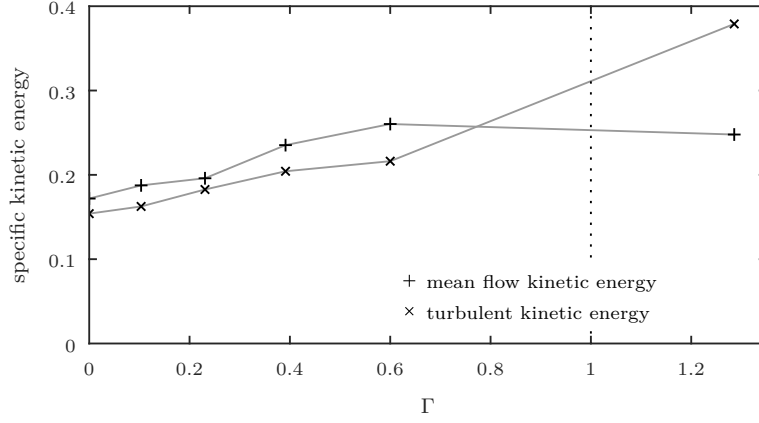


Figure 2.9: Mean flow and turbulent contribution to the specific kinetic energy in the domain.

condition is imposed (fig. 2.8b). The peak value of $\bar{w}$ at $z = 0$ decreases with increasing Γ , that is, with diminishing strength of the localised sources $F_\ell = (1 + \Gamma)^{-1}$. In contrast, the volume flux associated with $\bar{w}(x, 0)$ in fig. 2.8b should increase with Γ , since the volume fluxes corresponding to the velocities of fig. 2.8a and 2.8b are approximately equal for $\Gamma \leq 0.60$. This is because the mean velocity field is dominated by the vertical component $\bar{w}$ at $z = 0$ and by the horizontal component $\bar{u}$ at $x = 0$ and because the mean flow across the interface between the layers is weak for $\Gamma \leq 0.60$ (fig. 2.7). The opposite trends of volume flux and peak velocity in fig. 2.8b are possible, since the spatial distribution of $\bar{w}(x, 0)$ spreads in the horizontal with increasing Γ . The increase of the volume flux with Γ will be shown rigorously in §2.7.3.

The specific kinetic energy of the flow,

$$E_k = \frac{1}{2\Lambda} \int_{-\frac{\Lambda}{2}}^{\frac{\Lambda}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} \left(|\bar{\mathbf{u}}|^2 + |\mathbf{u}'|^2 \right) dz dx, \quad (2.12)$$

consists of a mean and a turbulent contribution, corresponding to the first and second term in the above expression, respectively. The turbulent kinetic energy increases with Γ (fig. 2.9), particularly at the transition from a stable ($\Gamma \leq 0.60$) to an unstable stratification ($\Gamma = 1.29$). The mean flow contribution to the kinetic energy increases with Γ while the two-layer stratification persists, but decreases slightly as the two-layer stratification breaks down. This decrease is consistent with the flow that we anticipate for a further increased value of Γ : because of the spontaneous reversal of direction occurring in the large-scale circulation of Rayleigh-Bénard convection [104], the mean flow velocity and associated kinetic energy should tend towards zero for $\Gamma \rightarrow \infty$ (for sufficiently long time averages).

2.5.3 Buoyancy transport between the layers

For $\Gamma \leq 0.60$, the buoyancy field is stably stratified in two layers, each supplied by a plume. The layers are separated by the isosurface of zero buoyancy, which also envelops the plumes (red dashed lines in fig. 2.7). For a precise definition of the two layers, we introduce a separating curve s which stretches over the full width of the domain (red solid lines in fig. 2.7). The curve s coincides with $\bar{b} = 0$ in the bulk and is continued to the left and right boundary by a horizontal line (see appendix B); the points where it departs from the isosurface are marked by red '+' markers in fig. 2.7.

Buoyancy exchanged between the two layers is either transported across the interface, defined as s between the ‘+’ markers, or via the plumes, i.e., across the two horizontal segments of s between the markers and the boundaries. We denote the buoyancy fluxes across the interface and the plumes as F_I and F_p , respectively (for a formal definition, see appendix B). In the steady state, the mean total buoyancy flux between the layers should equal the total buoyancy flux across the horizontal boundaries of the enclosure, $2 F_p + F_I = 1$. This equality holds to within an accuracy of 1% for all simulations $\Gamma \leq 0.60$. The simulation at $\Gamma = 1.29$ is excluded, since the buoyancy field does not show a clear two-layer stratification in this case.

Fig. 2.10 shows that the buoyancy transport between the layers is dominated by the plumes in all simulations $\Gamma \leq 0.60$. The value of the plumes’ buoyancy flux F_p is unaffected by the distribution of the buoyancy flux on the boundary Γ . Splitting the buoyancy flux of the plume into a turbulent buoyancy flux and a contribution of the mean flow (fig. 2.10), we find that the latter accounts for approximately 70% of the total F_p in the case of purely localised heating ($\Gamma = 0$). This is in agreement with experimental observations of planar plumes [53]. As Γ increases, the flow becomes increasingly turbulent (§2.5.2) and the turbulent buoyancy flux of the plume rises slightly, which is accompanied by a corresponding decrease in the mean flow contribution (fig. 2.10).

The buoyancy flux of each plume is slightly above 0.5. Thus, the equality $1 = 2 F_p + F_I$ is balanced by a negative buoyancy flux F_I across the interface due to turbulent mixing. The cross-interface buoyancy transport in the steady state has been studied by Chenvidyakarn and Woods [25] and Partridge and Linden [85] for other configurations of combined localised and distributed heating (fig. 1.2). Chenvidyakarn and Woods find a value of $F_I \approx 0.1 F_d$, whereas Partridge and Linden observe no mean buoyancy transport across the interface. Our results show a buoyancy flux of interfacial mixing that is negligibly small for all simulations $\Gamma \leq 0.60$, at about 5% of the total buoyancy flux of the boundaries. We did not observe a correlation between the value of the distributed buoyancy flux F_d and the cross-interface buoyancy flux F_I .

In spite of the Γ -independent and negligible value of F_I , the turbulent kinetic energy increases with Γ (fig. 2.9). Indeed, the behaviour of the turbulent kinetic energy might suggest an increase of the cross-interface buoyancy flux F_I with Γ , due to increased interfacial mixing. However, any increase of F_I would be counteracted by the behaviour of the buoyancy difference Δb between the layers of the stratification. The value of Δb decreases more rapidly with Γ than the turbulent kinetic energy rises with Γ (compare fig. 2.12 and fig. 2.9). Thus, a constant buoyancy flux across the interface can be consistent with a turbulent kinetic energy increasing with Γ .

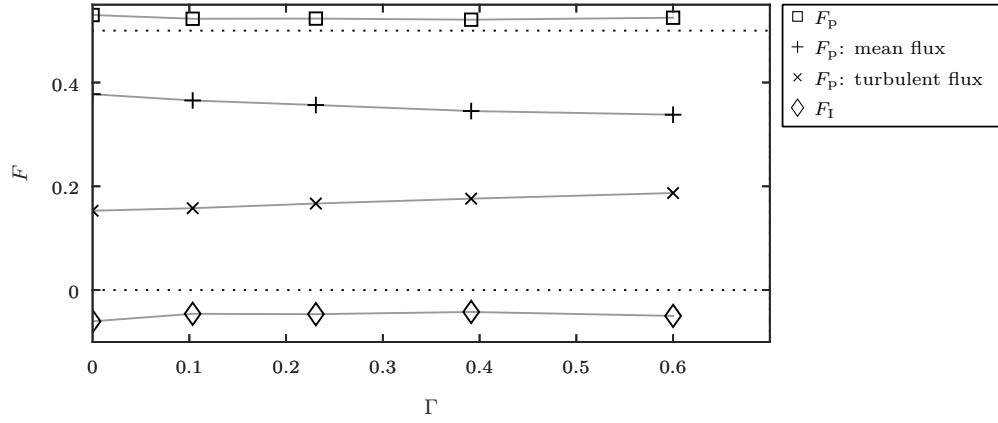


Figure 2.10: Buoyancy exchange between the two layers of the stable stratification (i.e., across the red solid lines in fig. 2.7). Depicted are the buoyancy fluxes F_p and F_l , corresponding to the discharge of one plume and mixing across the interface, respectively. In case of F_p , the total, the mean flow and the turbulent contribution are depicted.

2.6 Modelling the buoyancy field

We develop two models of the stably stratified buoyancy field found in a steady state using volume and buoyancy conservation. The models are defined in a piecewise manner; they each consist of four parts that correspond to the two plumes and the layers of the two-layer stratification (fig. 2.11). Model 1 uses a simple buoyancy structure by assuming that the buoyancy in each of the stratified layers is uniform. Model 2 includes a lateral buoyancy gradient in the layers and admits a tilt of the interface between the layers.

2.6.1 Model 1

We assume that each of the two layers of the stratification is well mixed and thus model the buoyancy of the layers, $\pm b_a$, as uniform in x and z (fig. 2.11a). Due to the symmetry of the problem, the buoyancy

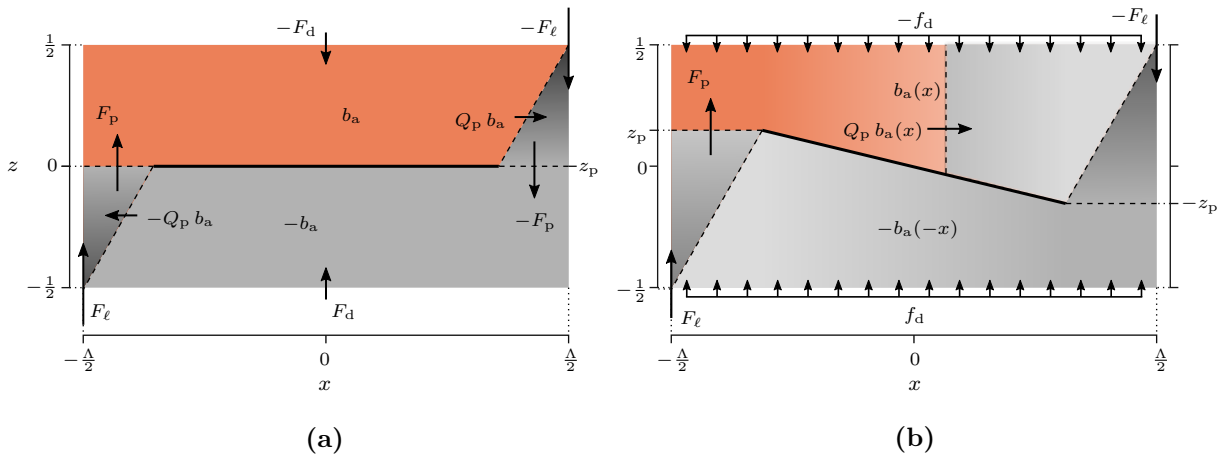


Figure 2.11: Schematics of the buoyancy structure for (a) model 1 of §2.6.1 and (b) model 2 of §2.6.2. The highlighted section is the control volume used. The volume flux across all dashed boundaries is equal Q_p .

of the two layers differs in sign only and it is sufficient to consider a single layer with its adjoining plumes. For the purpose of discussion, we will therefore focus on the upper layer of buoyancy b_a .

The upper layer is supplied by the left-hand plume with a mean buoyancy flux F_p . The top boundary of buoyancy flux F_d and the entraining right-hand plume act as buoyancy sinks. Consistent with §2.5.3, we neglect the buoyancy transport across the interface between the layers ($F_I = 0$) and hence set $F_p = \frac{1}{2}$ (cf. §2.5.3). In the steady state, the volume flux associated with entrainment into the right-hand plume equals the volume flux Q_p of the left-hand plume at the interface. Thus, we model the buoyancy flux into the right-hand plume as $Q_p b_a$. Using equation (2.5) for F_d , the buoyancy conservation of the upper layer in the steady state yields

$$\underbrace{\frac{1}{2}}_{F_p} = Q_p b_a + \underbrace{\frac{\Gamma}{1+\Gamma}}_{F_d} . \quad (2.13)$$

A plume from a source of strength $F_\ell = (1 + \Gamma)^{-1}$ placed at $z = -\frac{1}{2}$ penetrates the interface at z_p with a volume flux ([21], see appendix A)

$$Q_p = \alpha^{\frac{2}{3}} (1 + \Gamma)^{-\frac{1}{3}} \left(z_p + \frac{1}{2} \right) , \quad (2.14)$$

where α is the entrainment coefficient. We model the interface between the buoyancy layers as horizontal and hence the plume height as $z_p = 0$, neglecting the tilt that will be addressed in model 2 of §2.6.2.

Combining (2.13) and (2.14), we obtain the buoyancy b_a of the upper layer as $b_a = \alpha^{-\frac{2}{3}} (1 - \Gamma) (1 + \Gamma)^{-\frac{2}{3}}$. The corresponding buoyancy difference between the upper and lower layer is

$$\Delta b = b_a - (-b_a) = 2 \alpha^{-\frac{2}{3}} (1 - \Gamma) (1 + \Gamma)^{-\frac{2}{3}} . \quad (2.15)$$

Since the buoyancy is modelled as homogeneous in each layer, this difference is assumed to correspond to the difference between the peaks of the buoyancy field's PDF.

We defer discussion of the performance of the model to §2.7 and proceed with the construction of a second model, which incorporates a horizontal variation in both the buoyancy field and interface height.

2.6.2 Model 2

For the first model, we assumed the two layers of the stratification to be of homogeneous buoyancy $\pm b_a$. This results in a constant buoyancy flux $Q_p b_a$ across any vertical slice of the upper (or lower) layer, independent of its position in x . Thus, assuming layers of homogeneous buoyancy neglects the spatial distribution of the buoyancy flux F_d across the upper (and lower) boundary. For the second model, we allow the buoyancy in each layer to vary in x , but continue to assume the buoyancy layers to be well mixed over their smaller vertical dimension. The buoyancy of the upper layer at x is denoted as $b_a(x)$. Due to the antisymmetry of the buoyancy field, the buoyancy of the lower layer at position x equals $-b_a(-x)$.

We choose a segment of the upper layer as the control volume, stretching from the left-hand wall to an arbitrary position x (fig. 2.11b). The buoyancy flux across the top boundary in this segment is

the integral of the boundary's constant local buoyancy flux, $f_d = F_d \Lambda^{-1}$, over the respective interval:

$$\int_{-\frac{\Lambda}{2}}^x f_d dx = F_d \left(\frac{x}{\Lambda} + \frac{1}{2} \right). \quad (2.16)$$

Similarly to §2.6.1, the buoyancy flux at x is modelled as $Q_p b_a(x)$. The volume flux Q_p is given by (2.14) and is dependent on z_p . Combining these relations, the buoyancy conservation of the segment in the steady state gives

$$\underbrace{\frac{1}{2}}_{F_p} = Q_p b_a(x) + \underbrace{\frac{\Gamma}{1+\Gamma}}_{F_d} \left(\frac{x}{\Lambda} + \frac{1}{2} \right), \quad x \in \left[-\frac{\Lambda}{2}, \frac{\Lambda}{2} \right]. \quad (2.17)$$

In the construction of this model, we neglect the horizontal spatial extent of the right-hand plume and its source, assuming that the upper layer stretches from $-\frac{\Lambda}{2}$ to $\frac{\Lambda}{2}$ for all z and that F_d is distributed uniformly over this interval.

In contrast to the first model, z_p is not necessarily equal to zero. Consistent with a laterally dependent buoyancy, we consider the vertical position of the interface between the layers as an x -dependent function $z_I(x)$. The left- and right-hand plume penetrate the interface at z_p and $-z_p$, respectively, such that $z_I(\mp \frac{\Lambda}{2}) = \pm z_p$. To obtain $z_I(x)$, we assume that the vertical velocity in the bulk is sufficiently small for the pressure to be approximated as hydrostatic [112] and is approximately constant at the top and bottom of the domain. Thus, the pressure difference between the bottom and top boundary is

$$p|_{z=-\frac{1}{2}} - p|_{z=\frac{1}{2}} = \int_{-\frac{1}{2}}^{z_I(x)} -b_a(-x) dz + \int_{z_I(x)}^{\frac{1}{2}} b_a(x) dz \quad (2.18)$$

$$= -Q_p^{-1} (1 + \Gamma)^{-1} \left(z_I(x) + \Gamma \frac{x}{\Lambda} \right), \quad (2.19)$$

where we inserted b_a from (2.17). Due to the pressures being taken as constant in x , the above expression results in $z_I(x) = -\Gamma \frac{x}{\Lambda} + z_I(0)$. The offset is $z_I(0) = 0$ since $z_I(x)$ needs to be an antisymmetric function in x . Inserting $z_p = z_I(-\frac{\Lambda}{2})$ and (2.14) into (2.17), we find the buoyancy of the upper layer:

$$b_a(x) = \alpha^{-\frac{2}{3}} (1 + \Gamma)^{-\frac{5}{3}} \left(1 - \Gamma \frac{2x}{\Lambda} \right). \quad (2.20)$$

For the model, the peaks in the PDF correspond to the buoyancy over the deepest part of the layers. Thus, the buoyancy of the upper layer at $x = \frac{\Lambda}{2}$, $b_a(\frac{\Lambda}{2})$, corresponds to a peak in the buoyancy's PDF, as does the buoyancy at $x = -\frac{\Lambda}{2}$ in the lower layer, $-b_a(\frac{\Lambda}{2})$. Hence, the difference between the peaks in the buoyancy field's PDF is modelled as

$$\Delta b = b_a(\frac{\Lambda}{2}) - [-b_a(\frac{\Lambda}{2})] = 2 \alpha^{-\frac{2}{3}} (1 - \Gamma) (1 + \Gamma)^{-\frac{5}{3}}. \quad (2.21)$$

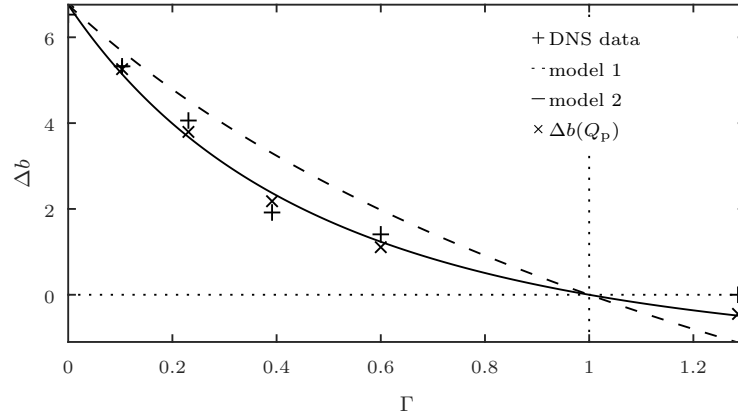


Figure 2.12: Difference Δb between the peaks of the buoyancy field's PDF: comparing simulation results and models. Depicted is the buoyancy difference from simulation data (fig. 2.4), and the predictions of model 1 and 2 (2.22). The value $\Delta b(Q_p)$ from (2.26) is a combination of modelling and observation (see §2.7.3). The models are valid for stable stratification corresponding to $\Gamma < 1$.

2.7 Model validation

2.7.1 Buoyancy difference between the layers

To summarize §2.6, the model predictions for the difference Δb between the peaks of the buoyancy field's PDF (see fig. 2.4) are

$$\Delta b = \begin{cases} 2\alpha^{-\frac{2}{3}}(1-\Gamma)(1+\Gamma)^{-\frac{2}{3}}, & \text{for } b_a = \text{const} \quad (\text{model 1}), \\ 2\alpha^{-\frac{2}{3}}(1-\Gamma)(1+\Gamma)^{-\frac{5}{3}}, & \text{for } b_a = b_a(x) \quad (\text{model 2}). \end{cases} \quad (2.22)$$

As discussed in §2.5.1, the buoyancy difference Δb is indicative of the stratification of the buoyancy field. Both models predict a stable stratification, $\Delta b > 0$, for boundary buoyancy flux ratios $\Gamma < 1$. Beyond the critical value $\Gamma_c = 1$, the buoyancy difference becomes negative, corresponding to an unstable stratification. Thus, the buoyancy flux ratio Γ on the boundary takes the role of a stability parameter within the models. Since both models are based on a stably stratified buoyancy field, their validity is restricted to $\Gamma < 1$.

A critical value of $\Gamma_c = 1$ is consistent with our observation of a stable stratification up to $\Gamma = 0.60$ and an unstable stratification at $\Gamma = 1.29$ (fig. 2.4). Wells, Griffiths and Turner [116] report the same critical value for other experimental configurations of competing localised and distributed buoyancy sources in an unventilated enclosure (fig. 1.2a,b, §2.5.1). To obtain numerical values from (2.22), we estimate the entrainment coefficient α based on the case of purely localised heating and using (2.14), which gives $\alpha = (2Q_p|_{\Gamma=0})^{\frac{3}{2}} \approx 0.16$ (see appendix A). We assume α to be independent of the buoyancy flux ratio Γ on the boundary.

Both models approximate the buoyancy difference Δb between the layers with comparable accuracy for the three lowest values of the boundary buoyancy flux ratio, $\Gamma \in \{0, 0.10, 0.23\}$ (fig. 2.12). In these configurations, secondary circulation cells are present and the PDF of the buoyancy field shows a near-uniform buoyancy in each of the two layers. Thus, the value of Δb is slightly overestimated by the homogeneous buoyancy model (model 1) and slightly underestimated when the lateral buoyancy gradient is based on the hydrostatic pressure at the bottom boundary (model 2).

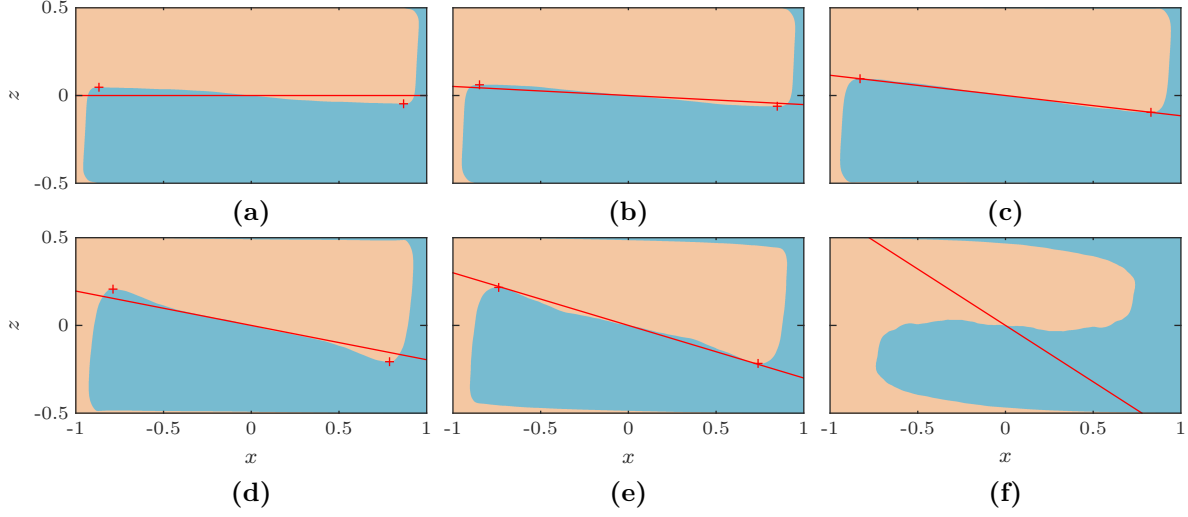


Figure 2.13: Tilt of the interface between the layers of the stratification: comparing simulation results and model 2. The buoyancy field is separated into values above (red) and below (blue) zero; we consider the resulting separation line between the ‘+’-markers as the interface (§2.5.3). The red curve shows the interface $z_I(x)$ of model 2 (§2.6.2). The individual figures correspond to (a) $\Gamma = 0$, (b) $\Gamma = 0.10$, (c) $\Gamma = 0.23$, (d) $\Gamma = 0.39$, (e) $\Gamma = 0.60$ and (f) $\Gamma = 1.29$.

As the secondary circulation breaks down, $\Gamma \geq 0.29$, the lateral buoyancy gradient in the bulk increases, and the assumption of homogeneous buoyancy layers used in model 1 is no longer suitable. In contrast, model 2 shows good agreement with the measurements, despite neglecting the marked vertical buoyancy gradient that establishes as the secondary circulation disappears (fig. 2.6).

2.7.2 The tilt of the interface

In §2.6, we model the position of the interface between the layers as

$$z_I = \begin{cases} 0, & \text{for model 1,} \\ -\frac{\Gamma}{\Lambda} x, & \text{for model 2.} \end{cases} \quad (2.23)$$

Using the corresponding height of the plume, $z_I|_{x=-\frac{\Lambda}{2} + \frac{1}{2}}$, Δb in (2.22) can be written as

$$\Delta b = \alpha^{-\frac{2}{3}} (1 - \Gamma) (1 + \Gamma)^{-\frac{2}{3}} \left(z_I|_{x=-\frac{\Lambda}{2} + \frac{1}{2}} + \frac{1}{2} \right)^{-1} \quad (2.24)$$

for both models. Thus, the difference between the two expressions in (2.22) originates from the different interface curves used in the models.

For $\Gamma > 0$, we find that the assumption of a hydrostatic environment and a constant pressure difference between the top and bottom boundary in model 2 (§2.6.2) lead to a tilt that is in good agreement with the interface curve defined in §2.5.3 from simulation data (fig. 2.13). The upper limit $\Gamma = 1$ to the model’s range of validity coincides with the interface touching the horizontal boundaries, $z_I(x = \mp \frac{\Lambda}{2}) = \pm \frac{1}{2}$. Thus, the breakdown of the model beyond $\Gamma = 1$ is reflected in the interface curve (fig. 2.13f) as well as in the buoyancy difference Δb (§2.7.1). For $\Gamma = 0$, the model diverges slightly from the simulation data (fig. 2.13a), predicting a horizontal interface whereas the DNS data show a

tilted interface.

Whilst the slope of the interface curve predicted by model 2 depends on the aspect ratio Λ (2.22), the corresponding plume height, $z_I|_{x=-\frac{\Lambda}{2}} + \frac{1}{2} = \frac{1}{2}(1 + \Gamma)$, is independent of Λ . In §2.5.2, we noted that the secondary circulations are driven by a flow that is similar to a jet in the statistical average. The vertical extent of the jet is limited by the depth remaining between the horizontal boundary and the position at which the plume penetrates the interface between the layers; the height of the jet thus decreases with a growing plume height. We therefore suspect a connection between the presence or absence of secondary circulation cells and the plume height. If this is the case, model 2 implies that the breakdown of secondary circulations is solely determined by the distribution Γ of boundary heating. The existence of secondary circulations at $\Gamma = 0$, however, is expected to depend on the aspect ratio of the domain, as is the case for confined axisymmetric plumes [29].

2.7.3 Volume flux

The volume flux Q_p of the plumes can be determined from the DNS data analogously to the plumes' buoyancy flux F_p in §2.5.3: we define Q_p as an integral of the vertical velocity taken over the separating curve s between the walls and the boundaries of the interface curve marked as '+' in fig. 2.7 (see appendix B). The resulting volume flux increases with Γ (fig. 2.14).

In the models, Q_p appears implicitly in the expression of the buoyancy difference (2.22) as

$$Q_p = \alpha^{\frac{2}{3}} (1 + \Gamma)^{-\frac{1}{3}} \left(z_I|_{x=-\frac{\Lambda}{2}} + \frac{1}{2} \right) = \begin{cases} \frac{1}{2} \alpha^{\frac{2}{3}} (1 + \Gamma)^{-\frac{1}{3}}, & \text{for model 1,} \\ \frac{1}{2} \alpha^{\frac{2}{3}} (1 + \Gamma)^{\frac{2}{3}}, & \text{for model 2.} \end{cases} \quad (2.25)$$

Notably, the models predict contrary trends for the volume flux with Γ . Model 1 is in conflict with the simulation data, showing a decrease of the volume flux with Γ , whereas model 2 correctly captures the observed trend of Q_p .

The decrease of the volume flux with growing Γ in model 1 is due to the decreasing velocity of the plumes (cf. fig. 2.8b), since the plume velocity obeys $w_m \propto (1 + \Gamma)^{-\frac{1}{3}}$ (see appendix A). In model 2, the decreasing plume velocity is countered by the growing height of the plume, $\frac{1}{2} + z_p \propto 1 + \Gamma$, and a correspondingly growing width of the plume at the interface level. The effect of the increasing area through which the plume discharges fluid to the adjoining layer on Q_p dominates over that of the decreasing plume velocity and leads to a volume flux increasing with Γ .

The volume flux of model 2 is in good agreement with the DNS data for buoyancy flux ratios $\Gamma \leq 0.23$, until the volume flux from the DNS data increases abruptly at $\Gamma = 0.39$ (fig. 2.14). The abrupt increase of the volume flux coincides with the disappearance of the secondary circulation cells and the increased vertical stratification of the buoyancy field in the layers between $\Gamma = 0.23$ and 0.39 in comparison to $\Gamma < 0.23$ (fig. 2.7, 2.6). The vertical stratification is not realised in the models and might account for the deviation of the second model's volume flux from the DNS data.

Combining (2.22) and (2.25), the buoyancy difference of model 1 and 2 is

$$\Delta b(Q_p) = 2 b_a|_{x=\frac{\Lambda}{2}} = (1 - \Gamma) (1 + \Gamma)^{-1} Q_p^{-1}. \quad (2.26)$$

Inserting the volume flux from the DNS data into the models (2.26), we find that the corrected volume flux has little impact on the value of Δb (fig. 2.12), since Q_p stands in the denominator in (2.26) and

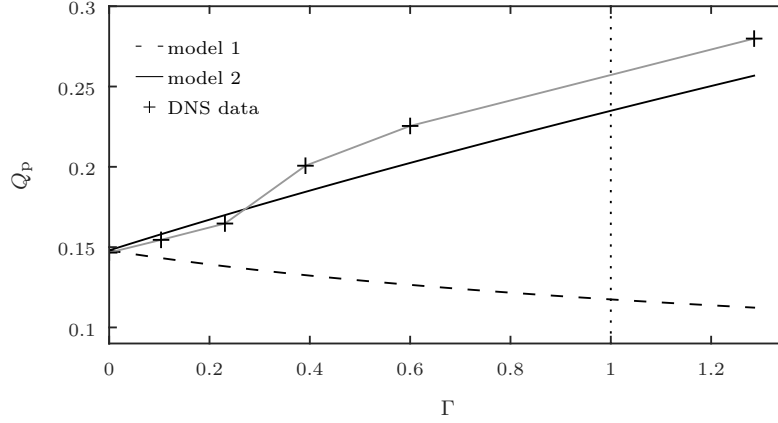


Figure 2.14: Volume flux Q_p of the plume where it penetrates the interface: comparing simulation results and models. Depicted are the predictions of models 1 and 2 (2.26) as well as the volume flux of the plumes from simulation data. The latter is defined as the volume flux through the horizontal continuation of the interface in fig. 2.7 (see appendix B for a formal definition).

the abrupt increase in Q_p is small relative to the overall magnitude of Q_p .

2.7.4 The gradient Richardson number at the interface

To investigate the impact of the shear flow on the interface between the layers, we define a gradient Richardson number:

$$\text{Ri}_g(x, z) \equiv \frac{\partial_z \bar{b}}{(\partial_z \bar{u})^2}. \quad (2.27)$$

In inviscid non-turbulent parallel flows, a stratified shear profile is linearly stable if the gradient Richardson number exceeds the critical value of $\frac{1}{4}$ everywhere [45, 68]. Gradient Richardson numbers with values approximately independent of time and the flow-normal direction [44, 91, 94, 97, 99, 101, 123] have been interpreted as an indicator of a turbulent equilibrium state [123]. In this context, it has been proposed that turbulent shear flows are attracted to a state of marginal instability, which is marked by a gradient Richardson number $\text{Ri}_g \approx \frac{1}{4}$ [101, 105].

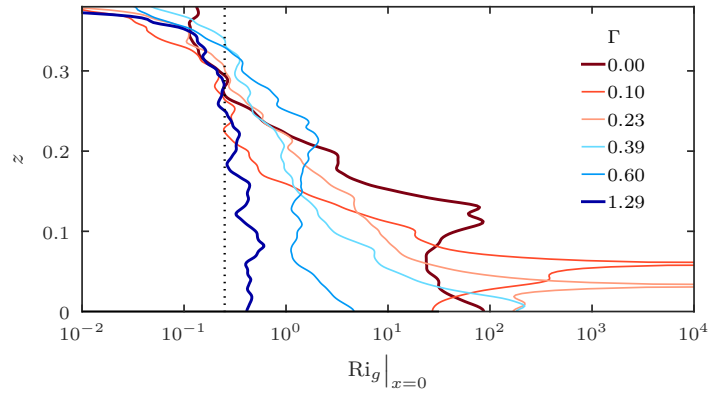


Figure 2.15: Gradient Richardson number Ri_g along a vertical slice in the middle of the domain ($x = 0$). The value $\text{Ri}_g = \frac{1}{4}$ is marked by a dotted line. At the chosen position $x = 0$, the interface elevation is $z = 0$ for all configurations.

In the present work, the profiles of the gradient Richardson number $\text{Ri}_g(0, z)$ in the horizontal middle of the domain far exceed those expected for marginal stability ($\frac{1}{4}$) at the interface ($z = 0$) and in its vicinity for all simulations for which $\Gamma \leq 0.39$ (fig. 2.15). Thus, the stabilising effect of the stratification is (significantly) larger than the destabilising effect of the shear flow. The reason is that the background stratification for the shear flow is not created by local mixing, but externally by the plumes on the side walls and the convection from the distributed buoyancy flux sources, which jointly determine both the horizontal velocity and the buoyancy difference. Equivalently, the turbulence that disturbs the buoyancy interface (fig. 2.5a-e) does not originate from the interface but arises from the plumes and the convection from distributed sources.

The gradient Richardson number $\text{Ri}_g(0, 0)$ at the interface changes with the buoyancy flux ratio Γ (fig. 2.15). For $\Gamma \leq 0.23$, there exists no monotonic relationship between $\text{Ri}_g(0, 0)$ and Γ , however, $\text{Ri}_g(0, 0)$ decreases with Γ for large $\Gamma \geq 0.39$. The non-monotonic behaviour of $\text{Ri}_g(0, 0)$ for $\Gamma \leq 0.23$ originates from the mean horizontal velocity $\bar{u}(0, z)$, the profile of which varies close to the interface due to the changing width of the secondary circulation cells with Γ (cf. 2.5.2). The peaks in $\text{Ri}_g(0, z)$ for $\Gamma = 0.10$ and 0.23 correspond to a sign change in $\partial_z \bar{u}(0, z)$ close to the interface (local minima in fig. 2.8a), which appears as the secondary circulation cells intersect the plane $x = 0$.

We can establish a relationship between Γ and the gradient Richardson number at the interface by denoting the width of the shear layer as ℓ_U and the width of the buoyancy interface as ℓ_b and estimating (2.27) at the interface as

$$\text{Ri}_g|_{z=z_1} \approx \frac{\Delta b}{\Delta U^2} \frac{\ell_U^2}{\ell_b} = \frac{1}{16} \frac{\Delta b}{Q_p^2} \frac{\ell_U^2}{\ell_b}. \quad (2.28)$$

Here, Δb and ΔU are the characteristic differences in buoyancy and horizontal velocity between the layers, respectively. The second identity in (2.28) results from estimating the absolute value of the horizontal velocity in the layers as $U = 2Q_p$, using the plume volume flux Q_p and the layer depth $\frac{1}{2}$ at $x = 0$, and taking $\Delta U = 2U$. Utilising model 2 for Δb (2.22) and Q_p (2.25) we obtain

$$\text{Ri}_g|_{z=z_1} \approx \frac{1}{2} \alpha^{-2} (1 - \Gamma) (1 + \Gamma)^{-3} \frac{\ell_U^2}{\ell_b}. \quad (2.29)$$

The layer depths ℓ_b and ℓ_U cannot be determined by the models. However, we expect them to depend on the turbulence from the plumes and the convective instabilities from the distributed buoyancy sources. As such, ℓ_b and ℓ_U would be functions of Γ , rather than emerging naturally without a dependence on Γ from a state of marginal stability.

2.8 Generalised models of the buoyancy field

So far, we examined steady states that arise from configurations where the strength of the localised sources is equal on the top and bottom boundary, as is the strength of the distributed sources. This symmetry in the boundary conditions results in steady state fields of the buoyancy and the velocity components that are (anti-) symmetric with respect to the axis $(x, z) = (0, 0)$ in the statistical average. While the symmetry of the system simplifies its description, a symmetric configuration is not necessary to allow for a steady state in an unventilated domain heated and cooled by localised and distributed sources.

In this section, we extend the models of §2.6 to configurations where the strength of the localised source on the top boundary is generally unequal to that of the localised source on the bottom boundary and the distributed sources on the top and bottom boundary are likewise generally of unequal strength. These models will not be validated with DNS data but rather serve as a tentative exploration of more general configurations than those studied in detail so far and provide a framework for the inverse problem in chapter 4.

2.8.1 Generalized model 1

We now consider an unventilated domain that is heated at the bottom by a localised source of strength $F_{\ell 1}$ and a distributed source of strength F_{d1} and cooled at the top by a localised source $F_{\ell 2}$ and a distributed source F_{d2} (see fig. 2.16). Generally, a steady state of the buoyancy field can be attained if the net buoyancy flux of the domain is zero. Thus, the buoyancy fluxes on the boundary need to satisfy

$$\underbrace{F_{\ell 1} + F_{d1}}_{F_1} = \underbrace{F_{\ell 2} + F_{d2}}_{F_2}. \quad (2.30)$$

As in the symmetric case, the total buoyancy flux on the bottom boundary F_1 and on the top boundary F_2 are used as a characteristic buoyancy flux for non-dimensionalisation, such that

$$F \equiv F_1 = F_2 = 1. \quad (2.31)$$

The symmetric configuration considered in the previous sections is a special case of the setup described here, corresponding to $F_{\ell 1} = F_{\ell 2}$ and $F_{d1} = F_{d2}$, and thus automatically satisfies (2.30).

As in §2.6, we model the buoyancy field as a two-layer stratification maintained by the plumes and consider distributed sources whose destabilising effect competes with the stabilising effect of the

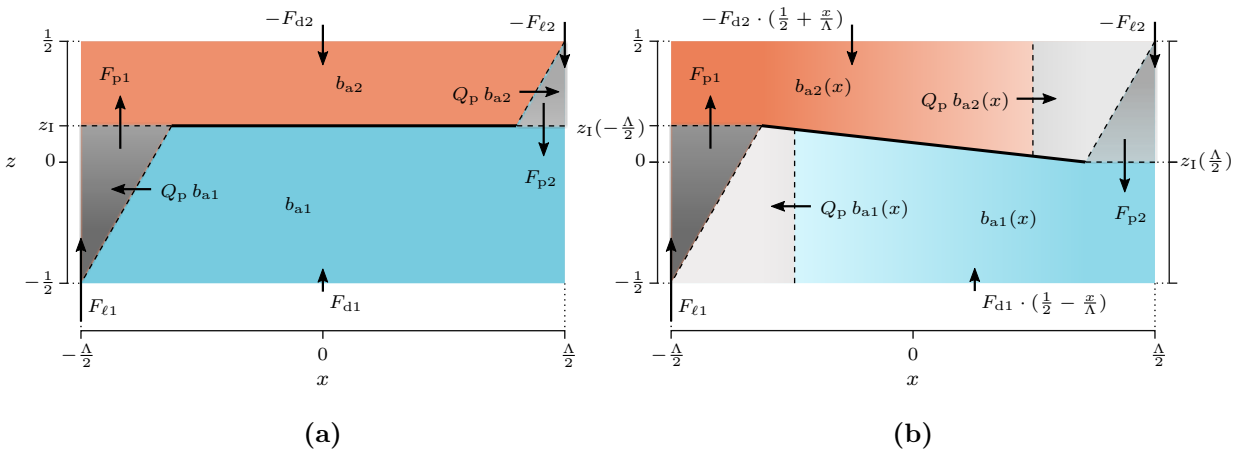


Figure 2.16: Schematics of the buoyancy structure for (a) the generalised model 1 of §2.8.1 and (b) the generalised model 2 of §2.8.2, where the localised sources on the top and bottom boundary and the distributed sources on the top and bottom boundary are generally unequal. The highlighted sections are the control volumes used. The volume flux across all dashed boundaries is equal Q_p .

localised sources,

$$F_{\ell 1} > 0, \quad F_{\ell 2} > 0, \quad F_{d1} \geq 0, \quad F_{d2} \geq 0. \quad (2.32)$$

In the current section, we construct an equivalent to model 1 of §2.6.1, i.e., we assume that each layer of the stratification is well-mixed. Hence, we model the stratification as consisting of a lower layer of uniform buoyancy b_{a1} and an upper layer of uniform buoyancy b_{a2} , separated by a horizontal interface at vertical position z_I that is now generally not located at the vertical middle $z = 0$ of the domain (see fig. 2.16a). The two plumes are connected by a global circulation of volume flux Q_p , which is modelled as the volume flux of each plume where it penetrates the interface according to plume scaling relations (see appendix A), i.e., at an elevation $\frac{1}{2} \pm z_I$ above or below their respective source:

$$Q_p = \alpha^{\frac{2}{3}} F_{\ell 1}^{\frac{1}{3}} \left(\frac{1}{2} + z_I \right) = \alpha^{\frac{2}{3}} F_{\ell 2}^{\frac{1}{3}} \left(\frac{1}{2} - z_I \right). \quad (2.33)$$

The plumes entrain fluid from their ambient and discharge fluid into the layer above or below them. We model the buoyancy flux associated with the plumes' entrainment as a product of the respective layer's mean buoyancy, b_{a1} or b_{a2} , and the volume flux Q_p of the global circulation, thus neglecting turbulent contributions to the buoyancy flux. Thus, the buoyancy fluxes F_{p1} and F_{p2} of the left- and right-hand plume, respectively, where they penetrate the interface can be obtained from buoyancy conservation of the plumes (see fig. 2.16a):

$$F_{p1} = F_{\ell 1} + Q_p b_{a1}, \quad F_{p2} = -F_{\ell 2} + Q_p b_{a2}. \quad (2.34)$$

To the upper layer, the left-hand plume acts as a buoyancy source (F_{p1}), while the distributed source on the top boundary (F_{d2}) and the entraining right-hand plume ($Q_p b_{a2}$) act as buoyancy sinks (see fig. 2.16a). Hence, buoyancy conservation of the upper layer results in

$$F_{p1} = F_{d2} + Q_p b_{a2} \quad (2.35)$$

and the equivalent consideration for the lower layer gives

$$F_{p2} = -F_{d1} + Q_p b_{a1}, \quad (2.36)$$

where we assumed that the buoyancy flux due to entrainment across the interface is negligible.

Combining equations (2.34), (2.35) and (2.36), we obtain the condition (2.30) for steady states and an expression for the buoyancy difference between the two layers of the stratification:

$$2 Q_p (b_{a2} - b_{a1}) = F_{\ell 1} - F_{d1} + F_{\ell 2} - F_{d2}. \quad (2.37)$$

Hence, the buoyancy fluxes on the boundary do not fully determine the buoyancy field within the domain, as we cannot give an expression of the upper and lower layer's buoyancy independently of each other. This is plausible, since the buoyancy fluxes only determine the rate of change of the

buoyancy field, and the volume integrated buoyancy B in the bulk, i.e., excepting the plumes,

$$B = \int_{-\frac{\Lambda}{2}}^{\frac{\Lambda}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} b_a dz dx \quad (2.38)$$

is not impacted by the buoyancy fluxes in the steady state,

$$\frac{dB}{dt} = F_{\ell 1} + F_{d1} - F_{\ell 2} - F_{d2}, \quad (2.39)$$

where the right-hand side is zero due to (2.30). In the symmetric configurations modelled in §2.6, the knowledge about the symmetry of the buoyancy field allowed us to express the buoyancy in each layer in dependence of the buoyancy fluxes on the boundary. Indeed, this symmetry information corresponds to including $B = 0$ into the model. Generally, the volume integrated buoyancy B is given for model 1 by

$$B = \int_{-\frac{\Lambda}{2}}^{\frac{\Lambda}{2}} \left[\int_{-\frac{1}{2}}^{z_1} b_{a1} dz + \int_{z_1}^{\frac{1}{2}} b_{a2} dz \right] dx = \Lambda \left[\frac{1}{2} (b_{a2} + b_{a1}) - z_1 (b_{a2} - b_{a1}) \right]. \quad (2.40)$$

Combining equations (2.33), (2.37) and (2.40), the modelled steady state buoyancy field is described by

$$z_1 = \frac{1}{2} \frac{(1 + \Gamma_1)^{\frac{1}{3}} - (1 + \Gamma_2)^{\frac{1}{3}}}{(1 + \Gamma_1)^{\frac{1}{3}} + (1 + \Gamma_2)^{\frac{1}{3}}}, \quad (2.41a)$$

$$\delta b = \frac{F^{\frac{2}{3}}}{\alpha^{\frac{2}{3}}} \left[(1 + \Gamma_1)^{\frac{1}{3}} + (1 + \Gamma_2)^{\frac{1}{3}} \right] \frac{1 - \Gamma_1 \Gamma_2}{(1 + \Gamma_1)(1 + \Gamma_2)}, \quad (2.41b)$$

$$\Sigma b = \frac{F^{\frac{2}{3}}}{\alpha^{\frac{2}{3}}} \left[(1 + \Gamma_1)^{\frac{1}{3}} - (1 + \Gamma_2)^{\frac{1}{3}} \right] \frac{1 - \Gamma_1 \Gamma_2}{(1 + \Gamma_1)(1 + \Gamma_2)} + \frac{2B}{\Lambda}, \quad (2.41c)$$

where

$$\delta b \equiv b_{a2} - b_{a1}, \quad \Sigma b \equiv b_{a2} + b_{a1}, \quad (2.42)$$

denote the buoyancy difference between the layers and the sum of the layers' buoyancies, respectively. The buoyancy flux on the boundaries is given in terms of the ratios Γ_1 and Γ_2 of the distributed to the localised source strength on the bottom and top boundary, respectively, and the total buoyancy flux F on the horizontal boundaries

$$\Gamma_1 \equiv \frac{F_{d1}}{F_{\ell 1}}, \quad \Gamma_2 \equiv \frac{F_{d2}}{F_{\ell 2}}, \quad F = F_{\ell 1} + F_{d1} = F_{\ell 2} + F_{d2}, \quad (2.43)$$

which, in accordance with (2.32), satisfy

$$\Gamma_1 \geq 0, \quad \Gamma_2 \geq 0, \quad F > 0. \quad (2.44)$$

From (2.33), the volume flux Q_p of the global circulation is modelled as

$$Q_p = \frac{\alpha^{\frac{2}{3}} F^{\frac{1}{3}}}{(1 + \Gamma_1)^{\frac{1}{3}} + (1 + \Gamma_2)^{\frac{1}{3}}}. \quad (2.45)$$

In (2.41), (2.43) and (2.45), we included the total buoyancy flux $F = 1$ on the horizontal boundaries for completeness, as Γ_1 , Γ_2 and F are the free parameters that describe the boundary buoyancy flux

for a configuration that permits steady states: the condition (2.30) is automatically satisfied in this parametrisation.

For the symmetric configurations, we found that the buoyancy field shows a stable two-layer stratification, if the difference Δb between the peaks of the buoyancy field's PDF is positive, $\Delta b > 0$. As we model the two layers of the stratification as uniform in this section, the characteristic buoyancy difference Δb equals δb and from (2.41b) and (2.44) we find that the condition $\Delta b > 0$ corresponds to

$$\Gamma_1 \cdot \Gamma_2 < 1. \quad (2.46)$$

Note, that δb and Σb describe the local buoyancy difference or buoyancy sum of the layers at a horizontal position x , whereas Δb is a property of the buoyancy field's PDF. Although $\Delta b = \delta b$ in model 1, we introduced δb in this section for consistent notation with §2.8.2 discussing model 2, where generally $\Delta b \neq \delta b$.

We defer the discussion of the predicted properties of the steady state buoyancy field in a generalised configuration to §2.8.3 and first consider a generalisation of model 2.

2.8.2 Generalized model 2

We now consider a configuration with the same boundary conditions as in the previous section but allow for a horizontal gradient in the buoyancy $b_{a1}(x)$ of the lower layer and in the buoyancy $b_{a2}(x)$ of the upper layer, though both layers are modelled as ideally mixed in the vertical (see fig. 2.16b). Likewise, the position $z_I(x)$ of the interface separating the layers is generally dependent on the position x in the horizontal.

The left-hand plume penetrates the interface at an elevation $\frac{1}{2} + z_I(-\frac{\Lambda}{2})$ and, equivalently, so does the right-hand plume at a distance $\frac{1}{2} - z_I(\frac{\Lambda}{2})$ below its source. The volume flux Q_p of the plumes where they penetrate the interface corresponds to the strength of the global circulation connecting both plumes:

$$Q_p = \alpha^{\frac{2}{3}} F_{\ell 1}^{\frac{1}{3}} \left(\frac{1}{2} + z_I(-\frac{\Lambda}{2}) \right) = \alpha^{\frac{2}{3}} F_{\ell 2}^{\frac{1}{3}} \left(\frac{1}{2} - z_I(\frac{\Lambda}{2}) \right). \quad (2.47)$$

We model the buoyancy flux corresponding to entrainment into the plumes with assumptions equivalent to those used in §2.8.1, where the left-hand plume entrains fluid at a buoyancy $b_{a1}(-\frac{\Lambda}{2})$ and the fluid entrained into the right-hand plume is of buoyancy $b_{a2}(\frac{\Lambda}{2})$. Thus, buoyancy conservation of the plumes results in (see fig. 2.16b):

$$F_{p1} = F_{\ell 1} + Q_p b_{a1}(-\frac{\Lambda}{2}), \quad F_{p2} = -F_{\ell 2} + Q_p b_{a2}(\frac{\Lambda}{2}). \quad (2.48)$$

We now consider a segment of the upper layer between the left-hand wall at $-\frac{\Lambda}{2}$ and an arbitrary position x in the horizontal. The left-hand plume discharging into the upper layer acts as a buoyancy source to this control volume (F_{p1}), while the distributed source on the top boundary ($F_{d2} (\frac{1}{2} + \frac{x}{\Lambda})$, cf. §2.6.2) and the fluid advected with the global circulation through the right-hand boundary of the control volume ($Q b_{a2}(x)$) constitute buoyancy sinks. Buoyancy conservation in this segment of the upper layer and an equivalent segment of the lower layer gives (see fig. 2.16b):

$$F_{p1} = F_{d2} \left(\frac{1}{2} + \frac{x}{\Lambda} \right) + Q_p b_{a2}(x), \quad F_{p2} = -F_{d1} \left(\frac{1}{2} - \frac{x}{\Lambda} \right) + Q_p b_{a1}(x). \quad (2.49)$$

In terms of the difference $\delta b(x)$ and the sum $\Sigma b(x)$ of the buoyancy of the upper and lower layer (2.42), equations (2.48) and (2.49) correspond to the equation set

$$\frac{F_{d1} - F_{d2}}{\Lambda} = Q_p \partial_x \delta b(x), \quad F_{\ell 1} = Q_p \delta b(-\frac{\Lambda}{2}), \quad F_{\ell 2} = Q_p \delta b(\frac{\Lambda}{2}), \quad (2.50a)$$

$$-\frac{F_{d1} + F_{d2}}{\Lambda} = Q_p \partial_x \Sigma b(x), \quad -(F_{d1} + F_{d2}) = Q_p (\Sigma b(\frac{\Lambda}{2}) - \Sigma b(-\frac{\Lambda}{2})), \quad (2.50b)$$

together with the condition (2.30) for steady states. Using the expression of the volume integrated buoyancy B according to model 1,

$$B = \int_{-\frac{\Lambda}{2}}^{\frac{\Lambda}{2}} \left[\int_{-\frac{1}{2}}^{z_1(x)} b_{a1}(x) dz + \int_{z_1(x)}^{\frac{1}{2}} b_{a2}(x) dz \right] dx, \quad (2.51a)$$

$$= \int_{-\frac{\Lambda}{2}}^{\frac{\Lambda}{2}} \left[\frac{1}{2} \Sigma b(x) - z_1(x) \delta b(x) \right] dx, \quad (2.51b)$$

we may give a preliminary solution to (2.50):

$$\delta b(x) = \frac{1}{2 Q_p} \left[F_{\ell 1} \left(1 - \frac{2x}{\Lambda} \right) + F_{\ell 2} \left(1 + \frac{2x}{\Lambda} \right) \right], \quad (2.52a)$$

$$\Sigma b(x) = -\frac{1}{2 Q_p} (F_{d1} + F_{d2}) \frac{2x}{\Lambda} + \frac{2}{\Lambda} \int_{-\frac{\Lambda}{2}}^{\frac{\Lambda}{2}} z_1(x) \delta b(x) dx + \frac{2B}{\Lambda}. \quad (2.52b)$$

As in §2.6.2, the position of the interface z_1 , and likewise the volume flux Q_p , cannot be obtained solely from volume conservation (2.47) and a closure assumption is required. Note, however, that a linear spatial dependence of the buoyancy values in the layers in x is already determined in the preliminary solution (2.52). Indeed, the character of the spatial dependence of δb and Σb in the horizontal is independent of any closure assumption.

As in §2.6.2, we close the model by assuming that the pressure p in the domain can be approximated as hydrostatic, and that the pressure difference between the top and bottom boundary satisfies

$$0 = \partial_x \left(p|_{z=-\frac{1}{2}} - p|_{z=\frac{1}{2}} \right) = \partial_x \left(\frac{1}{2} \Sigma b(x) - z_1(x) \delta b(x) \right). \quad (2.53)$$

Combining equations (2.47), (2.52) and (2.53), the modelled steady state is described by

$$z_1(x) = -\frac{1}{2} \left(\frac{1 - \frac{2x}{\Lambda}}{1 + \Gamma_1} + \frac{1 + \frac{2x}{\Lambda}}{1 + \Gamma_2} \right)^{-1} \left[\frac{1 + \frac{2x}{\Lambda} \Gamma_1}{1 + \Gamma_1} - \frac{1 - \frac{2x}{\Lambda} \Gamma_2}{1 + \Gamma_2} + 2 \frac{(1 + \Gamma_1)^{\frac{2}{3}} - (1 + \Gamma_2)^{\frac{2}{3}}}{(1 + \Gamma_1)^{\frac{2}{3}} + (1 + \Gamma_2)^{\frac{2}{3}}} \right], \quad (2.54a)$$

$$\delta b(x) = \frac{F^{\frac{2}{3}}}{2 \alpha^{\frac{2}{3}}} \left(\frac{1}{(1 + \Gamma_1)^{\frac{2}{3}}} + \frac{1}{(1 + \Gamma_2)^{\frac{2}{3}}} \right) \left(\frac{1 + \frac{2x}{\Lambda} \Gamma_1}{1 + \Gamma_1} + \frac{1 - \frac{2x}{\Lambda} \Gamma_2}{1 + \Gamma_2} \right), \quad (2.54b)$$

$$\begin{aligned} \Sigma b(x) = & -\frac{F^{\frac{2}{3}}}{2 \alpha^{\frac{2}{3}}} \left[\left(\frac{1}{(1 + \Gamma_1)^{\frac{2}{3}}} + \frac{1}{(1 + \Gamma_2)^{\frac{2}{3}}} \right) \left(\frac{1 + \frac{2x}{\Lambda} \Gamma_1}{1 + \Gamma_1} - \frac{1 - \frac{2x}{\Lambda} \Gamma_2}{1 + \Gamma_2} \right) \right. \\ & \left. - 2 \left(\frac{1}{(1 + \Gamma_1)^{\frac{2}{3}}} - \frac{1}{(1 + \Gamma_2)^{\frac{2}{3}}} \right) \right] + \frac{2B}{\Lambda}, \end{aligned} \quad (2.54c)$$

where the buoyancy flux ratios Γ_1 and Γ_2 on the bottom and top boundary, respectively, and the total buoyancy flux $F = 1$ on each horizontal boundary are defined as given in (2.43). The volume flux Q_p

of the global circulation is modelled as

$$Q_p = \frac{\alpha^{\frac{2}{3}} F^{\frac{1}{3}}}{(1 + \Gamma_1)^{-\frac{2}{3}} + (1 + \Gamma_2)^{-\frac{2}{3}}} . \quad (2.55)$$

As for the symmetric case, it can be shown that the upper layer is deepest at the right-hand wall ($x = \frac{\Lambda}{2}$) and the lower layer is deepest at the left-hand wall ($x = -\frac{\Lambda}{2}$),

$$z_I(-\frac{\Lambda}{2}) \geq z_I(x) \geq z_I(\frac{\Lambda}{2}), \quad x \in [-\frac{\Lambda}{2}, \frac{\Lambda}{2}], \quad (2.56)$$

and thus, the difference Δb between the peaks of the modelled buoyancy field's PDF corresponds to

$$\Delta b = b_{a2}(\frac{\Lambda}{2}) - b_{a1}(-\frac{\Lambda}{2}) = \frac{F^{\frac{2}{3}}}{\alpha^{\frac{2}{3}}} \left(\frac{1}{(1 + \Gamma_1)^{\frac{2}{3}}} + \frac{1}{(1 + \Gamma_2)^{\frac{2}{3}}} \right) \frac{1 - \Gamma_1 \Gamma_2}{(1 + \Gamma_1)(1 + \Gamma_2)} . \quad (2.57)$$

Hence, as in the generalized model 1, the condition $\Delta b > 0$ corresponds to $\Gamma_1 \cdot \Gamma_2 < 1$.

2.8.3 Predicted properties of the buoyancy field in the generalised case

The configurations we focused on in this chapter have symmetric boundary conditions, i.e., the buoyancy flux ratio on the bottom boundary Γ_1 is equal to that on the top boundary, $\Gamma \equiv \Gamma_1 = \Gamma_2$. Symmetric boundary conditions result in an antisymmetric steady state buoyancy field $b = g(\rho_0 - \rho)$ in the sense that we can find a reference density ρ_0 , such that the buoyancy field satisfies $b(x, z) = -b(-x, -z)$ in the statistical average.

Modelling the buoyancy field that arises from more general boundary conditions, $\Gamma_1 \neq \Gamma_2$, highlights that the same boundary conditions can maintain different buoyancy fields in the steady state, which differ in the value of the corresponding volume-integrated buoyancy B . Vice versa, this means that the buoyancy field in the considered configuration is not fully determined by the buoyancy fluxes on the boundary. In contrast, the modelled local buoyancy difference δb between the layers at any position

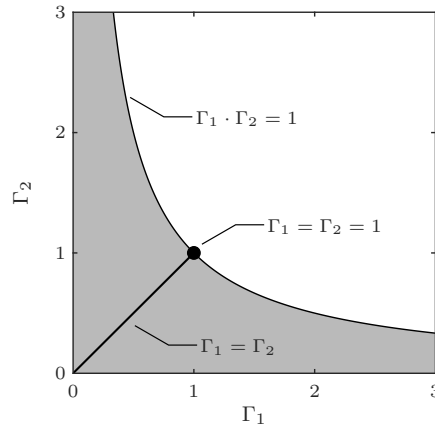


Figure 2.17: Range of the ratio of the distributed to the localised buoyancy flux on the bottom and top boundary, Γ_1 and Γ_2 , respectively, in which the generalised models 1 and 2 are consistent (grey shaded). The range of permissible values is bounded by $\Gamma_1 \cdot \Gamma_2 < 1$ in the general case (thin black line), which corresponds to $\Gamma < 1$ in the symmetric case $\Gamma \equiv \Gamma_1 = \Gamma_2$ (‘•’-marker). The bold black line shows the range of permissible values in the symmetric case.

in the horizontal is solely dependent on the buoyancy fluxes on the boundary, as is the position of the interface z_1 . However, the modelled buoyancy difference δb does not have a clearly defined measurable equivalent, since the models presented in this section are constructed under the assumption that each layer is ideally mixed in the vertical. A measurable equivalent to the modelled interface position is more easily defined, where, according to our models, the interface position is solely determined by the ratio of the buoyancy fluxes on each boundary and is independent of the total buoyancy flux F on each boundary. In the general case $\Gamma_1 \neq \Gamma_2$, the modelled interface is no longer at the vertical centre $z = 0$ of the domain or rotated around the line $(x, z) = (0, 0)$. Moreover, if we account for a horizontal buoyancy gradient (model 2), the modelled interface resulting from asymmetric boundary conditions is not linear in the horizontal x (see (2.54a)), where the curvature is typically small for $\Gamma_1 < 1$ and $\Gamma_2 < 1$:

$$\frac{\partial^2 z_1}{\partial x^2} = \frac{1}{\Lambda^2} (\Gamma_1^2 - \Gamma_2^2) + \mathcal{O}((\Gamma_i \Gamma_j)^3), \quad i, j \in \{1, 2\}. \quad (2.58)$$

In the symmetric case, the models are consistent up to a limit of $\Gamma = 1$, which corresponds to the difference Δb between the peaks of the buoyancy field's PDF becoming zero. This limit represents a special case of the more general condition $\Gamma_1 \cdot \Gamma_2 < 1$ found from the generalised models in the previous sections. Fig.2.17 illustrates the corresponding permissible range of the buoyancy flux ratios on the top and bottom boundary (grey shaded area), where symmetric configurations, $\Gamma_1 = \Gamma_2$, are marked by a bold black line. The condition $\Gamma_1 \cdot \Gamma_2 < 1$ allows for an arbitrarily strong distributed source on one boundary, relative to the localised source on the same boundary, provided the distributed source on the opposite boundary is sufficiently small compared to the localised source on the same boundary. It is not realistic that we find a two-layer stratification in any such configuration, and hence, $\Gamma_1 \cdot \Gamma_2 < 1$ should be understood as an upper limit to the buoyancy flux ratios that may produce a two-layer stratification in the steady state, rather than as a requirement for the stratification to be destroyed.

2.9 Conclusions

Localised sources of buoyancy at the top and bottom boundary of a closed domain produce turbulent plumes that maintain a stable two-layer stratification in the steady state. The addition of distributed heating leads to a competition between the stabilising effect of the localised sources and the destabilising effect of the distributed sources. The ratio of the distributed to the localised buoyancy flux, Γ , determines the system's response. At $\Gamma < 1$, the stabilising effect of the localised sources dominates and the buoyancy field is stably stratified in two layers. The buoyancy difference between the layers decreases with increasing Γ , until the two-layer stratification is destroyed for $\Gamma > 1$. These remarks are consistent with the results of Wells, Griffiths and Turner [116] for different configurations of combined localised and distributed heating in a closed domain (fig. 1.2a,b).

The buoyancy transport between the layers of the two-layer stratification ($\Gamma < 1$) is dominated by the plumes and interfacial buoyancy transport outside the plumes is negligible. This agrees with the negligible interfacial buoyancy flux inferred by Partridge and Linden [85, fig. 1.2d] for a ventilated domain heated by a localised and a distributed source and is in contrast to the results of Chenvidyakarn and Woods [25, fig. 1.2c]. In this context, we note that Chenvidyakarn and Woods [25] considered a mechanically ventilated domain where the direction of the mean inflow and outflow was perpendicular to the interface between the layers, whereas Partridge and Linden [85] studied natural ventilation through openings in the sidewalls, which promote a mean inflow and outflow approximately parallel

to the interface. With regard to the orientation of the mean flow, the case considered in this chapter is closer to that of Partridge and Linden [85] than to the one of Chenvidyakarn and Woods [25] and the difference in the mean flow structure may be partly responsible for the different observations of the buoyancy transport between the layers.

Despite its focus on stably stratified states dominated by localised sources ($\Gamma < 1$), our work demonstrates the significance of distributed heating in determining the flow circulation and buoyancy structure. Distributed heating produces a lateral buoyancy gradient in each layer, which increases with Γ . A result of the lateral buoyancy gradient is a tilting of the interface separating the two layers, which increases with Γ . The tilt of the interface affects the secondary circulations that develop within each layer and the strength of the primary large-scale circulation. We presume that the lateral buoyancy gradient is a result of the horizontal mean flow over the distributed sources, where the increasing (or decreasing) buoyancy value of the fluid in the mean flow direction is an accumulative effect of the distributed source of positive (or negative) buoyancy flux. Hence, the mean flow structure crucially influences the buoyancy field. In configurations of confined equal and opposite plumes, the mean flow structure in the steady state depends on the aspect ratio of the domain [29] and, likewise, we expect the structure of the buoyancy field for combined localised and distributed heating and cooling to depend on the aspect ratio.

In predictions of the buoyancy difference Δb between the layers, the lateral buoyancy gradient can be neglected for small values of Γ , but plays an essential role when $\Gamma \gtrsim 0.23$. In contrast, the lateral buoyancy gradient is crucial in predictions of the strength of the large-scale circulation for all values of $\Gamma < 1$. Indeed, our model predicts that the height at which the plumes penetrate the interface, which determines their volume flux, is solely a function of Γ . In this regard we note that the two-layer stratification disappears as the plume height becomes comparable to the domain height. We extended the models to steady states from configurations where the ratio of the distributed to the localised source strength is generally unequal on the top and bottom boundary, $\Gamma_1 \neq \Gamma_2$. The models indicate that the steady state is in this case determined by the buoyancy flux ratios of both boundaries, Γ_1 and Γ_2 , and that $\Gamma_1 \cdot \Gamma_2 < 1$ poses an upper boundary for the maintenance of a two-layer stratification. In cases of unequal sources on the top and bottom boundary, the interface would not necessarily be located at the domain's mid-plane, but rather position itself such as to balance the interfacial volume flux from each plume.

The configuration considered here is relatively simple and might therefore provide a useful starting point in the investigation of non-uniformly heated domains. In all such cases we would expect to find a buoyancy structure that is more stably stratified than the well-mixed environments produced by uniform heating.

Chapter 3

Transient states

3.1 Introduction

In this chapter, we study transient states that result from an abrupt change in the distribution of heating or cooling of the boundaries. As in chapter 2, we consider a box that is heated and cooled by a combination of localised and distributed sources of buoyancy flux. We focus on distributions of boundary heating where the plumes from the localised sources produce a stable stratification in the bulk.

A related configuration is that of a single localised heat source on the bottom boundary of a box, resulting in a plume that produces a stable stratification in its ambient. The filling box mechanism, first described by Baines and Turner [9], is a simple transient state of this configuration that occurs when localised heating is turned on in an initially unstratified environment. Fluid above the localised source is heated and rises, resulting in a turbulent plume. As the plume reaches the ceiling, buoyant fluid from the plume spreads out and forms a buoyant layer above the unstratified fluid in the ambient of the plume, where the interface between the layers is marked by a density step. Since the plume entrains fluid from the newly formed buoyant layer, the buoyancy of the plume where it reaches the ceiling is subsequently higher than the buoyant layer and the fluid discharged by the plume spreads above the existing layer. Thus, a stratified buoyant layer develops which deepens over time, corresponding to a descending interface between stratified and unstratified fluid, and increases in its average buoyancy [117]. The density stratification of the buoyant layer typically has a high vertical density gradient close to the interface and a low density gradient away from the interface through much of the buoyant layer [9, 117].

If the interior of such a box with a localised buoyancy source is connected to a uniform and quiescent environment by ventilation openings on the top and bottom boundary, the buoyant layer drives a draining flow through the upper ventilation opening, which is balanced by an inflow through the lower opening (‘emptying-filling box’) [63]. The non-dimensional flow is then determined by two parameters: the buoyancy flux F_ℓ of the localised source and the effective opening areas A^* of the vents. These two parameters determine the time scale of the transient period before a steady state is reached and the transient depth of the buoyant layer, which is supplied by the plume’s volume flux (F_ℓ) and depleted by outflow through the upper ventilation opening (A^*) [50]. The transient depth of the buoyant layer can at times exceed the eventually approached steady state layer depth [38, 50],

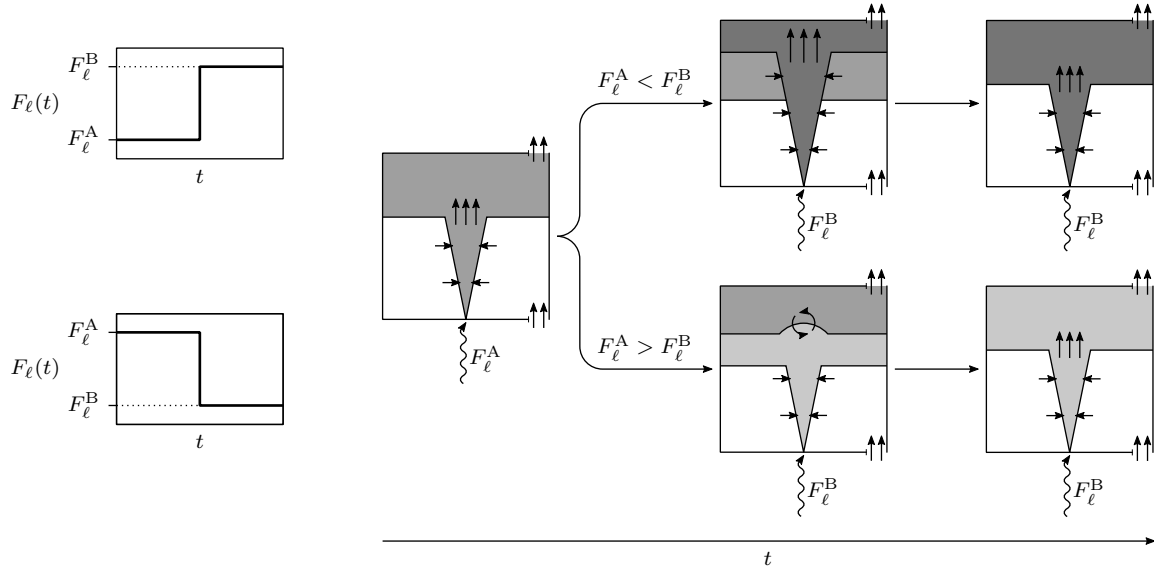


Figure 3.1: Types of transient flow resulting from an abrupt change in the source strength of a plume in a ventilated box. Depicted are the flows resulting from an increase (upper row) and decrease (lower row) of the localised source buoyancy flux F_ℓ , which takes the values F_ℓ^A and F_ℓ^B before and after the step change, respectively. The figure is based on fig. 1 in Bower et al. [20].

which is solely determined by the ventilation openings [63].

If the plumes source strength F_ℓ in an emptying-filling box configuration with a steady stable stratification is changed abruptly from F_ℓ^A to F_ℓ^B , two different types of flows can arise, depending on whether the source strength is increased or decreased [20]. Following an increase of the localised buoyancy flux ($F_\ell^A < F_\ell^B$), the density of fluid in the plume decreases, such that the fluid discharged by the plume after the step change of F_ℓ spreads above the buoyant layer of the previous stratification [20] (fig. 3.1, upper row). The new buoyant upper layer resulting from the ‘filling flow’ increases in depth as the plume entrains fluid from the two lower layers and thus develops a stratified density profile [20]. The buoyant layer of the initial stable stratification is depleted by the plume, such that the steady state eventually approached after the step change resembles the initial steady state with an upper layer of increased buoyancy (fig. 3.1).

If the plumes source strength is decreased to a positive value $F_\ell^B > 0$ of buoyancy flux ($F_\ell^A > F_\ell^B$), the density of fluid in the plume increases. Whilst the density of fluid in the plume is smaller than the density of the unstratified environment, it exceeds the density of the buoyant layer from the initial stratification, such that fluid discharged by the plume forms an intruding layer between the two layers of the initial stratification [20] (fig. 3.1, lower row). The fluid in the plume becomes neutrally buoyant relative to its ambient when it reaches the buoyant layer of the initial stratification and the plume becomes a fountain at the level of zero relative buoyancy [51, 55]. The fountain impinges on the overlying layer and thus entrains fluid from the latter [8, 10, 16, 55, 60, 67]. Thus, the volume of the upper layer is depleted by entrainment into the intruding layer and by outflow through the upper ventilation opening, until a steady state stratification corresponding to that of an emptying-filling box is regained.

How does this dynamic change if distributed sources are included in the configuration? In this chapter, we consider configurations where the step change of the strength of the localised plume

sources is accompanied by a step increase or decrease of added distributed heating and cooling on the horizontal boundaries.

3.2 Problem description

Equivalently to chapter 2, we consider a box that is heated and cooled by a combination of localised and distributed sources of buoyancy flux, where the source strengths now undergo an abrupt change at time $t = 0$. The dimensions of the box are as in chapter 2, as are the boundary conditions on the flow velocity (see fig. 2.1). All quantities in this chapter are non-dimensionalised according to chapter 2.

As in chapter 2, each horizontal boundary is heated (or cooled) by a localised source of buoyancy flux F_ℓ and a distributed source of buoyancy flux F_d , where the area of the localised source corresponds to a strip of dimensionless width λ and the area of the distributed source covers the remaining horizontal boundary area (see fig. 2.1). The buoyancy fluxes F_ℓ and F_d assume the same values on the top and bottom boundary and the buoyancy flux across the side walls is zero.

We consider step changes of the buoyancy flux ratio at $t = 0$

$$\frac{F_d(t)}{F_\ell(t)} = \Gamma(t) = \begin{cases} \Gamma^A & \text{for } t < 0, \\ \Gamma^B & \text{for } t \geq 0, \end{cases} \quad (3.1)$$

where the total buoyancy flux on the top and bottom boundary is equal and constant at all times

$$F_\ell^A + F_d^A = F_\ell^B + F_d^B = 1. \quad (3.2)$$

Before the step change of Γ , the system is statistically steady at Γ^A and stably stratified, since $\Gamma^A < 1$ (see chapter 2). Likewise, the buoyancy flux ratio Γ^B after the step change satisfies $\Gamma^B < 1$, such that we expect the system to develop a stable stratification for $t \rightarrow \infty$. Hence, the transient state resulting from the step change of Γ corresponds to a transition between two stably stratified steady states, provided it is observed for a sufficiently long duration. The buoyancy difference between the two layers of the stratification is determined by the same characteristic parameters as given in chapter 2.

3.3 Simulation details

We investigate the configuration described in the previous section using DNS, where the methods and characteristic parameters, apart from Γ , are as in chapter 2 (see §2.4). We consider step changes between a configuration of purely localised heating and cooling ($\Gamma = 0$) and a configuration where a significant fraction of the buoyancy flux is provided by the distributed sources ($\Gamma = 0.60$). Specifically, we consider a step increase

$$\Gamma(t) = \begin{cases} 0 & \text{for } t < 0 \\ 0.60 & \text{for } t \geq 0 \end{cases} \quad (3.3)$$

and a step decrease

$$\Gamma(t) = \begin{cases} 0.60 & \text{for } t < 0 \\ 0 & \text{for } t \geq 0 \end{cases} \quad (3.4)$$

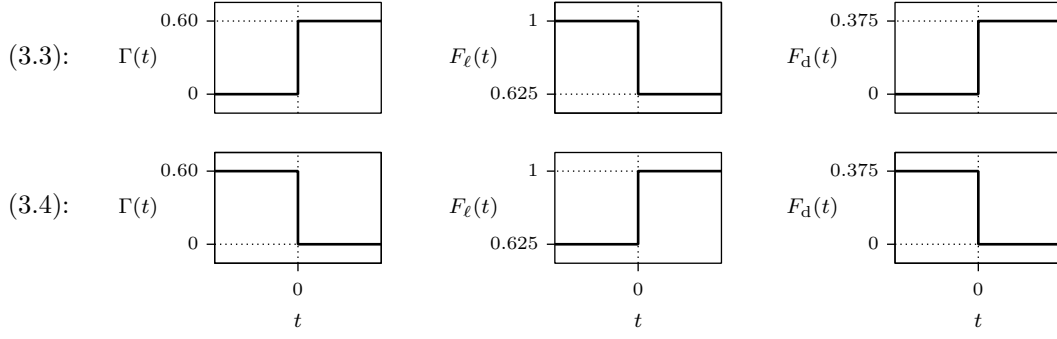


Figure 3.2: Visualisation of the boundary conditions associated with the step changes defined in (3.3) and (3.4): depicted are the buoyancy flux ratio Γ , the localised buoyancy flux F_ℓ and the distributed buoyancy flux F_d over time.

of the buoyancy flux ratio. Since the total buoyancy flux $F_\ell + F_d$ on each boundary is kept constant, a step change in Γ corresponds to a simultaneous step change in the localised and distributed buoyancy flux, F_ℓ and F_d , respectively (see fig. 3.2). The DNS data for $t < 0$ corresponds to the simulations of the steady state at $\Gamma \in \{0, 0.60\}$ presented in chapter 2. For the criterion employed to determine a state as statistically steady, see §2.4.

As in chapter 2, we refer to $b = g(\rho_0 - \rho)/\rho_0$ as buoyancy, where ρ is the fluid density, ρ_0 is a reference density and g is the absolute value of the gravitational acceleration. This definition of buoyancy is not necessarily the same as the relative buoyancy of a fluid parcel to its ambient, which corresponds to the buoyancy force acting on the fluid parcel.

We define the mean of a field $h(t, x, y, z)$ over the homogeneous direction y as

$$\langle h \rangle(t, x, z) \equiv \frac{1}{\Lambda_y} \int_{-\frac{\Lambda_y}{2}}^{\frac{\Lambda_y}{2}} h(t, x, y, z) dy. \quad (3.5)$$

Moving averages at time t over a time interval Δt are calculated as

$$\frac{1}{\Delta t} \int_{t-\frac{\Delta t}{2}}^{t+\frac{\Delta t}{2}} h(t, x, y, z) dt, \quad (3.6)$$

where we choose $\Delta t = 0.04$ in dimensionless time units. As in chapter 2, the mean of a field $h(t, x, y, z)$ over the homogeneous direction y and time is denoted as $\bar{h}(x, z)$ (see §2.4).

3.4 Results

3.4.1 Step increase of the buoyancy flux ratio

In the current section, we consider the transient state resulting from a step change (3.3) from a configuration with purely localised heating and cooling ($\Gamma^A = 0$) to a configuration with heating and cooling from localised and distributed sources ($\Gamma^B = 0.60$).

The transition in spatially dependent quantities

We first consider the transient state in terms of the corresponding time and spatially dependent buoyancy field. The transient state studied in this section can be considered as a transition between the steady state at $\Gamma = 0$, which constitutes its initial state for $t < 0$, and the steady state at $\Gamma = 0.60$, which the system would approach for $t \rightarrow \infty$. Let us briefly recapitulate the buoyancy structure of the initial and ‘final’ steady states of the transition, as presented in chapter 2. In the initial steady state at $\Gamma = 0$, the buoyancy field is stably stratified into two layers of approximately uniform buoyancy in the bulk, which are separated by a horizontal interface (fig. 3.3 at $t = 0$). In the ‘final’ steady state at $\Gamma = 0.60$, the buoyancy difference between the layers is reduced compared to $\Gamma = 0$. The steady state buoyancy field at $\Gamma = 0.60$ possesses a finite and oppositely oriented horizontal buoyancy gradient in its two layers and the interface between the two layers is tilted (cf. §2.5.1).

To study the transient state resulting from the step change (3.3), we first consider instances of the buoyancy field over a duration of 5 time units (fig. 3.3). With the step change to $\Gamma^B = 0.60$, convection from the horizontal boundaries develops (fig. 3.3 at $t = 1$) which results in the formation of small plumes transporting cool or warm fluid into the former approximately homogeneous upper or lower layers of the stratification, respectively. The fluid in the upper (lower) layer, which is thus

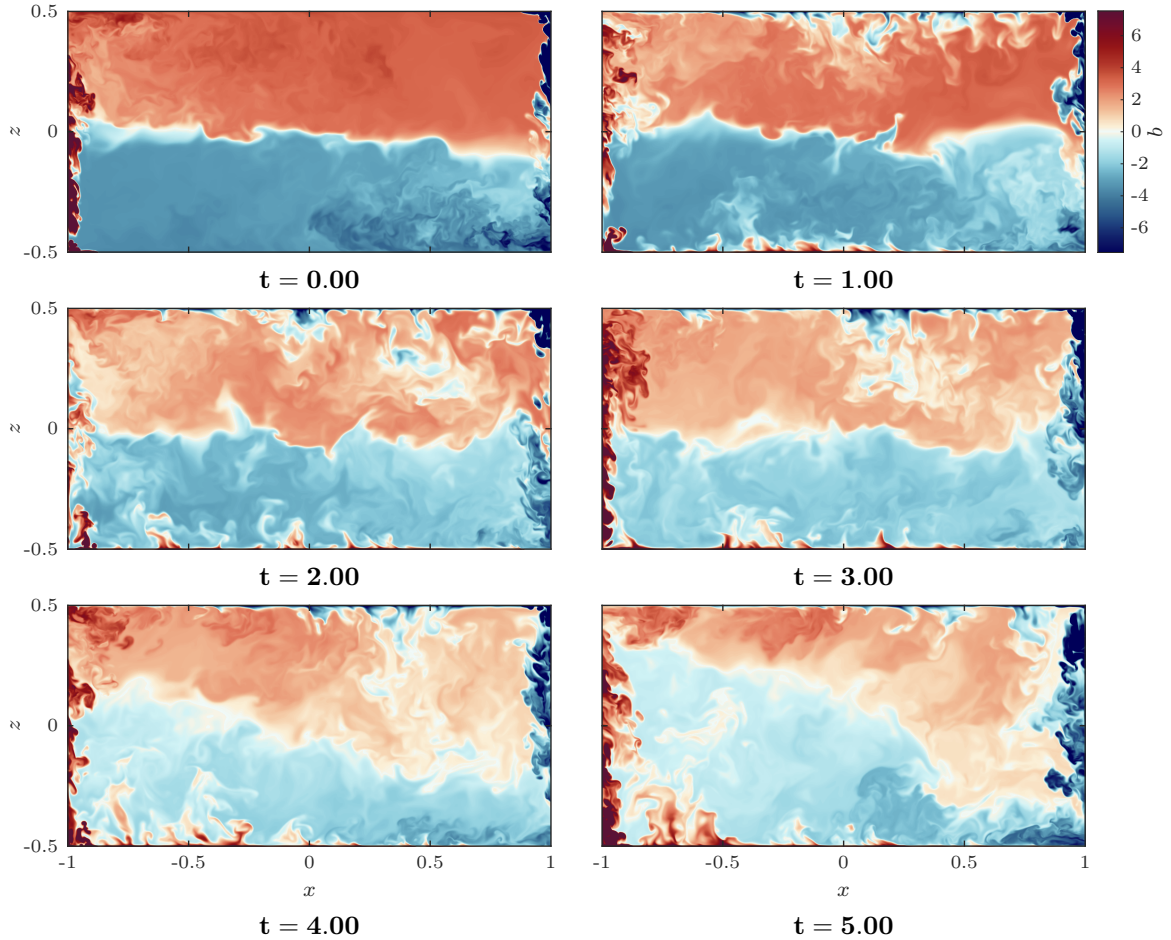


Figure 3.3: Instances of the transient buoyancy field for the step increase of Γ (3.3) considered at time steps of 1 time unit for the duration $t \in [0, 5]$.

cooled (heated) by the horizontal boundaries, is entrained into the plumes, whose source strength has been reduced by the step change. Consequently, the buoyancy of the upper layer gradually decreases, while the lower layer's buoyancy increases. At $t = 4$, a horizontal buoyancy gradient is evident in the two layers of the stratification and the interface between the layers is tilted (fig. 3.3). Subsequently, the tilt of the interface increases further until the interface qualitatively resembles that of the steady state at $\Gamma = 0.60$ (fig. 3.3 at $t = 5$, cf. §2.5.1, fig. 2.5e).

It is noticeable that the transient state shown in fig. 3.3 represents a smooth transition between the initial steady state and the expected final steady state in the sense that the buoyancy field at each instant in time resembles the instantaneous buoyancy field of a steady state (cf. fig. 3.3 and 2.5). The buoyancy difference between the two layers decreases gradually and the buoyancy field appears to be stratified into two layers at all times. In contrast to the transient buoyancy field following a reduction of the strength of a localised source in an enclosure [20, fig. 3.1, bottom row], we do not observe intermediate ‘intruding’ layers from the plumes below the original warm upper layer or above the original cool lower layer in fig. 3.3. However, a step increase in Γ corresponds to a step decrease in the strength of the localised sources and the wall-bounded plumes introduce fluid of lower

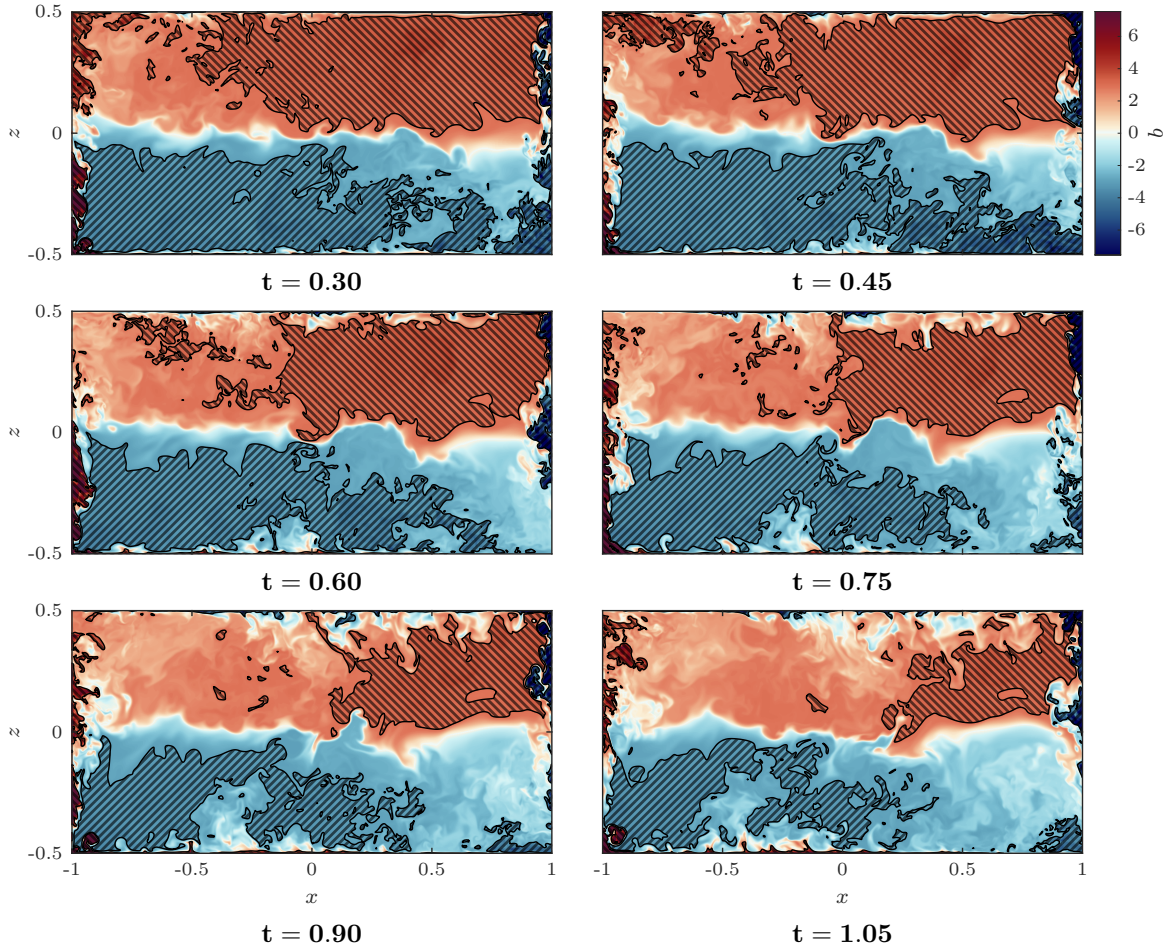


Figure 3.4: Instances of the transient buoyancy field shortly after the step increase of Γ (3.3) considered at time steps of 0.15 time units for the duration $t \in [0.30, 1.05]$. Fluid at buoyancy $b > 3$ and $b < -3$ is marked by parallel hatching in order to visualise the change of buoyancy in the bulk.

(higher) buoyancy into the original upper (lower) steady state layer, following the step change. We presume that the absence of intermediate layers is a result of the distributed heating and cooling of the horizontal boundaries. The convection from the distributed sources promotes mixing and thus prevents the formation of intermediate layers. This is supported by fig. 3.4, which visualises the change of buoyancy in the bulk following the step increase of Γ . Fluid at absolute buoyancy $|b| > 3$ (parallel hatched regions in fig. 3.4), which originally dominates the bulk, is replaced by fluid at lower absolute buoyancy both from the plumes and from convection from the distributed sources. Particularly in instances taken at $t = 0.90$ and 1.05 , both processes appear to contribute equally to the change of buoyancy in the bulk.

Whilst we do not observe intermediate layers in the transient state considered here, they might occur for other step increases of Γ . It is conceivable that, under suitable boundary conditions, intermediate layers develop whose buoyancy is lower (higher) than the buoyancy of the fluid convecting downward (upward) from the distributed sources. In this case, the small plumes from the distributed sources would not penetrate deeply into the intermediate layers, acting as fountains at a density interface as discussed in §3.1, and the intermediate layers would thus not be destroyed by convection from the distributed sources.

The step change of the buoyancy flux ratio Γ corresponds to a simultaneous change of the localised and distributed buoyancy flux on the boundaries, F_ℓ and F_d , respectively (fig. 3.2). We expect that the change in the localised and distributed source strengths affects the buoyancy in the bulk on different time scales, since both types of sources produce different dynamics. A change in F_d results in a buoyancy transport into the bulk via convection, thus directly affecting the buoyancy in the bulk adjoining the distributed source. However, since F_d is zero before the step change (3.3), the transport of cooled or heated fluid from the distributed sources into the bulk is delayed by the time required for the onset of convection. In contrast, the simultaneous reduction of the localised source strength F_ℓ with the step increase of Γ (3.3) results in a change of the buoyancy of fluid at the base of the plumes, where the fluid parcels of changed buoyancy are immediately transported towards the interface by the established plume. However, the change of F_ℓ can affect the buoyancy in the bulk only after the buoyancy change in the plume has propagated to the interface between the layers. The dimensionless time scale T_p required for a fluid parcel to travel from the source of a plume to the interface between the layers can be approximated as

$$T_p = \frac{\frac{1}{2}}{w_m} = \frac{1}{2} \alpha^{\frac{1}{3}} (1 + \Gamma^B)^{\frac{1}{3}} \approx 0.32, \quad (3.7)$$

where $\frac{1}{2}$ corresponds to the initial height of the plume and w_m is the vertical velocity in the plume assuming a top-hat profile (see appendix A). This approximation roughly agrees with the behaviour of the y -averaged buoyancy in the plumes observed at the horizontal mid-plane: in fig. 3.5, the absolute value of the peak buoyancy in the left- and right-hand plume becomes visibly reduced at $t = 0.36$ for the first time.

We would like to know whether the change of the localised and the distributed source strengths affects buoyancy timelines in a characteristic, distinguishable manner. This is of particular interest with regard to inferring boundary heating distributions from measurements. To this end, we consider the buoyancy at three points in the lower boundary ($z = -0.25$), placed at different positions $x \in \{0.6, -0.1, -0.8\}$ in the horizontal (fig. 3.6). We expect that the onset of convection due to $F_d^B > 0$

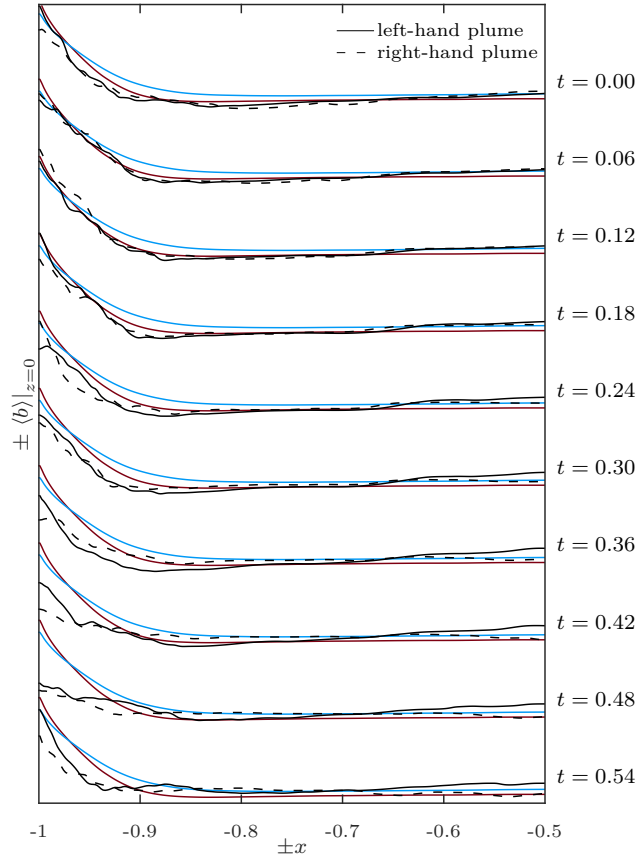


Figure 3.5: Qualitative behaviour of the y -averaged buoyancy (black) in the left- (solid line) and right-hand plume (dashed line) at the horizontal mid-plane ($z = 0$) shortly after the step increase of Γ (3.3) at times $t \in \{0, 0.06, \dots, 9 \times 0.06\}$. For the left-hand plume, $\langle b \rangle(x)$ is depicted, in case of the right-hand plume the plot shows $-\langle b \rangle(-x)$. At each time, the mean buoyancy $\bar{b}$ of the steady states corresponding to the boundary condition before $\Gamma^A = 0$ (red) and after $\Gamma^B = 0.60$ (blue) the step change is added for reference.

results in a near simultaneous change in buoyancy at all points in fig. 3.6, since the considered points are placed at the same distance from the bottom boundary and the distributed source. In contrast, fluid shed by the right-hand plume, whose source strength decreases at $t = 0$, spreads out horizontally across the domain and thus the corresponding change in buoyancy propagates in the lower layer from the right to the left, reaching the points at $x \in \{0.6, -0.1, -0.8\}$ at increasingly later times. This is indeed the behaviour observed in fig. 3.6. The changed buoyancy of the fluid spreading from the plume results both from the change in F_ℓ and F_d , since fluid cooled or heated by the distributed sources is entrained into the plumes and contributes to the buoyancy of the subsequently shed fluid.

While fluid shed by the plume and spreading across the layer affects the buoyancy timelines in fig 3.6 as expected, a simultaneous change in buoyancy at all positions x , associated with convection from distributed sources, cannot be identified in fig. 3.6. The reason might be that while the magnitude of the change of the localised and distributed buoyancy flux at $t = 0$ is equal, $F_d^B - F_d^A = F_\ell^B - F_\ell^A$, the change of buoyancy flux per unit length is smaller for the distributed sources than for the localised ones

$$\Lambda^{-1} (F_d^B - F_d^A) \approx 0.38, \quad \left(\frac{1}{2}\right)^{-1} (F_\ell^B - F_\ell^A) \approx -1.5. \quad (3.8)$$

In the right-hand approximation, we assume that the fluid shed by the plumes fills one layer in the vertical as it spreads out horizontally, hence, half the domain height is used as a length scale. Since the lateral propagation of a buoyancy change in the layers with fluid shed from the plumes (fig. 3.4) results from the step change in both F_ℓ and F_d , the approximation of the localised buoyancy fluxes should be interpreted in terms of a lower limit: the effect of fluid shed by the plumes on the buoyancy in the bulk, in comparison with the effect of convection from distributed sources, differ by at least a factor ≈ 4 in the considered transient state. This might explain why we cannot identify the effect of convection from distributed sources in fig. 3.6

From fig. 3.6, we can approximate the velocity of the global circulation in the bulk shortly after the step change of Γ . The approximate times at which the buoyancies at $x \in \{0.6, -0.1, -0.8\}$ depart from their initial value (vertical dashed and dotted lines) suggest an absolute dimensionless velocity of ≈ 2 . Based on this estimate, the time required for fluid to propagate across the domain from one plume to another shortly after the step change is one dimensionless time unit.

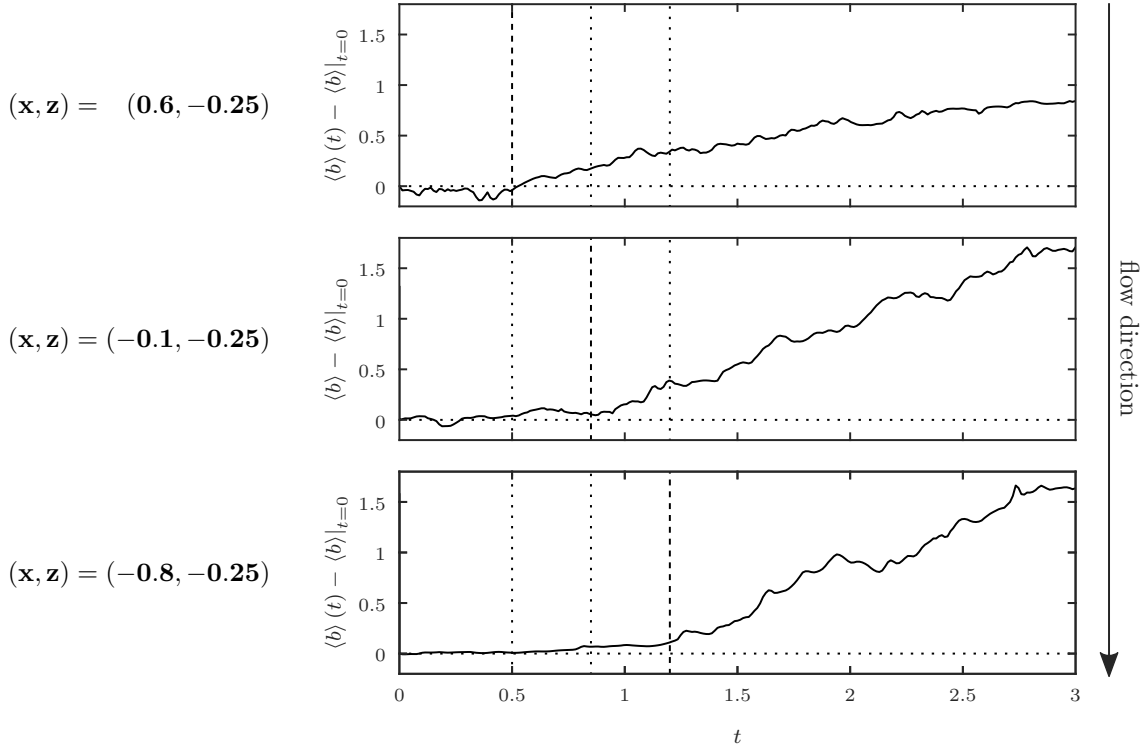


Figure 3.6: The y -averaged buoyancy in the lower layer after the step increase of Γ (3.3) at different positions $x \in \{0.6, -0.1, -0.8\}$ over time. The figures are displayed from top to bottom in the order in which a fluid parcel advected by the global circulation would reach them. The buoyancies are subtracted by their value at the time $t = 0$ of the step change (dotted horizontal lines). The approximate time at which a buoyancy departs from its $t = 0$ value is marked by a vertical dashed line in the respective figure. For reference, the corresponding times are marked in all figures as vertical dotted lines.

The transition in global quantities

In the following, we will describe the transient state in terms of global quantities of the system, those being the PDF of the buoyancy field, the specific kinetic energy in the domain

$$E_k = \frac{1}{2\Lambda\Lambda_y} \int_{-\frac{\Lambda}{2}}^{\frac{\Lambda}{2}} \int_{-\frac{\Lambda_y}{2}}^{\frac{\Lambda_y}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} |\mathbf{u}|^2 dz dy dx, \quad (3.9)$$

and the strength of the global circulation, quantified as the mean volume flux over the horizontal mid-plane

$$Q_g \equiv \frac{1}{2} \left[\int_{-\frac{\Lambda}{2}}^0 \langle w \rangle dx - \int_0^{\frac{\Lambda}{2}} \langle w \rangle dx \right], \quad (3.10)$$

where we assume an antisymmetry of the vertical velocity at $z = 0$, $\langle w \rangle(t, x, 0) = -\langle w \rangle(t, -x, 0)$.

In the initial steady state, the buoyancy field is stably stratified into two layers of near-homogeneous buoyancy. This stratification manifests in the buoyancy field's PDF as a pair of narrow peaks (red shaded area in fig. 3.7a), where the distance Δb between the peaks of the PDF is indicative of the buoyancy difference between the two layers. In the 'final' steady state, which is approached for $t \rightarrow \infty$, the buoyancy difference Δb (blue shaded PDF in fig. 3.7a) is reduced compared to Δb in the initial steady state and the buoyancy of each layer is less homogeneous, resulting in wider peaks.

In accordance with the initial and 'final' steady states of the transient state, the step change of Γ at $t = 0$ results in a buoyancy difference Δb between the layers that decreases in time over a duration of 4 time units, for $1 \lesssim t \lesssim 5$ (fig. 3.7b). However, the effect of the changed boundary conditions on Δb is delayed, as the buoyancy difference between the layers remains approximately constant for $t \lesssim 1$. When the transition of Δb begins at $t \approx 1$, the peaks of the buoyancy field initially decrease in amplitude and increase in width (fig. 3.7a). This is a result of inhomogeneity of the buoyancy field in the early transient state. As time progresses, the buoyancy in the layers grows first more homogeneous, manifesting in narrower buoyancy peaks ($t = 3$ in fig. 3.7a), before the peaks again increase in width, due to developing horizontal buoyancy gradients in the layers ($t \geq 4$ in fig. 3.7a, cf. fig. 3.3 at $t = 4$).

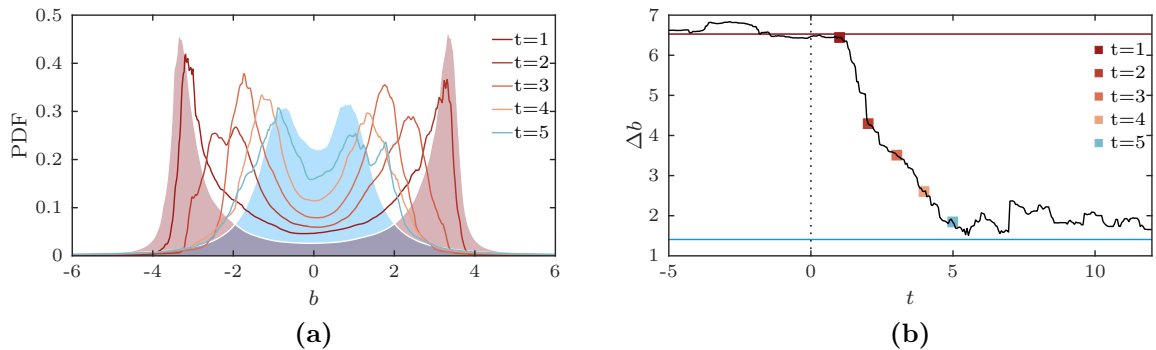


Figure 3.7: PDF of the transient buoyancy field for the step increase of Γ (3.3) over time (moving average). (a) shows the transient PDF at times $t \in \{1, 2, 3, 4, 5\}$, together with the PDFs of the steady states corresponding to the boundary condition before $\Gamma^A = 0$ (red) and after $\Gamma^B = 0.60$ (blue) the step change (cf. fig. 2.4). (b) depicts the distance Δb between the PDF peaks over time, where the times at which the PDF is plotted in (a) are marked for reference. The buoyancy difference of the steady state at $\Gamma = 0$ and 0.60 is marked as a red and a blue horizontal line, respectively, and corresponds to the mean values presented in chapter 2 (see fig. 2.12).

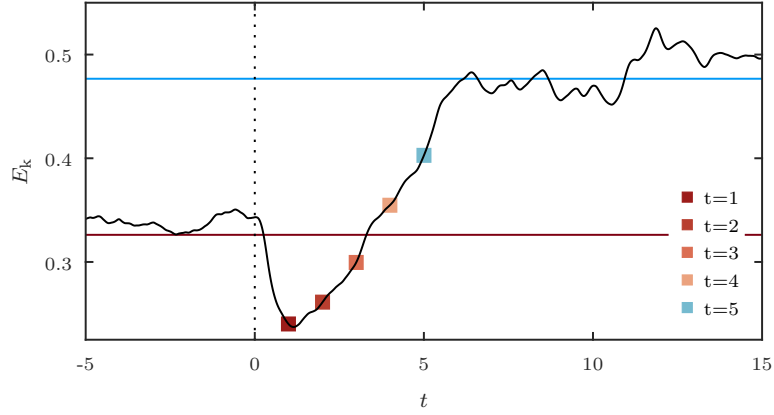


Figure 3.8: Specific kinetic energy for the step increase of Γ (3.3) over time. The specific kinetic energy of the steady state corresponding to the boundary condition before $\Gamma^A = 0$ and after $\Gamma^B = 0.60$ the step change are marked as red and blue lines, respectively. The times $t \in \{1, 2, 3, 4, 5\}$ are marked for reference (cf. fig. 3.7).

At all times, we can identify two major peaks in the buoyancy field's PDF (fig. 3.7a), confirming our earlier statement that the buoyancy field is stably stratified into two layers throughout the transition.

The specific kinetic energy E_k (fig. 3.8) and the volume flux Q_g associated with the global circulation (fig. 3.9) ultimately increase as a result of the step change (3.3), as is to be expected from their values in the initial and ‘final’ steady state (red and blue line, respectively, in fig. 3.8 and 3.9). However, E_k and Q_g initially decrease immediately after the step change, up until $t \approx 1$ and $t \approx 1.5$, respectively, before reversing their former trend and increasing towards their steady state value. The strength of the global circulation appears to assume its ‘final’ steady state value at $t = 4$ (fig. 3.9), while the specific kinetic energy reaches the steady state value at $t \approx 6$ (fig. 3.8).

The curve of Q_g over time, which mainly corresponds to the volumes flux of the plumes at $z = 0$, is qualitatively similar to the curve of E_k . In plumes, the mean flow dominates the kinetic energy. As the strength of the localised sources exceeds that of the distributed sources in the considered

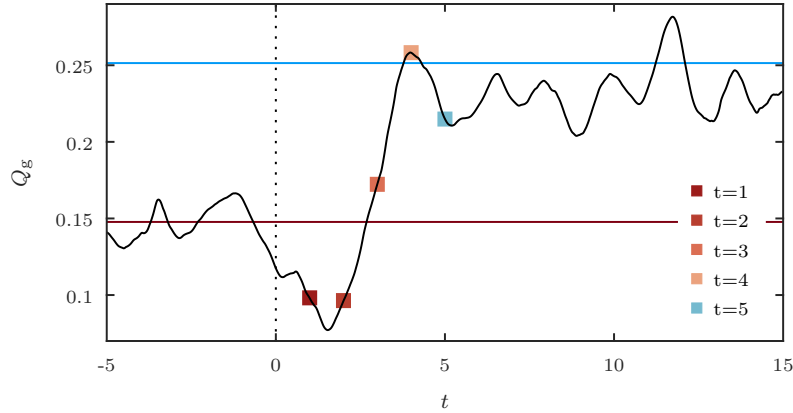


Figure 3.9: Volume flux (3.10) associated with the global circulation for the step increase of Γ (3.3) over time. The volume flux of the steady state corresponding to the boundary condition before $\Gamma^A = 0$ and after $\Gamma^B = 0.60$ the step change are marked as red and blue lines respectively. The times $t \in \{1, 2, 3, 4, 5\}$ are marked for reference (cf. fig. 3.7).

configuration ($\Gamma < 1$), we assume that the correlation between Q_g and E_k arises because the mean flow of the plumes dominates the specific kinetic energy of the domain, although a correlation between turbulent fluctuations and the mean flow may contribute to the similar behaviour of Q_g and E_k . Some disagreement between the curves of Q_g and E_k in fig. 3.8 and fig. 3.9 may arise because the former results from an integral over the horizontal mid-plane, whilst the latter corresponds to a volume integral over the entire domain, making the volume flux more prone to fluctuations than the specific kinetic energy.

We would like to understand the processes responsible for the observed behaviour of Δb , E_k and Q_g over time, in particular regarding the non-monotonic behaviour of E_k and Q_g and the delay in the transition of Δb . In the following, we will attempt to connect the observations made in the transients of these three quantities. As Γ is abruptly increased from $\Gamma = 0$ to 0.60 at $t = 0$, the strength of the localised plume sources is decreased and consequently the buoyancy difference between a fluid parcel in the plumes and the fluid in the ambient layer decreases. This corresponds to a reduced buoyancy force acting on fluid parcels in the plumes relative to the fluid ambient to the plume. Shortly after the step change, we expect the buoyancy of the ambient fluid to be unchanged from its value before the step change. The reduced buoyancy force on fluid parcels in the plumes, whose entrainment of fluid drives the global circulation in the domain, results in a decrease of the corresponding volume flux, which takes effect immediately after the step change and lasts up until approximately 1.5 time units after the step change (fig. 3.9). Likewise, the specific kinetic energy, which is dominated by the mean flow of the plumes, decreases over $0 \lesssim t \lesssim 1$ (fig. 3.8).

During the time in which the specific kinetic energy decreases, $0 \lesssim t \lesssim 1$, the buoyancy difference Δb between the peaks of the PDF remains approximately constant (fig. 3.7a). It might be argued that this delay corresponds to the time required for a change of buoyancy to propagate from the plume sources to the interface or to the duration between the step change of Γ and the onset of convection from the distributed sources. However, as was shown earlier, the corresponding time scale $T_p \approx 0.32$ is significantly shorter than the observed delay of one time unit. To interpret the delay, we have to consider that the position of the buoyancy field's PDF peaks is a measure for the buoyancy value assumed by the majority of fluid parcels in the bulk. Thus, a shift of the PDF peaks requires the circulation and mixing of fluid over the entire domain. This interpretation of the delay is in agreement with the observed delay of one time unit, which matches the duration approximated from fig. 3.6 for a parcel of fluid to traverse the domain. Since the boundary conditions on the top and bottom are equal, only a half circulation is necessary for the majority of the points in the bulk to be affected by the change in the boundary conditions. The circulation is possibly slowed down by the decreased volume flux of the global circulation.

At $t \gtrsim 1$, the buoyancy in the bulk has changed sufficiently for the peaks of the buoyancy field's PDF to move in b (fig. 3.7). Since the upper and the lower layer are cooled and heated, respectively, by a distributed source, the buoyancy difference Δb between the layers decreases until it reaches the value corresponding to the 'final' steady state at $t \approx 5$ (fig. 3.7b).

We presume that the increase of the specific kinetic energy and the volume flux of the global circulation, setting in at $t \approx 1$ and $t \approx 1.5$, respectively (fig. 3.9 and 3.8), is caused by a change of the buoyancy in the bulk, which is marked by the decrease of Δb starting at $t \approx 1$. The decrease in Δb might suggest a decrease in the global circulation strength, instead of the observed increase, since a continually increasing (or decreasing) buoyancy in the fluid ambient to the plume in the lower (or

upper) layer will reduce the buoyancy difference between plume and ambient and thus the buoyancy force acting on fluid parcels in the plumes. In the steady state, we found that the volume flux of the plumes increases with increasing Γ because the height of the plumes increases due to the tilted interface. The effect of the increased plume height on the volume flux counteracts the effect of the reduced buoyancy difference Δb and the accordingly reduced buoyancy force on fluid parcels in the plume with increasing Γ (see §2.7.3). However, fig. 3.3 implies that a tilting of the interface between the layers occurs only from $t \approx 4$ onwards and cannot be responsible for the increase of Q_g at $t \approx 1$, though it might affect the volume flux at later times.

Whilst a decreasing Δb reduces the buoyancy force on the fluid in the plumes below a horizontal interface, it increases the buoyancy force on the fluid in the flow that replaces the plumes upon penetrating the interface. In the steady state at $\Gamma = 0$, the plume is replaced by a flow similar to a jet in the statistical average upon penetrating the interface (see appendix A). With $\Gamma^B > 0$, the formerly jet-like flow becomes a forced plume, since the distributed heating creates a buoyancy difference between the fluid discharged by the plume into a layer and the fluid in the layer. Thus, the fluid heated or cooled by the localised sources is accelerated over a longer distance, although with smaller forcing, as Δb decreases, resulting in an increase of the volume flux of the global circulation even before the interface is tilted. The mean flow contribution to the specific kinetic energy rises with Q_g .

3.4.2 Step decrease of the buoyancy flux ratio

In this section, we examine the reverse transition to the one studied in the previous section, constituting of a step change from combined localised and distributed buoyancy flux sources ($\Gamma^A = 0.60$) to purely localised buoyancy flux sources ($\Gamma^B = 0$).

The transition in spatially dependent quantities

To study the transient state resulting from the step decrease of Γ (3.4), we first consider instances of the buoyancy field over a duration of 9 dimensionless time units following the change of the buoyancy fluxes at $t = 0$ (fig. 3.10, 3.11 and 3.12). With the step change from $\Gamma^A = 0.60$ to $\Gamma^B = 0$, the buoyancy flux of the distributed sources is reduced to zero (fig. 3.2). Thus, convection from the horizontal boundaries in the bulk, as observed for the initial steady state at $\Gamma = 0.60$ (cf. fig. 3.10 at $t = 0$), does not occur in the transient state after the step change.

The decrease of Γ corresponds to an increase of the localised source strength F_ℓ at $t = 0$ (fig. 3.2), resulting in an increased buoyancy force acting on fluid parcels in the plume. Due to the increase of F_ℓ , the fluid in the left-hand plume becomes more buoyant than the upper layer of the initial two-layer stratification and the plume rises to the top boundary of the domain. Fluid in the left-hand plume where it reaches the top boundary has been accelerated over a longer distance than fluid discharged by the plumes before the step change of Γ and with a higher buoyancy force. Thus, shortly after the step change of Γ , the left-hand plume discharged buoyant fluid with an increased volume flux compared to the global circulation of the initial steady state. This results in a front of buoyant fluid propagating below the top boundary across the width of the domain (fig. 3.11 and fig. 3.10 at $t = 1$). Similarly, we observe a cold front propagating along the bottom boundary of the domain. These propagating warm and cold fronts are driven by their initial momentum and the global circulation resulting from entrainment into the plumes. Moreover, the fluid spreading from the plumes is subjected to a buoyancy

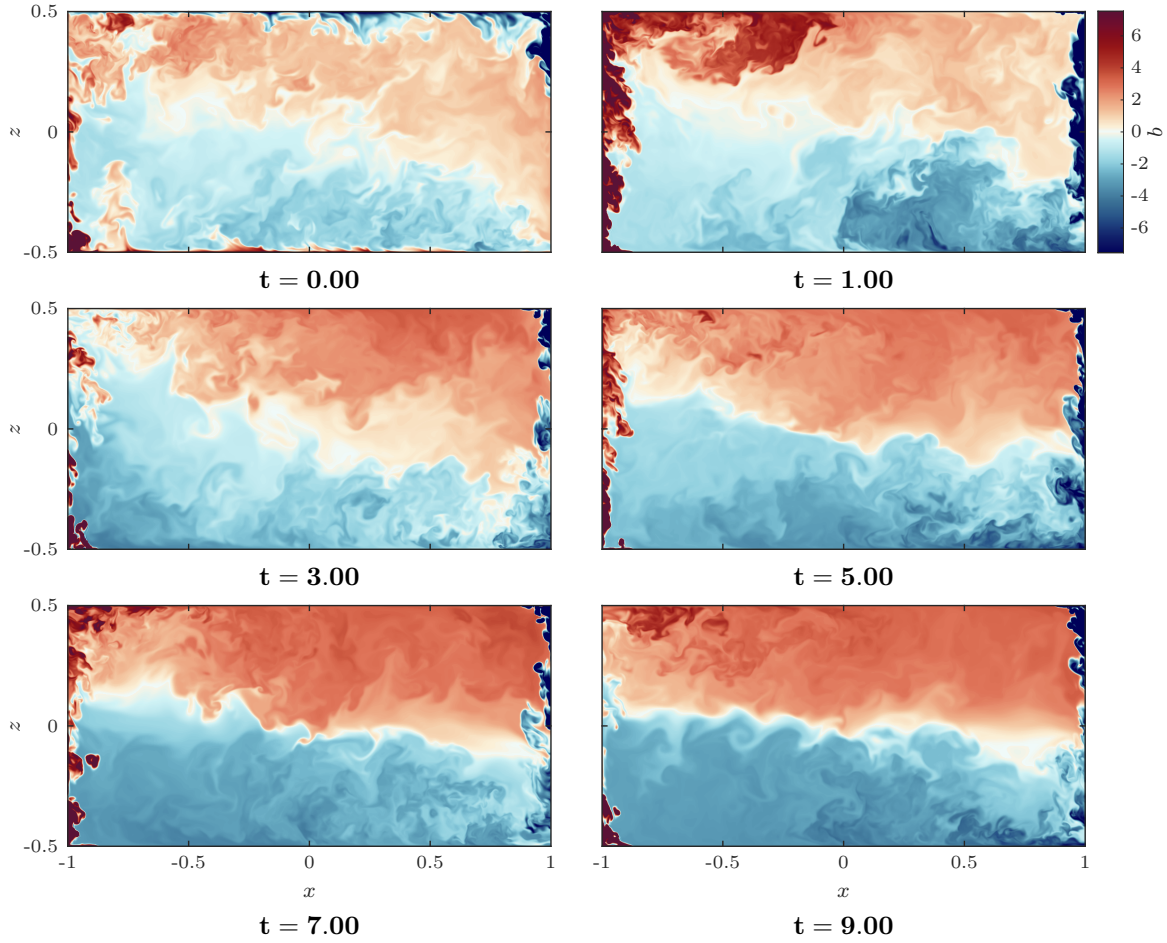


Figure 3.10: Instances of the transient buoyancy field for the step increase of Γ (3.3) considered at $t = 0$ and at time steps of 2 time units for the duration $t \in [1, 9]$.

force, due to the horizontal buoyancy difference to the fluid of the previous stratification. Thus, the spreading warm and cold fluid could be considered as a gravity current with a finite source momentum flux in a background flow, due to entrainment by the plumes.

The fluid discharged by the plumes after the step decrease of Γ results in the formation of a layer at the top and at the bottom of the domain $t \approx 1.80$ (fig. 3.12), which are distinct from the fluid of the initial steady state stratification. At times $1.80 \leq t \leq 2.25$, a horizontal stratification of the buoyancy field is visible in fig. 3.12 between the top and bottom layer, representing a remainder of the initially tilted stratification (cf. fig. 3.10 at $t = 0$). At $t = 3$, the fluid at intermediate buoyancies between the top and bottom layer is no longer clearly discernible, having been entrained by the plumes, and the buoyancy field appears as a two-layer stratification with a tilted interface for $5 \leq t \leq 9$ in fig. 3.12. At $t = 9$, the interface between the layers in fig. 3.12 has become approximately horizontal, matching the steady state stratification for $\Gamma = 0$ (cf. §2.5.1).

The transient stratification resulting from a step decrease of Γ differs from the transient stratification following a step increase of Γ in §3.4.1. The spread of a hot and cold layer above and below fluid of the previous stratification, respectively, following a decrease of Γ , corresponds to the filling flow observed for plumes in confinement whose source strength has been abruptly increased [17, 20]

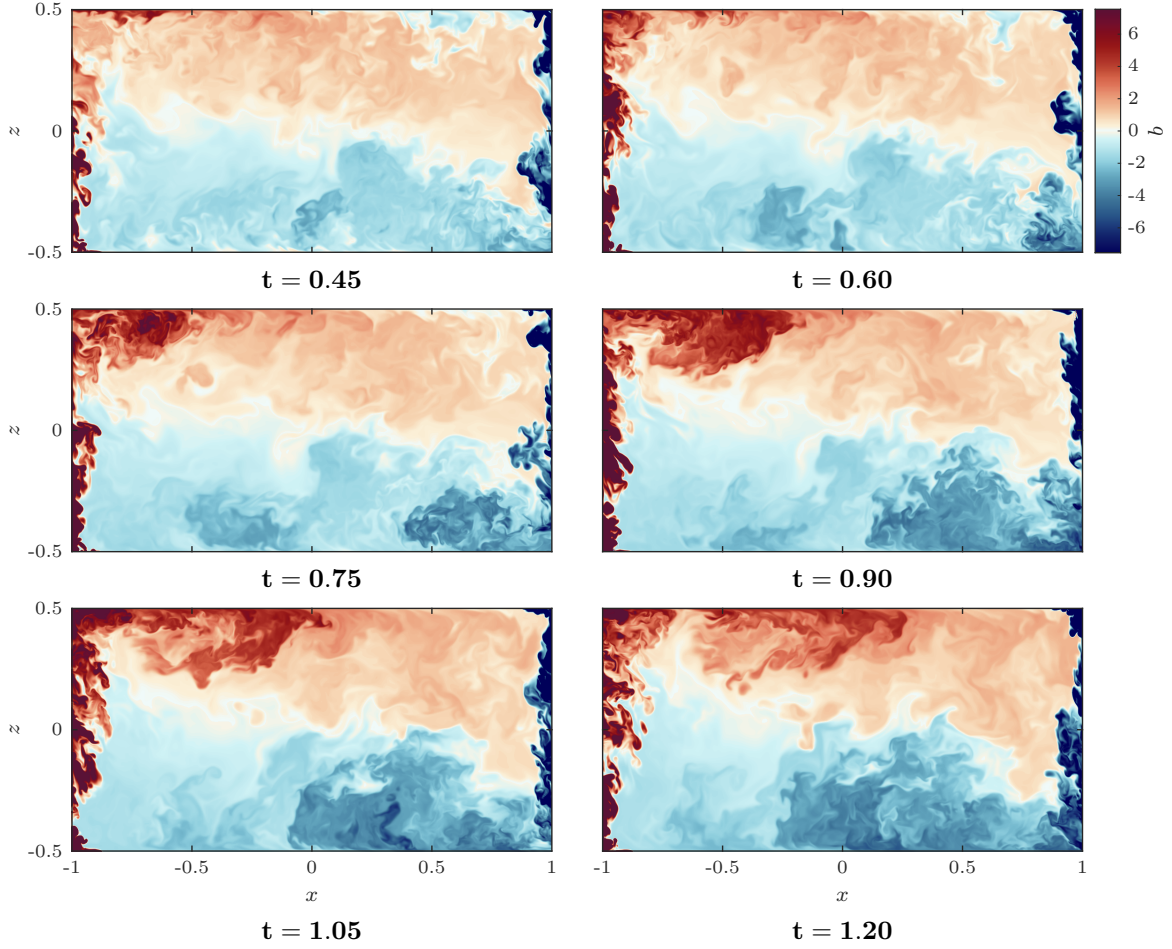


Figure 3.11: Instances of the transient buoyancy field shortly after the step decrease of Γ (3.4) considered at time steps of 0.15 time units for the duration $t \in [0.45, 1.20]$, showing gravity currents in each layer.

(cf. fig. 3.1). In contrast, the transient resulting from a step increase of Γ (§3.4.1) shows a two-layer stratification at all times instead of the intruding flow that occurs in the equivalent case of a plume with abruptly decreased source strength in confinement [17, 20]. The reason for the different stratifications for a step increase and decrease of Γ is the corresponding strength F_d^B of the distributed sources following the step change. For the considered step increase of Γ , F_d^B is finite, causing convection from the top and bottom boundary and thus promoting mixing in the upper and lower layer. In case of the considered step decrease of Γ , the distributed buoyancy flux F_d^B after the step change is zero and the domain is heated and cooled purely by localised sources. The boundary conditions after the step decrease of Γ are thus closely related to those of a plume from a source of increased strength, such as considered by Bower et al. [20], and result in an equivalent filling flow. However, a step decrease of Γ to a finite value and thus to a finite distributed buoyancy flux F_d^B would result in convection from the top and bottom boundary after the step change. This would prevent the formation of additional layers from a filling flow or decrease the time for which such layers can persist during the transient.

Comparing the time scales associated with the transient from a step increase and decrease of Γ , we find that the transition to a new steady state takes longer after the decrease of Γ than for the increase

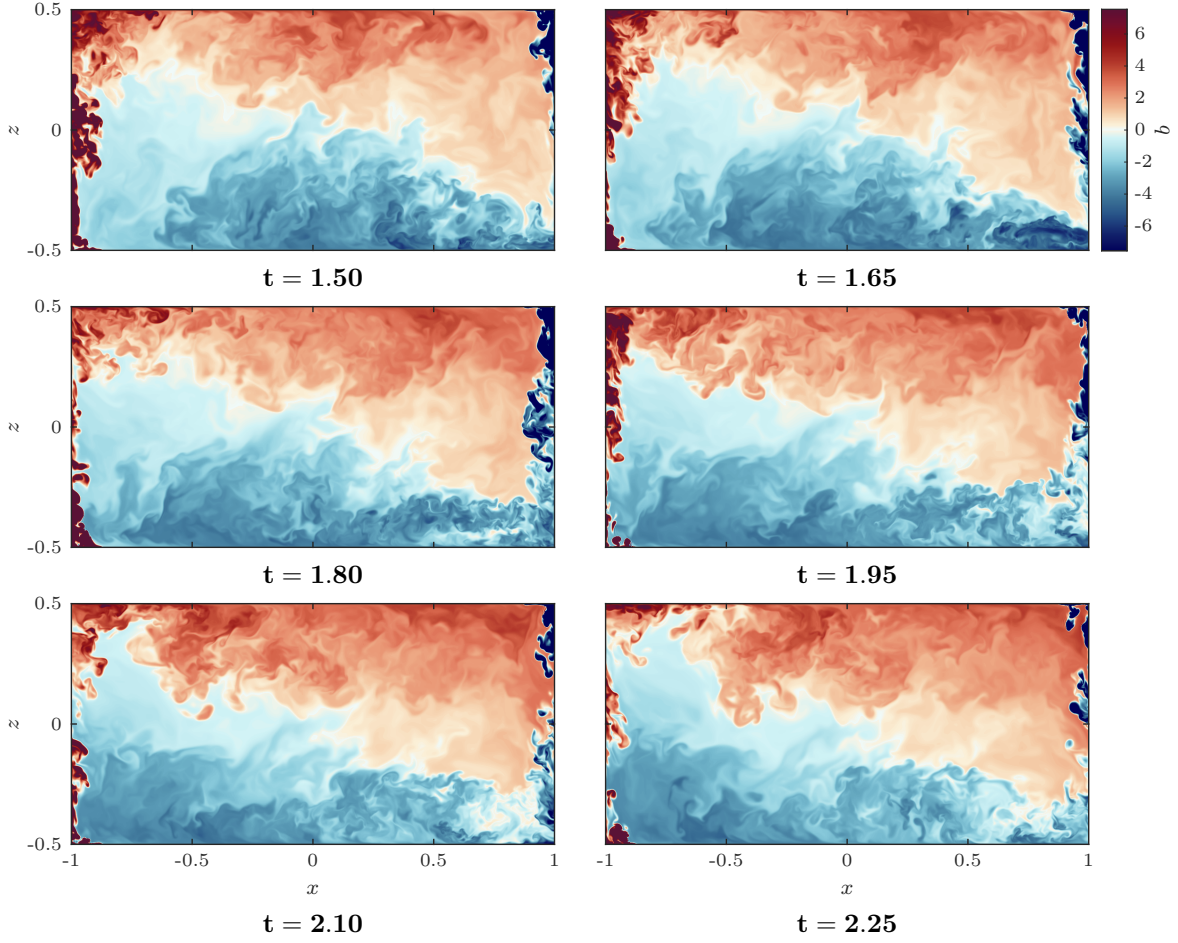


Figure 3.12: Instances of the transient buoyancy field for the step decrease of Γ (3.4) considered at time steps of 0.15 time units for the duration $t \in [1.50, 2.25]$, showing the formation of new layers above and below the original stratification.

of Γ (cf. fig. 3.3 and 3.10). The behaviour of the transition time with Γ is consistent with the plume volume flux Q_p that corresponds to the ‘final’ steady state at Γ^B : the steady state volume flux that is approached after the step change of Γ is greater for $\Gamma^B = 0.60$ than for $\Gamma^B = 0$ (cf. §2.7.3, fig. 2.14). The plumes’ volume flux impacts the rate with which fluid is exchanged between the upper and lower layer of the transient stable stratification and thus affects the time scale of the transition between two steady states. The plume volume flux is, however, not the only factor determining the speed of the transition. As observed earlier, convection from distributed sources of buoyancy causes mixing in the upper and lower layer of the stratification and thereby accelerates the transition to a new equilibrium at Γ^B .

The transition in global quantities

Equivalent to §3.4.2, we now shift our focus from the spatially dependent buoyancy field to global quantities of the domain, specifically the buoyancy field’s PDF, the specific kinetic energy E_k (3.9) and the volume flux of the global circulation Q_g (3.10).

In the initial steady state at $\Gamma = 0.60$, the buoyancy field is stratified into an upper and lower layer,

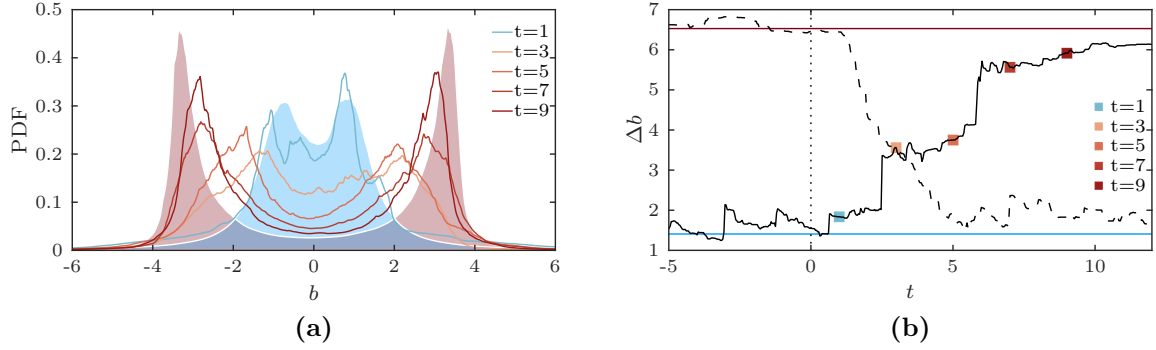


Figure 3.13: PDF of the transient buoyancy field for the step decrease of Γ (3.4) over time (moving average). (a) shows the transient PDF at times $t \in \{1, 3, 5, 7, 9\}$, together with the PDFs of the steady states corresponding to the boundary condition before $\Gamma^A = 0.60$ (blue) and after $\Gamma^B = 0$ (red) the step change (cf. fig. 2.4). (b) depicts the distance Δb between the PDF peaks over time (solid line), where the times at which the PDF is plotted in (a) are marked for reference. The transient buoyancy difference for the step change (3.3) is added for comparison (dashed line). The buoyancy difference of the steady state at $\Gamma = 0$ and 0.60 is marked as a red and a blue horizontal line, respectively, and corresponds to the mean values presented in chapter 2 (see fig. 2.12).

where each of the layers shows a lateral buoyancy gradient (cf. fig. 3.10 at $t = 0$). In the buoyancy field's PDF of the initial steady state (blue shaded PDF in fig. 3.13a), the two layers corresponds to a pair of broad peaks that overlap, such that the PDF's amplitude between the peaks is large compared with the peak height. After the step change of Γ , the PDF should eventually approach the PDF that we observe in the steady state at $\Gamma^B = 0$ (red shaded PDF in fig. 3.13a). The latter is characterised by a pair of two distinct and narrow peaks, corresponding to the steady state stratification of two near homogeneous layers at $\Gamma = 0$ (cf. §2.5.1, fig. 2.5a). Accordingly, the distance Δb between the PDF peaks should eventually increase from its initial steady state value (blue horizontal line in fig. 3.13b) to the steady state value at $\Gamma = 0$ (red horizontal line in fig. 3.13b).

In contrast to the transient that occurs following a step decrease of Γ (black dashed line in fig. 3.13b), the buoyancy difference Δb between the PDF peaks following a step decrease of Γ does not change smoothly from its initial to its 'final' steady state value (black solid line in fig. 3.13b). After the step decrease of Γ at $t = 0$, Δb remains initially unchanged, before increasing abruptly by 0.5 units of buoyancy at $t \approx 0.7$. For $t \gtrsim 0.7$, the value of Δb stays approximately constant before undergoing a further abrupt increase at $t \approx 2.5$. A third jump of Δb occurs at $t \approx 5.8$, after which Δb increases further towards the final steady state value, though the steady state value is not reached during the simulation of the transient state over 12 directionless time units.

The reason for the jumps in the transient buoyancy difference Δb is the shape of the transient PDF of the buoyancy field and the definition of Δb . After the step decrease of Γ , two fronts of hot and cold fluid spread from the plumes and develop into additional layers above and below the initial stratification, as is shown in instances of the buoyancy field in fig. 3.10, 3.11 and 3.12. In the PDF of the buoyancy field, the additional layers manifest as additional peaks in the PDF whose height increases as the layer deepens. In order for the buoyancy difference Δb displayed in fig. 3.13b to be defined uniquely for a PDF with more than two peaks, we chose to define Δb as the distance between the highest peak of the PDF above and below zero. Hence, abrupt jumps in Δb occur, when in a PDF of multiple peaks with changing height one peak overtakes another in height.

Due to the irregular behaviour of Δb in fig. 3.13b, we introduce a new quantity to study the characteristic buoyancy difference between the upper and lower part of the stratification. We obtain a mean value of the positive and negative buoyancies in the bulk, $\bar{b}_+$ and $\bar{b}_-$, respectively, by separately integrating over the buoyancy field's PDF above and below zero buoyancy. The plumes are excluded from these integrals by defining $\bar{b}_+$ and $\bar{b}_-$ as integrals over the PDF where the PDF exceeds a value $\gamma \cdot \max(\text{PDF})$, where $\gamma \in [0, 1]$ is a given threshold factor and $\max(\text{PDF})$ corresponds to the time-dependent maximum value of the PDF. Fig. 3.14b shows the resulting areas of integration in the PDFs of the steady state at $\Gamma = 0$ and 0.60 (red and blue areas in fig. 3.14b, respectively) for a threshold factor of $\gamma = 0.05$ (uniform shading) and 0.20 (parallel hatching). The difference between the mean positive and negative buoyancy is denoted as $\Delta\bar{b}_\gamma \equiv \bar{b}_+(\gamma) - \bar{b}_-(\gamma)$.

It is difficult to interpret $\Delta\bar{b}_\gamma$ quantitatively, since the value of $\Delta\bar{b}_\gamma$ depends on the chosen value of γ . We aim to choose the threshold factor γ such that the plumes are excluded from the integrals used in the definition of $\Delta\bar{b}_\gamma$, whilst buoyancies corresponding to the bulk are included. Fig. 3.14c and 3.14d show instances of the steady state buoyancy field at $\Gamma = 0$ and 0.60, respectively, where the buoyancies excluded by the threshold factor γ are highlighted. For a threshold factor $\gamma = 0.05$ (uniform grey shading in fig. 3.14c and 3.14d), virtually no buoyancies in the bulk are excluded, apart from small plumes from the boundary layers. However, the planar plumes at the left and right boundary are not

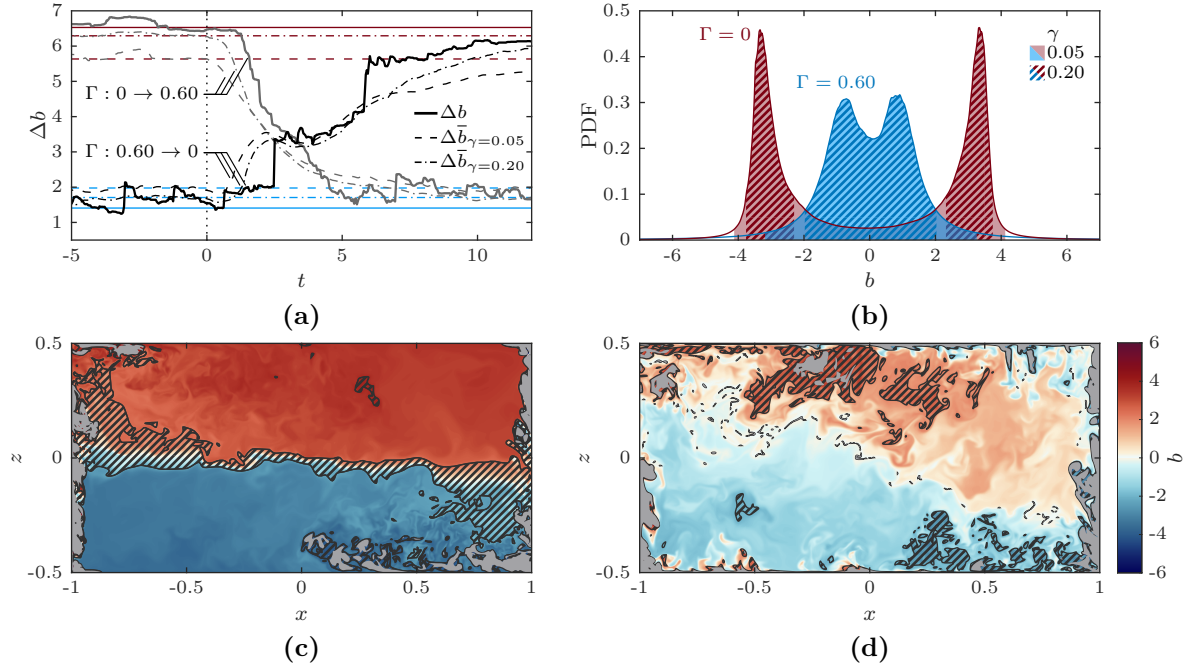


Figure 3.14: Buoyancy difference $\Delta\bar{b}_\gamma$ between the layers defined via integrals over the buoyancy field's PDF for a given threshold factor $\gamma \in \{0.05, 0.20\}$ (see text). Depicted are (a) the transient buoyancy difference Δb between PDF peaks (cf. fig. 3.7 and 3.13) and the transient buoyancy difference $\Delta\bar{b}_\gamma$ from integrals over the PDFs for a step increase (3.3) and decrease (3.4) of Γ . The values for the initial and 'final' steady state for the different definitions are obtained from PDFs averaged over 10 time units and shown as red ($\Gamma = 0$) and blue ($\Gamma = 0.60$) horizontal lines in (a). Plot (b) shows the PDFs of the initial and 'final' steady state with the areas considered in the definition of $\Delta\bar{b}_\gamma$ shaded. The impact of γ is visualised in instantaneous slices of the buoyancy field for the initial and final steady state at (c) $\Gamma = 0$ and (d) $\Gamma = 0.60$, where the buoyancies excluded by the threshold γ are highlighted ($\gamma = 0.05$: uniform grey, $\gamma = 0.20$: parallel hatching).

completely excluded in this case. At a larger threshold such as $\gamma = 20$ (parallel hatching), although buoyancies in the bulk are excluded, the planar plumes can be excluded more rigorously. Hence, it might not be possible to choose the threshold factor γ such that the resulting mean buoyancy difference $\Delta\bar{b}_\gamma$ is representative of the mean buoyancy difference between the upper and lower part of the stratification in the bulk. In the following, we will therefore focus on the qualitative behaviour of $\Delta\bar{b}_\gamma$.

The mean buoyancy difference $\Delta\bar{b}_\gamma$ (dashed and dashed dotted black line in fig. 3.14a) shows behaviours of the transient buoyancy field after the step decrease of Γ that are not visible in the buoyancy difference Δb between the PDF peaks (solid black line in fig. 3.14a). Due to the irregular behaviour of Δb , we cannot use Δb to identify a delay in the response of the buoyancy field to the changed boundary conditions. In contrast, $\Delta\bar{b}_\gamma$ shows that the buoyancy in the bulk does not increase immediately after the step change of Γ at $t = 0$. However, we cannot deduce a time scale for this delay, since it depends on the threshold factor γ : if γ is reduced to zero, the buoyancy in the plumes is included in the definition of $\Delta\bar{b}_\gamma$ and $\Delta\bar{b}_\gamma$ increases immediately after the step decrease of Γ .

After the first step increase of $\Delta\bar{b}_\gamma$ (dashed and dashed dotted black line in fig. 3.14a), the mean buoyancy difference peaks and subsequently decreases slightly, before continually increasing towards its ‘final’ steady state value. The transient of $\Delta\bar{b}_\gamma$ confirms that the buoyancy field is not fully converged to a steady state at $t = 12$, since the transient buoyancies for $\gamma = 0.05$ and 0.20 do not align with their respective steady state values at this time (dashed and dashed dotted red line in fig. 3.14a). In contrast, the mean buoyancy differences $\Delta\bar{b}_\gamma$ following a step increase of Γ (dashed and dashed dotted grey line in fig. 3.14a) match their steady state values at $t \approx 8$. In this regard, we note that the qualitative behaviour of Δb and $\Delta\bar{b}_\gamma$ generally agrees well for the step increase (3.3) of Γ (grey lines in fig. 3.14a), such that Δb can be considered a sufficient measure for the behaviour of the buoyancy in the bulk in this case.

The transient behaviour of the specific kinetic energy E_k and the volume flux Q_g of the global circulation after the step decrease (3.4) of Γ (solid lines in fig. 3.15 and 3.16, respectively) appears in some respects as a reversed equivalent to the observed transient behaviour resulting from a step

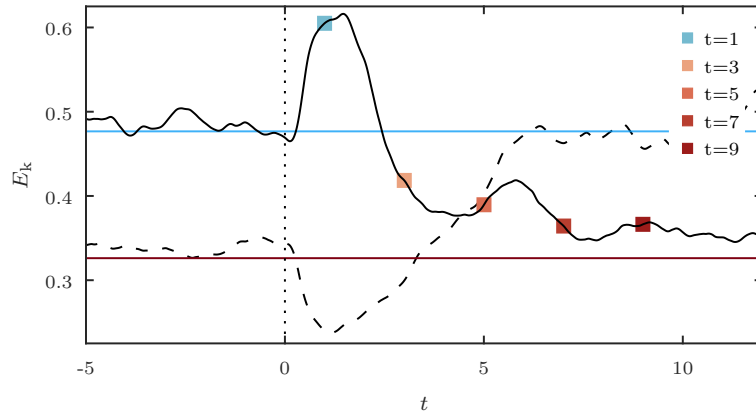


Figure 3.15: Specific kinetic energy for the step decrease of Γ (3.4) over time (solid line), with the specific kinetic energy for (3.3) added for comparison (dashed line). The specific kinetic energy of the steady state corresponding to the boundary condition before $\Gamma^A = 0.60$ and after $\Gamma^B = 0$ the step change are marked as blue and red lines, respectively. The times $t \in \{1, 3, 5, 7, 9\}$ are marked for reference (cf. fig. 3.13).

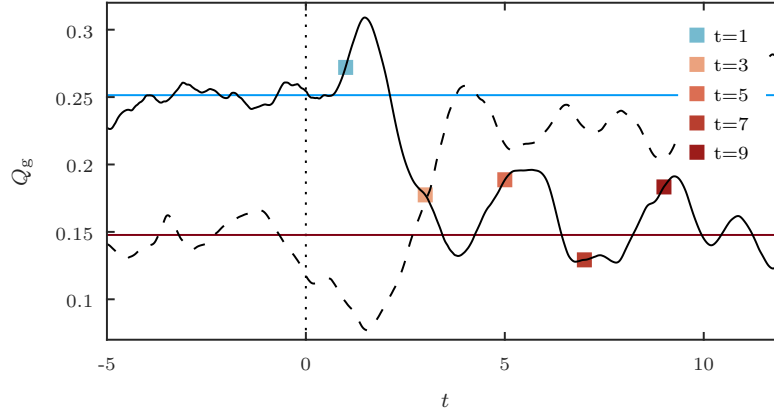


Figure 3.16: Volume flux (3.10) associated with the global circulation for the step decrease of Γ (3.4) over time (solid line), with the volume flux for (3.3) added for comparison (dashed line). The volume flux of the steady state corresponding to the boundary condition before $\Gamma^A = 0.60$ and after $\Gamma^B = 0$ the step change are marked as blue and red lines respectively. The times $t \in \{1, 3, 5, 7, 9\}$ are marked for reference (cf. fig. 3.13).

increase of Γ (dashed lines in fig. 3.15 and 3.16). Instead of an initial decrease of E_k and Q_g , their values now increase immediately after the step change and peak at $t \approx 1.5$, before decreasing towards their respective ‘final’ steady state values (red horizontal line in fig. 3.15 and 3.16). The specific kinetic energy does not converge monotonically towards its ‘final’ steady state value, but shows a second, weaker peak at $t \approx 6$ and a further broad peak of even lower amplitude at $t \approx 9$ (fig. 3.15). Both peaks of the specific kinetic energy are matched by peaks in the strength of the global circulation at approximately the same times (fig. 3.16), though identifying peaks in Q_g is complicated by its noisier behaviour in comparison with E_k (see §3.4.1). The qualitative correlation between E_k and Q_g implies, as in the case of the step increase of Γ , that the specific kinetic energy is dominated by the mean flow of the plumes. Similarly to §3.4.1, we observe that the volume flux Q_g reaches its ‘final’ steady state value significantly earlier (at $t \approx 3.5$) than the specific kinetic energy, which indeed does not reach its ‘final’ steady state value during the simulated transient.

With the decrease of Γ , the localised buoyancy flux of the plume sources is increased, increasing the buoyancy force on fluid parcels in the plume relative to their ambient, which is yet unchanged from its buoyancy in the initial steady state. Due to the increased localised source strength, the plumes extend to the full height of the domain. Thus, immediately after the step decrease of Γ , fluid parcels in the plumes are accelerated with increased buoyancy force over the full height of the domain, resulting in an initially increasing volume flux Q_g and specific kinetic energy. The fluid discharged by the plumes spreads as a front of hot and cold fluid below the top boundary and above the bottom boundary, respectively. When the cold (or hot) front reaches a plume and is entrained, the fluid in the plumes is subsequently of lower (or higher) buoyancy than the fluid the plumes previously supplied to the respective layer. Thus, the fluid in the plumes is accelerated over a shorter distance and the plumes’ volume flux and the specific kinetic energy begin to decrease at $t \approx 1.5$. It is possible that the initial propagating warm and cold fronts reappear in a weaker form, as the corresponding fluid is entrained, mixed and transported across the interface by the plumes. This might be the cause of the second and third, lower peak in E_k and Q_g at $t \approx 6$ and $t \approx 9$. As the buoyancy field approaches the steady state at $\Gamma = 0$, the interface between the layers becomes horizontal and the plume height reduces to

approximately half the domain height, resulting in a volume flux that is decreased relative to its initial value.

3.5 Modelling the transient state

In this section, we develop two types of models of the buoyancy field by assuming different stratifications following the step change of Γ . In §3.5.1, we assume that the fluid discharged by the plumes after the step change mixes ideally with the upper or lower layer of the original stratification, despite the buoyancy difference between the fluid discharged by the plumes before and after the change in Γ . This corresponds to a model where the two-layer buoyancy structure of the steady state persists in the transient state. In §3.5.2 and §3.5.3, we assume that the step change of Γ results in additional layers of lower or higher buoyancy than the layers of the original stratification, equivalent to the transient models of Bower et al. [20]. For an increase of Γ , fluid from the plumes spreads between the existing layers (intruding regime, §3.5.2), whereas it spreads along the top and bottom boundary for a decrease of Γ (filling regime, §3.5.3).

In all the models constructed in this chapter, we neglect the lateral buoyancy gradient in the bulk. Thus, the initial steady state at $t < 0$ and the steady state that is approached by the transient models for $t \rightarrow \infty$ correspond to a buoyancy field modelled by the steady state model 1 of §2.6.1. Constructing a model of the transient state that allows for a lateral buoyancy gradient, i.e., extending the steady state model 2 of chapter 2 to transient states, is non-trivial. If the plumes are modelled as quasi-steady, a step change of the buoyancy flux ratio Γ would result in a discontinuity of the buoyancy values and of the interface position with respect to the lateral dimension x and the discontinuities would propagate in x . Hence, a physically meaningful model that is two-dimensional in space would require us to model the plumes as unsteady or to model the mixing processes in the layers that smooth the discontinuity introduced by the step change. The resulting model would take the form of a non-linear partial differential equation. This would be more computationally demanding to solve than the spatially one-dimensional models constructed in the following sections, which correspond to ordinary differential equations.

3.5.1 Model 1: transient two-layer stratification

We assume that the buoyancy structure in the bulk can be modelled as a two-layer stratification throughout the transient state. In modelling the buoyancy field, we follow the approach for model 1 in chapter 2 (see §2.6.1) and extend the assumptions made there to the transient state. The model developed in this section is therefore referred to as model 1. When a distinction between the model 1 of §2.6.1 and the model 1 of the present section is necessary, the terms ‘steady state model 1’ and ‘transient state model 1’ are used, respectively. In accordance with §2.6.1, we assume that the buoyancy field in the transient state consist of a stable two-layer stratification, where the upper and lower layer are of uniform buoyancy, b_{a1} and b_{a2} , respectively (fig. 3.17). Modelling the buoyancy field as a two-layer stratification is physically consistent if the stratification is stable, $b_{a2} > b_{a1}$. As in the steady state, the interface between the layers at elevation z_1 is assumed to be horizontal and the interfacial buoyancy flux between the layers is neglected.

The upper layer of the two-layer stratification is supplied by the left-hand plume with a volume flux Q_{p1} and a buoyancy flux $Q_{p1} b_{p1}$ (see fig. 3.17), where b_{p1} is the characteristic top-hat buoyancy of

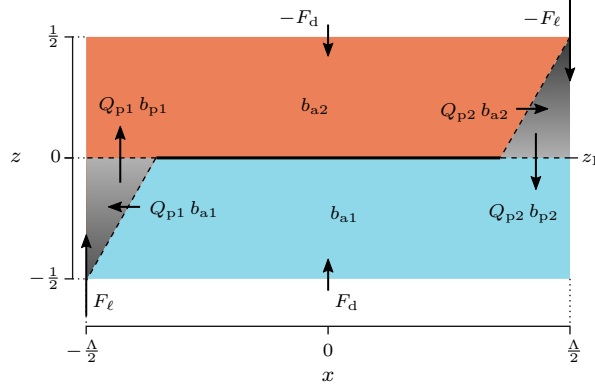


Figure 3.17: Schematics of the buoyancy structure for model 1 of the transient state, assuming a two-layer stratification with well-mixed layers. The highlighted sections are the time-dependent control volumes used; the arrows indicate the buoyancy flux between segments of the domain.

the left-hand plume at the interface height. Fluid in the upper layer is cooled by the distributed source of buoyancy flux F_d and entrained by the right-hand plume with volume flux Q_{p2} . Thus, conservation of the volume $V = \Lambda \left(\frac{1}{2} - z_I \right)$ and total buoyancy $V b_{a2}$ of the upper layer result in

$$\frac{d}{dt} \left[\Lambda \left(\frac{1}{2} - z_I \right) \right] = Q_{p1} - Q_{p2}, \quad (3.11a)$$

$$\frac{d}{dt} \left[\Lambda \left(\frac{1}{2} - z_I \right) b_{a2} \right] = Q_{p1} b_{p1} - F_d - Q_{p2} b_{a2}. \quad (3.11b)$$

Likewise, volume and buoyancy conservation of the lower layer result in

$$\frac{d}{dt} \left[\Lambda \left(\frac{1}{2} + z_I \right) \right] = Q_{p2} - Q_{p1}, \quad (3.12a)$$

$$\frac{d}{dt} \left[\Lambda \left(\frac{1}{2} + z_I \right) (-b_{a1}) \right] = Q_{p2} (-b_{p2}) - F_d - Q_{p1} (-b_{a1}), \quad (3.12b)$$

where b_{p2} is the characteristic top-hat buoyancy of the right-hand plume where it penetrates the interface. We drop the time-dependence of the interface height, the buoyancies and the volume and buoyancy fluxes in the model construction for better readability.

If the buoyancy in a plume evolves significantly faster than the buoyancy in its ambient, the plume can be considered as quasi-steady [27]. From our observations of the DNS data following a step increase of Γ , this condition is satisfied: the approximate time of $T_p \approx 0.32$ dimensionless time units that is required for a fluid parcel to travel from the plume source to the top of the plume is significantly smaller than the time required for a fluid parcel to be advected by the global circulation from the left to the right-hand plume (or vice versa), which we approximated as one time unit (§3.4.1). Equivalent assumptions of quasi-steady transient plumes have been used in the filling box and emptying-filling box model of Baines and Turner [9] and Linden, Lane-Serff and Smeed [63], respectively, as well as in models of confined plumes with time-dependent source strengths [17, 18, 20, 51]. Note, however, that the relevant time scales depend on the aspect ratio $\Lambda = \frac{L_z}{H}$ of the domain and that a quasi-steady plume model may not be appropriate in configurations of smaller aspect ratio.

Modelling the plumes as quasi-steady, their volume and buoyancy flux at the position z_I of the

interface between the layers corresponds to that of a steady planar plume in an unstratified environment (see appendix A):

$$Q_{p1} = \alpha^{\frac{2}{3}} F_{\ell}^{\frac{1}{3}} \left(\frac{1}{2} + z_I \right), \quad F_{\ell} = Q_{p1} (b_{p1} - b_{a1}), \quad (3.13a)$$

$$Q_{p2} = \alpha^{\frac{2}{3}} F_{\ell}^{\frac{1}{3}} \left(\frac{1}{2} - z_I \right), \quad F_{\ell} = -Q_{p2} (b_{p2} - b_{a2}). \quad (3.13b)$$

Note that the assumption of quasi-steady plumes is already implicitly used in (3.11), (3.12) and fig. 3.17, since the volume flux associated with entrainment into the plume and the volume flux of fluid discharged from the plume are modelled as equal.

Combining equations (3.11), (3.12) and (3.13), we obtain

$$\frac{dz_I}{dt} = -\frac{2\alpha^{\frac{2}{3}}}{\Lambda} F_{\ell}^{\frac{1}{3}} z_I, \quad (3.14a)$$

$$\frac{d\delta b}{dt} = \frac{1}{\Lambda} \frac{1}{\frac{1}{4} - z_I^2} \left[(F_{\ell} - F_d) - 2\alpha^{\frac{2}{3}} F_{\ell}^{\frac{1}{3}} \left(\frac{1}{4} + z_I^2 \right) \delta b \right], \quad (3.14b)$$

$$\frac{d\Sigma b}{dt} = \frac{1}{\Lambda} \frac{2z_I}{\frac{1}{4} - z_I^2} \left[(F_{\ell} - F_d) - \alpha^{\frac{2}{3}} F_{\ell}^{\frac{1}{3}} \delta b \right], \quad (3.14c)$$

where the buoyancy field is expressed in terms of the buoyancy difference $\delta b = b_{a2} - b_{a1}$ between the layers and the sum of buoyancies $\Sigma b = b_{a2} + b_{a1}$ of both layers (see §2.8).

From (3.14a), it is apparent that if the interface is at any time positioned at the horizontal mid-plane, $z_I = 0$, it remains at this elevation. This is not an artefact of the coordinate system but also occurs for a translated z -coordinate. Since we consider transient systems that are initially in a steady state, where $z_I = 0$ (see §2.6.1), equation (3.14) can be simplified to

$$\frac{dz_I}{dt} = 0, \quad (3.15a)$$

$$\frac{d\delta b}{dt} = \frac{4}{\Lambda} \left[(F_{\ell} - F_d) - \frac{\alpha^{\frac{2}{3}}}{2} F_{\ell}^{\frac{1}{3}} \delta b \right], \quad (3.15b)$$

$$\frac{d\Sigma b}{dt} = 0. \quad (3.15c)$$

The sum of buoyancies of both layers Σb^A is zero before the step change, since the volume integrated buoyancy of the domain is zero in the initial steady states. As the strength of the buoyancy flux sources of the top and bottom boundary are equal, Σb remains at zero for all times in the transient state (3.15c). Consequently, the buoyancy of the lower layer corresponds to the negative buoyancy of the upper layer, $b_{a1} = -b_{a2}$. Thus, the buoyancy field in the transient state displays the same antisymmetry that was present in the steady state (§2.6.1) at all times.

As the total buoyancy flux over each horizontal boundary remains constant over time

$$F_{\ell}(t) + F_d(t) = 1, \quad (3.16)$$

the buoyancy fluxes in equation (3.15b) can be written solely in terms of the time-dependent buoyancy

flux ratio Γ :

$$\frac{d\delta b(t)}{dt} = \frac{4}{\Lambda} \left[\frac{1 - \Gamma(t)}{1 + \Gamma(t)} - \frac{\alpha^{\frac{2}{3}}}{2} \frac{\delta b(t)}{(1 + \Gamma(t))^{\frac{1}{3}}} \right]. \quad (3.17)$$

For a step change of Γ according to (3.1), (3.17) can be solved analytically:

$$\delta b(t) = \begin{cases} \delta b^A & \text{for } t < 0, \\ (\delta b^B - \delta b^A) \left[1 - \exp \left(-\frac{2\alpha^{\frac{2}{3}}}{\Lambda} \frac{t}{(1 + \Gamma^B)^{\frac{1}{3}}} \right) \right] + \delta b^A & \text{for } t \geq 0. \end{cases} \quad (3.18)$$

Here, δb^A is the initial buoyancy difference corresponding to the steady state at Γ^A and δb^B is the buoyancy difference corresponding to the steady state at Γ^B , which is approached as $t \rightarrow \infty$. The steady state buoyancy differences are given by (2.15) as

$$\delta b(t) = \delta b^A = \frac{2}{\alpha^{\frac{2}{3}}} \frac{1 - \Gamma^A}{(1 + \Gamma^A)^{\frac{2}{3}}} \quad \text{for } t < 0, \quad \lim_{t \rightarrow \infty} \delta b(t) = \delta b^B = \frac{2}{\alpha^{\frac{2}{3}}} \frac{1 - \Gamma^B}{(1 + \Gamma^B)^{\frac{2}{3}}}. \quad (3.19)$$

In the construction of this model, we assumed that the buoyancy field is stably stratified at all times ($\delta b(t) > 0$). The resulting model is in accordance with this assumption, since $\delta b(t)$ in (3.18) satisfies $\delta b(t) > 0$ at all times if the initial and asymptotic final state are stably stratified ($\delta b^A, \delta b^B > 0$), which is true for the simulated step changes (3.3) and (3.4). In terms of the time-dependent buoyancy flux ratio Γ , the model is consistent if the initial and final buoyancy fluxes in a step change of Γ satisfy $\Gamma^A, \Gamma^B < 1$ (cf. §2.6).

To compare the model with the DNS data presented in fig. 3.7 and fig. 3.13, we need to extract the distance Δb between the peaks of the buoyancy field's PDF from the model. However, since model 1 describes a stratification in two homogeneous layers, the position of the peaks of the PDF corresponds to b_{a1} and b_{a2} and their distance equals δb , $\Delta b = \delta b$, as given in (3.18) (cf. §2.6.1).

3.5.2 Model 1a: transient intruding regime

As discussed in §3.1, the abrupt change of the source strength of a confined plume typically leads to the development of an additional layer above or below the buoyant layer of the original stratification (fig. 3.1). In this and the following section, we consider an equivalent transient stratification of the buoyancy field adapted to our configuration of combined localised and distributed boundary heating and cooling. In the present section, we model the transient state arising from a step increase of Γ .

Construction of the model

In §3.5.1, we demonstrated that the transient buoyancy field resulting from buoyancy flux sources of equal strength at the top and bottom boundary and an initial steady state of zero volume integrated buoyancy is antisymmetric to $z = 0$, equivalent to the steady state model 1 (§2.6.1). In the present section, we utilise the antisymmetry of the buoyancy field and consider only the upper half of the buoyancy field in the bulk, consisting of an upper and an upper intermediate layer, and the left-hand plume. The lower half of the buoyancy field in the bulk and the right-hand plume follow from the antisymmetry of the buoyancy field (see fig. 3.18).

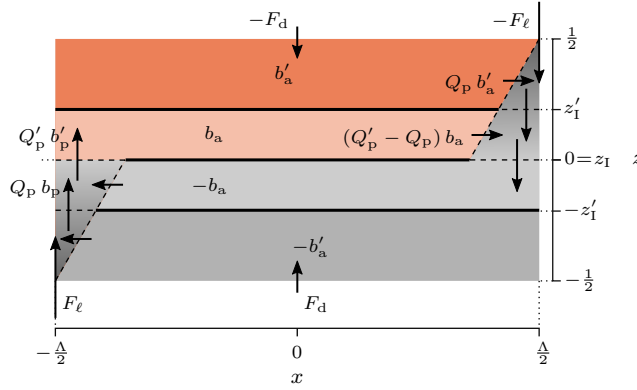


Figure 3.18: Schematics of the buoyancy structure for model 1a (intruding regime) of the transient state, assuming a four-layer stratification with well-mixed layers. The highlighted sections are the time-dependent control volumes used; the arrows indicate the buoyancy flux between segments of the domain.

A step increase of Γ at $t = 0$ corresponds to a decrease of the strength F_ℓ of the localised sources (fig. 3.2). Due to the abruptly decreased localised buoyancy flux, the buoyancy of fluid in the left-hand plume at the height of the interface is decreased at $t = 0$ and the fluid discharged by the plume spreads along the interface of the original stratification $z_I = 0$, forming a new layer of higher density below the upper layer of the original stratification (intruding regime, fig. 3.18). Both the upper layer and the newly formed upper intermediate layer are modelled as well-mixed layers of uniform buoyancy b'_a and b_a , respectively, and are separated by a horizontal interface at z'_1 . The plumes are modelled as quasi-steady. An equivalent model for a plume of abruptly decreased source strength has been considered by Bower et al. [20]. In the following, this model of the intruding regime is referred to as model 1a.

The upper layer is not supplied by a mass source, but is depleted by entrainment of fluid into the right-hand plume at a volume flux Q_p . The entrainment volume flux Q_p equals the volume flux of the right-hand plume at the position z'_1 of the density step between the upper and the upper intermediate layer (see fig. 3.18). Both the distributed buoyancy flux source at the top boundary and the entraining right-hand plume act as buoyancy sinks on the upper layer, corresponding to a buoyancy flux F_d and $Q_p b'_a$, respectively. Thus, volume and buoyancy conservation of the upper layer yield

$$\frac{d}{dt} \left[\Lambda \left(\frac{1}{2} - z'_1 \right) \right] = -Q_p, \quad (3.20a)$$

$$\frac{d}{dt} \left[\Lambda \left(\frac{1}{2} - z'_1 \right) b'_a \right] = -F_d - Q_p b'_a. \quad (3.20b)$$

The upper intermediate layer at buoyancy b_a is supplied by the left-hand plume with a volume flux Q'_p and a buoyancy flux $Q'_p b'_p$ (fig. 3.18), where b'_p is the characteristic top-hat buoyancy of the left-hand plume at the density step between the two intermediate layers at $z_I = 0$. Fluid from the upper intermediate layer is entrained into the right-hand plume. The volume flux of the entrainment corresponds to the difference between the volume fluxes Q'_p and Q_p of the right-hand plume at the density steps that border the upper intermediate layer at z_I and z'_1 , respectively (fig. 3.18). Volume

and buoyancy conservation of the upper intermediate layer thus result in

$$\frac{d}{dt} (\Lambda z'_1) = Q'_p - (Q'_p - Q_p) , \quad (3.21a)$$

$$\frac{d}{dt} (\Lambda z'_1 b_a) = Q'_p b'_p - (Q'_p - Q_p) b_a , \quad (3.21b)$$

where equations (3.20a) and (3.21a) contain the same information, since the joint depth of the upper and upper intermediate layer is fixed to $\frac{1}{2}$ at all times by the antisymmetry of the buoyancy field.

In the conservation equations, (3.20) and (3.21), we neglect entrainment between the upper and the upper intermediate layer. Entrainment between the two layers can occur as a result of the left-hand plume, which becomes a fountain at the elevation z_1 where the buoyancy of fluid parcels in the plume is zero relative to the ambient fluid [51]. Depending on the momentum flux of the plume at $z = 0$ and the depth z'_1 of the upper intermediate layer, the resulting fountain can overshoot into the upper layer and subsequently fall back into the upper intermediate layer, thereby entraining fluid from the upper layer [20]. Our choice to neglect this possible entrainment will be discussed in §3.6.

We consider the left-hand plume as a composite of two segments, $-\frac{1}{2} \leq z \leq -z'_1$ and $-z'_1 < z \leq z_1$, separated by the density step in the ambient of the plume at $-z'_1$ (see fig. 3.18). The plume evolves in each segment in an environment of homogenous buoyancy and thus the relative buoyancy flux of the plume to its ambient is conserved within each segment. The volume flux and characteristic top-hat buoyancy at the upper boundary of the segments are denoted as Q_p and b_p at $-z'_1$ and as Q'_p and b'_p at z_1 (fig. 3.18)). Buoyancy conservation in the two plume segments corresponds to

$$F_\ell + Q_p (-b'_a) = Q_p b_p , \quad (3.22a)$$

$$Q_p b_p + (Q'_p - Q_p) (-b_a) = Q'_p b'_p , \quad (3.22b)$$

which can be combined to give

$$Q'_p b'_p = F_\ell - Q_p b'_a - (Q'_p - Q_p) b_a . \quad (3.23)$$

Thus, the governing equations of model 1a can be obtained from (3.20), (3.21) and (3.23) as

$$\Lambda \frac{dz'_1}{dt} = Q_p , \quad (3.24a)$$

$$\Lambda z'_1 \frac{db_a}{dt} = F_\ell + Q_p (b_a - b'_a) - 2 Q'_p b_a , \quad (3.24b)$$

$$\Lambda \left(\frac{1}{2} - z'_1 \right) \frac{db'_a}{dt} = -F_d . \quad (3.24c)$$

The volume and momentum flux, Q_p and M_p , of the left-hand plume at $z = -z'_1$ are given by plume scaling relations (A.3) as

$$Q_p = \alpha^{\frac{2}{3}} F_\ell^{\frac{1}{3}} \left(\frac{1}{2} - z'_1 \right) , \quad M_p = \alpha^{\frac{1}{3}} F_\ell^{\frac{2}{3}} \left(\frac{1}{2} - z'_1 \right) . \quad (3.25)$$

To determine the volume flux Q'_p of the left-hand plume at z_1 , we follow Cooper and Linden [28] and model the upper segment of the plume ($-z'_1 < z \leq z_1$) as a plume from an area source of finite

volume and momentum flux at $-z'_1$, where the source volume and momentum flux match the volume and momentum flux, Q_p and M_p (3.25), of the lower segment of the plume at $-z'_1$. Generally, for a density step positioned at an elevation ζ_{ds} , the volume flux $Q(\zeta)$ of the plume at an arbitrary elevation $\zeta - \zeta_{ds}$ above the density step obeys the relation (see appendix A)

$$\zeta - \zeta_{ds} = \frac{\Omega}{\alpha^{\frac{2}{3}} F_{ds}^{\frac{1}{3}}} \int_{\frac{Q_{ds}}{\Omega}}^{\frac{Q(\zeta)}{\Omega}} [1 + q^{-3}]^{-\frac{1}{3}} dq, \quad (3.26)$$

where Q_{ds} and M_{ds} correspond to the volume and momentum of the plume at the density step, F_{ds} denotes the plume's buoyancy flux relative to its ambient just above the density step and Ω is defined as

$$\Omega \equiv \left(\frac{\alpha}{F_{ds}} M_{ds}^3 - Q_{ds}^3 \right)^{\frac{1}{3}}. \quad (3.27)$$

Using these analytical expressions to model the behaviour of a plume at a density step allows us to write model 1a of the buoyancy field in the bulk as a set of ordinary differential equations and we avoid numerical derivatives of a discontinuous ambient buoyancy field.

For the volume flux Q'_p of the left-hand plume at $z_1 = 0$, i.e. at a distance $[0 - (-z'_1)]$ above the density step at $-z'_1$, equation (3.26) results in

$$z'_1 = \frac{\Omega'}{\alpha^{\frac{2}{3}} F'_{ds}{}^{\frac{1}{3}}} \int_{\frac{Q_p}{\Omega'}}^{\frac{Q'_p}{\Omega'}} [1 + q^{-3}]^{-\frac{1}{3}} dq, \quad (3.28)$$

with

$$F'_{ds} \equiv Q_p [b_p - (-b_a)] = F_\ell - Q_p (b'_a - b_a), \quad \Omega' \equiv \left(\frac{\alpha}{F'_{ds}} M_p^3 - Q_p^3 \right)^{\frac{1}{3}}, \quad (3.29)$$

where the second equality in the left-hand expression results from (3.22a).

Initial conditions for numerical solution

The governing equations (3.24) of model 1a need to be solved numerically. Hence, we require initial conditions that correspond to the system's state immediately after the step change of Γ at $t = 0$.

The initial layer depth in a filling box mechanism is typically modelled as infinitesimal [20, 39, 63]. At a time δt immediately after the step change, the plumes extend over half the domain height ($z'_1(\delta t) = 0$) and the buoyancy of the top and bottom layer is yet unchanged from its value before the step change ($b'_a(\delta t) = b_a^A$). The buoyancy of the newly formed upper intermediate layer can then be estimated as the characteristic buoyancy b'_p of the plume at z_1 , $b_a(\delta t) = b'_p(\delta t)$. We neglect entrainment from the infinitesimally thin lower intermediate layer at buoyancy $-b_a$ into the left-hand plume, and thus model the plume as developing in a homogeneous ambient of buoyancy $-b'_a(\delta t) = -b_a^A$. Utilising (3.22b) and plume scaling relations (A.3), we obtain

$$F_\ell^B + Q'_p(\delta t) (-b_a^A) = Q'_p(\delta t) b_a(\delta t), \quad Q'_p(\delta t) = \alpha^{\frac{2}{3}} (F_\ell^B)^{\frac{1}{3}} \frac{1}{2}, \quad (3.30)$$

which can be combined to give

$$b_a(\delta t) = 2 \alpha^{-\frac{2}{3}} (F_\ell^B)^{\frac{2}{3}} - b_a^A. \quad (3.31)$$

In the numerical implementation, we have to choose a small finite initial value for the initial depth of the newly formed layers, $0 < z'_1(\delta t) \ll 1$, to avoid a singularity in the governing equation (3.24b).

Measure of the buoyancy difference in the bulk

The transient intruding regime as modelled by model 1a is stratified into four layers. However, the initial and asymptotic final steady state of this transient show a two-layer stratification in the bulk and are separated by an interface at $z_I = 0$ (see §2.6.1). Hence, we separate the four-layer stratification of model 1a at the density step z_I into an upper and a lower segment and characterize the transient buoyancy field via the difference between the mean buoyancy of the upper segment and the mean buoyancy of the lower segment:

$$\Delta b \equiv 2 \left[\int_0^{z'_1(t)} b_a(t) dz + \int_{z'_1(t)}^{\frac{1}{2}} b'_a(t) dz \right] - 2 \left[\int_{-\frac{1}{2}}^{-z'_1(t)} (-b'_a(t)) dz + \int_{-z'_1(t)}^0 (-b_a(t)) dz \right] \quad (3.32a)$$

$$= 4 \left[z'_1(t) b_a(t) + \left(\frac{1}{2} - z'_1(t) \right) b'_a(t) \right]. \quad (3.32b)$$

Note, that employing an equivalent definition for model 1 of §3.5.1 would result in the characteristic buoyancy difference $\Delta b = b_{a2} - b_{a1}$ defined there, i.e., the definition of Δb chosen here is consistent with the one in §3.5.1.

3.5.3 Model 1b: transient filling regime

In this section, we consider a transient state where a step decrease of Γ results in two additional layers in the stratified buoyancy field, equivalent to the filling regime discussed in §3.1

Construction of the model

As for the intruding regime in §3.5.2, we utilise the antisymmetry of the buoyancy field with respect to $z = 0$ to restrict our considerations to the upper and upper intermediate buoyancy layer in the bulk and the left-hand plume (see fig. 3.19).

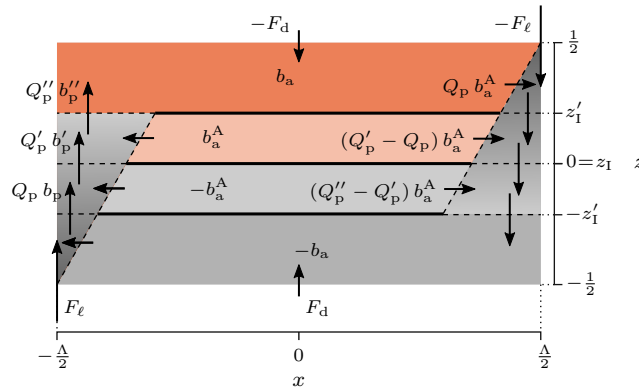


Figure 3.19: Schematics of the buoyancy structure for model 1b (filling regime) of the transient state, assuming a four-layer stratification with well-mixed layers. The highlighted sections are the time-dependent control volumes used; the arrows indicate the buoyancy flux between segments of the domain.

Before the step decrease of Γ at $t = 0$, the buoyancy field in the bulk is stratified into two layers, which we model as homogeneous according to the steady state model 1 (§2.6.1). Each layer is supplied by a plume from a localised source, where the buoyancy of fluid parcels in the plume at the interface height ($z_I = 0$) equals the buoyancy b_a^A of fluid of the layer the plume is discharging into. A step decrease of Γ corresponds to an increase of the localised buoyancy flux F_ℓ (fig. 3.2) and results in an increase of the buoyancy of fluid parcels in the left-hand plume at z_I . Thus, fluid parcels in the left-hand plume are positively buoyant relative to the ambient fluid of the original upper layer and the plume extends upwards to the top boundary. The fluid discharged by the plume spreads below the top boundary and forms a new layer of buoyancy b_a (filling regime, fig. 3.19). The fluid of the original upper layer at buoyancy b_a^A now forms an upper intermediate layer. The elevation of the interface separating the upper and upper intermediate layer is denoted as z'_I . The plumes are modelled as quasi-steady. This model of the filling regime is equivalent to a model by Bower et al. [20] of a plume of abruptly increased source strength and will be referred to as model 1b.

The upper layer at buoyancy b_a is supplied by the left-hand plume with a volume flux Q_p'' and a buoyancy flux $Q_p'' b_p''$ (fig. 3.19), where b_p'' corresponds to the characteristic top-hat buoyancy of the left-hand plume where it penetrates the interface at z'_I . The top boundary at buoyancy flux F_d and the entraining right-hand plume act as buoyancy sinks on the top layer, where the latter corresponds to a buoyancy flux $Q_p b_a$. The volume flux with which the right-hand plume entrains fluid from the upper layer equals the volume flux Q_p of the right-hand plume at z'_I . Thus, volume and buoyancy conservation of the upper layer give:

$$\frac{d}{dt} \left[\Lambda \left(\frac{1}{2} - z'_I \right) \right] = Q_p'' - Q_p, \quad (3.33a)$$

$$\frac{d}{dt} \left[\Lambda \left(\frac{1}{2} - z'_I \right) b_a \right] = Q_p'' b_p'' - F_d - Q_p b_a. \quad (3.33b)$$

The upper intermediate layer is not subjected to buoyancy sources or sinks and thus remains at its initial buoyancy, which corresponds to the steady state buoyancy b_a^A of the upper layer of a two-layer stratification before the step change (see (3.19)). The upper intermediate layer is depleted by entrainment into the left- and right-hand plume (fig. 3.19),

$$\frac{d}{dt} [\Lambda z'_I] = -[Q_p' - Q_p] - [Q_p'' - Q_p'], \quad (3.34)$$

where Q_p' corresponds to the volume flux of the left or right-hand plume at the density step z_I . However, since the joint volume of the upper and upper intermediate layer is fixed by the antisymmetry of the buoyancy field ($z_I = 0$), equations (3.33a) and (3.34) contain the same information.

As in model 1a of the intruding regime (§3.5.2), we consider the left-hand plume as a composite of segments in which the plume's buoyancy flux relative to its ambient is constant (fig. 3.19), resulting in three plume segments in the z -intervals $[-\frac{1}{2}, -z'_I]$, $(-z'_I, z_I]$ and $(z_I, z'_I]$. Buoyancy conservation in the segments corresponds to

$$F_\ell + Q_p (-b_a) = Q_p b_p, \quad (3.35a)$$

$$Q_p b_p + (Q_p' - Q_p) (-b_a^A) = Q_p' b_p', \quad (3.35b)$$

$$Q_p' b_p' + (Q_p'' - Q_p') b_a^A = Q_p'' b_p'', \quad (3.35c)$$

where Q_p and b_p are the volume flux and characteristic top-hat buoyancy of the left-hand-plume at the density step at $-z'_1$ and the equivalent quantities at z_1 and z'_1 are denoted as Q'_p , b'_p and Q''_p , b''_p , respectively (see fig. 3.19).

The conservation equations above can be combined to give

$$Q''_p b''_p = F_\ell - Q_p b_a + (Q''_p - 2Q'_p + Q_p) b_a^A, \quad (3.36)$$

which can be inserted into (3.33) to obtain the governing equations of model 1b:

$$\Lambda \frac{dz'_1}{dt} = Q_p - Q''_p, \quad (3.37a)$$

$$\Lambda \left(\frac{1}{2} - z'_1 \right) \frac{db_a}{dt} = F_\ell - F_d - (Q''_p + Q_p) (b_a - b_a^A) - 2Q'_p b_a^A. \quad (3.37b)$$

As in §3.5.2, the volume and momentum flux, Q_p and M_p , of the left-hand plume at $-z'_1$ are given by (3.25). To obtain the volume flux of the left-hand plume at the density steps at z_1 and z'_1 , we again use the approach of Cooper and Linden [28] and model the plume segments in the intervals $z \in (-z'_1, z_1]$ and $z \in (z_1, z'_1]$ as plumes from area sources of finite volume and momentum flux.

For the volume flux Q'_p of the left-hand plume at z_1 , i.e. at a distance $0 - (-z'_1)$ above the respective closest upstream density step at $-z'_1$, equation (3.26) gives

$$z'_1 = \frac{\Omega'}{\alpha^{\frac{2}{3}} F'_{ds}{}^{\frac{1}{3}}} \int_{\frac{Q_p}{\Omega'}}^{\frac{Q'_p}{\Omega'}} [1 + q^{-3}]^{-\frac{1}{3}} dq, \quad (3.38)$$

with

$$F'_{ds} \equiv Q_p (b_p - (-b_a^A)) = F_\ell - Q_p (b_a - b_a^A), \quad \Omega' \equiv \left(\frac{\alpha}{F'_{ds}} M_p^3 - Q_p^3 \right)^{\frac{1}{3}}. \quad (3.39)$$

where the second equality in the left-hand expression results from (3.35a).

The corresponding momentum flux M'_p at $z = 0$ is given by the relation (see appendix A)

$$M_p'^3 = \frac{F'_{ds}}{\alpha} [Q_p'^3 + \Omega'^3]. \quad (3.40)$$

Equivalent to Q'_p , we obtain for the volume flux Q''_p of the left-hand plume at z'_1 from (3.26) the relationship

$$z'_1 = \frac{\Omega''}{\alpha^{\frac{2}{3}} F''_{ds}{}^{\frac{1}{3}}} \int_{\frac{Q'_p}{\Omega''}}^{\frac{Q''_p}{\Omega''}} [1 + q^{-3}]^{-\frac{1}{3}} dq, \quad (3.41)$$

with

$$F''_{ds} \equiv Q'_p (b'_p - b_a^A) = F'_{ds} - 2Q'_p b_a^A, \quad \Omega'' \equiv \left(\frac{\alpha}{F''_{ds}} M_p'^3 - Q_p'^3 \right)^{\frac{1}{3}}, \quad (3.42)$$

where the second equality in the left-hand expression results from (3.35a), (3.35b) and (3.39).

Initial conditions for numerical solution

At a time δt immediately after the step change of Γ , the plumes extend over the entire height of the domain ($z'_1(\delta t) = \frac{1}{2}$). The buoyancy of the newly formed top layer can then be estimated as the buoyancy b_p'' of the plume where it touches the top boundary of the domain. Inserting $b_a(\delta t) = b_p''(\delta t)$ into (3.35c), we obtain

$$Q'_p(\delta t) b'_p(\delta t) + [Q''_p(\delta t) - Q'_p(\delta t)] b_a^A = Q''_p(\delta t) b_a(\delta t). \quad (3.43)$$

We neglect entrainment from the infinitesimally thin bottom layer at buoyancy $-b_a$ into the left-hand plume. Thus, buoyancy conservation in the left-hand plume for $-\frac{1}{2} \leq z \leq z_I$ gives

$$F_\ell^B + Q'_p(\delta t) (-b_a^A) = Q'_p(\delta t) b'_p(\delta t) \quad (3.44)$$

and the volume and momentum flux of the plume at z_I can be estimated as those of a plume in a homogeneous ambient of buoyancy $-b_a^A$ (A.3):

$$Q'_p(\delta t) = \alpha^{\frac{2}{3}} (F_\ell^B)^{\frac{1}{3}} \frac{1}{2}, \quad M'_p(\delta t) = \alpha^{\frac{1}{3}} (F_\ell^B)^{\frac{2}{3}} \frac{1}{2}. \quad (3.45)$$

Combining (3.43) and (3.44), we obtain the buoyancy of the top layer as

$$b_a(\delta t) = \frac{1}{Q''_p(\delta t)} [F_\ell^B - 2 Q'_p(\delta t) b_a^A] + b_a^A, \quad (3.46)$$

where the volume flux $Q''_p(\delta t)$ of the left-hand plume where it touches the top boundary is determined by (cf. (3.41)):

$$\frac{1}{2} = \frac{\Omega''(\delta t)}{\alpha^{\frac{2}{3}} F_{ds}''(\delta t)^{\frac{1}{3}}} \int_{\frac{Q'_p(\delta t)}{\Omega''(\delta t)}}^{\frac{Q''_p(\delta t)}{\Omega''(\delta t)}} [1 + q^{-3}]^{-\frac{1}{3}} dq, \quad (3.47)$$

and

$$F_{ds}''(\delta t) = Q'_p(\delta t) (b'_p(\delta t) - b_a^A) = F_\ell^B - 2 Q'_p(\delta t) b_a^A, \quad (3.48)$$

$$\Omega''(\delta t) = \left(\frac{\alpha}{F_{ds}''(\delta t)} M'_p(\delta t)^3 - Q'_p(\delta t)^3 \right)^{\frac{1}{3}}. \quad (3.49)$$

The initial interface height $z'_1(\delta t)$ has to be chosen as a value slightly smaller than $\frac{1}{2}$, to avoid a singularity in the governing equation (3.37b).

Measure of the buoyancy difference in the bulk

As for model 1a of the intruding regime in §3.5.2, we define a characteristic buoyancy difference Δb as the difference between the mean buoyancy of the upper and lower half of the bulk:

$$\Delta b \equiv 2 \left[\int_0^{z'_1(t)} b_a^A dz + \int_{z'_1(t)}^{\frac{1}{2}} b_a(t) dz \right] - 2 \left[\int_{-\frac{1}{2}}^{-z'_1(t)} (-b_a(t)) dz + \int_{-z'_1(t)}^0 (-b_a^A) dz \right] \quad (3.50)$$

$$= 4 \left[z'_1(t) b_a^A + \left(\frac{1}{2} - z'_1(t) \right) b_a(t) \right]. \quad (3.51)$$

3.6 Model comparison and validation for the transient state

In §3.5, we constructed two types of models for the transient state: the transient model 1, which describes a two-layer stratification with homogeneous layers in the bulk, and models 1a and 1b, which are characterised by the appearance of two additional homogeneous layers after the step change of Γ . The models 1a and 1b are equivalent to models of the intruding and filling regime, respectively, as considered by Bower et al. [20] for a plume of abruptly decreased or increased source strength (see §3.1). The initial and asymptotic final state of the transient buoyancy field is described by the steady state model 1 (§2.6.1) for all transient models of §3.5.

Modelling the transient buoyancy field as a two-layer stratification (model 1) or a four-layer stratification (model 1a and 1b) can be understood as representing two extremal cases of the mixing in the bulk following a step change of Γ : model 1a and 1b describe a transient state where mixing between the original stratification and the fluid discharged by the plumes after the step change of Γ occurs only in the plumes. In contrast, model 1 is based on the assumption that the fluid of the original stratification mixes ideally with fluid discharged by the plumes after the step change in each layer. The actual flow behaviour may correspond to neither of these mixing assumptions, but rather lie within a range of behaviours bounded by model 1 and model 1a or 1b. This is the concept on which we base the comparison between the models and the DNS data in this section. This interpretation of the models is based on existing work concerning stratifications that arise from a confined unsteady plume. Considering a confined plume of abruptly decreased source strength experimentally, Bower et al. [20] found that the real system shows features of a model with and without interfacial entrainment between the original and the intruding layer, concluding that these models should be considered as “end-members bracketing the actual flow behaviour” [20, p. 23]. Similarly, Bolster, Maillard and Linden [18] describe their experimental observations of the stratification resulting from a unsteady plume in a ventilated enclosure as displaying “neither perfect mixing nor idealised stratification” [18, p. 2109].

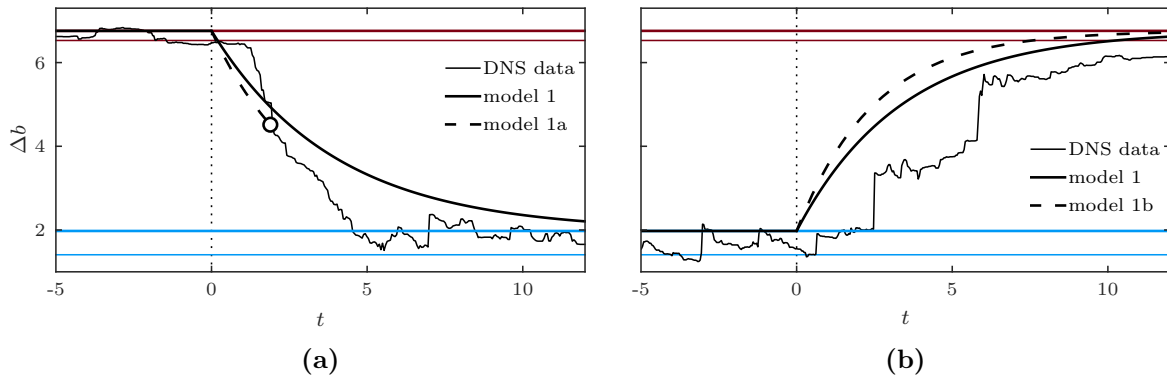


Figure 3.20: Characteristic buoyancy difference Δb of the stratification for (a) a step increase (3.3) and (b) a step decrease (3.4) of Γ : comparing the DNS data (thin lines) and model solutions (thick lines). The DNS data of the transient state is depicted as black thin lines (moving average), with the buoyancy difference of the steady state at $\Gamma = 0$ and 0.60 marked as a thin red and blue horizontal line, respectively (see fig. 3.7 and 3.13 for details). The characteristic buoyancy differences Δb of the stratifications as given by the models are depicted as thick black lines (see §3.5 for the definitions of Δb in each model); ‘o’ marks the point at which model 1a becomes inconsistent (see text). The buoyancy differences for the steady states, according to model 1 (2.15), are depicted as thick red and blue horizontal lines for $\Gamma = 0$ and 0.60 , respectively.

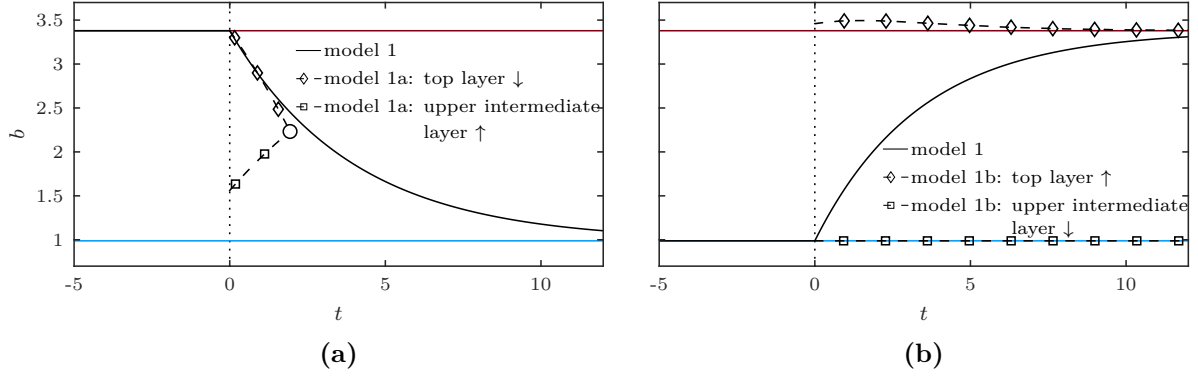


Figure 3.21: Comparing transient models 1, 1a and 1b for (a) a step increase (3.3) and (b) a step decrease (3.4) of Γ . Depicted are the transient buoyancies b of the layers in the upper half of the domain (black lines, cf. fig. 3.18 and fig. 3.19); ‘o’ marks the point at which model 1a becomes inconsistent (see text). The arrows in the legends indicate whether the respective layer is increasing ($\uparrow$) or decreasing ($\downarrow$) in depth. The buoyancies for the steady states, according to model 1 (2.15), are depicted as red and blue horizontal lines for $\Gamma = 0$ and 0.60, respectively.

To compare the models with the DNS data, we characterise the modelled buoyancy fields with the difference Δb between the mean buoyancy of the upper and lower half of the stratification (fig. 3.20). For two-layer stratifications, i.e., for the transient model 1, the initial steady state and the asymptotic final steady state, Δb corresponds to the buoyancy difference between the two layers. Fig. 3.21 shows the buoyancies of the individual layers of the stratification to clarify the behaviour of the models.

According to model 1 (3.18), a step change of the buoyancy flux ratio from Γ^A to Γ^B at $t = 0$ results in a characteristic buoyancy difference $\Delta b(t)$ that converges exponentially from the steady state value of Δb at Γ^A towards the steady state value at Γ^B for $t \rightarrow \infty$ (fig. 3.20, thick solid line)

$$\Delta b(t) = (\Delta b^B - \Delta b^A) \left[1 - \exp\left(-\frac{t}{T^{AB}}\right) \right] + \Delta b^A \quad \text{for } t \geq 0. \quad (3.52)$$

Here, Δb^A and Δb^B correspond to the initial and asymptotic final characteristic buoyancy difference, respectively, (see (3.19)) and the time scale of the transition between steady states is determined by

$$T^{AB} = \frac{\Lambda}{2\alpha^{\frac{2}{3}}} (1 + \Gamma^B)^{\frac{1}{3}}. \quad (3.53)$$

This behaviour is qualitatively the same for an increase or decrease of the buoyancy flux ratio Γ .

In contrast to model 1, the transient buoyancy field represented by model 1a develops two new layers between the layers of the initial two-layer stratification following a step increase of Γ . However, since the top layer of the original stratification is cooled by the distributed source and the newly formed upper intermediate layer increases in buoyancy over time (fig. 3.21a), the latter becomes eventually more buoyant than the layer above it and the layers in the upper half of the domain mix at $t \approx 1.9$ (‘o’-marker in fig. 3.20a and 3.21a). Likewise, the stratification in the lower half of the domain becomes unstable and mixes at $t \approx 1.9$. Thus, the transient buoyancy field becomes a two-layer stratification and is no longer described by model 1a after $t \approx 1.9$, though the transient could be continued by switching to model 1, starting from an initial value (‘o’) that matches the buoyancy of model 1a at breakdown. Indeed, it can be shown that the transient four-layer stratification of model 1a will always

reduce to a two-layer stratification before a steady state is reached.

Although model 1 and model 1a describe different stratifications which contain fluid parcels at notably different buoyancies (fig. 3.21a), their behaviour in terms of a characteristic buoyancy difference Δb between the upper and lower half of the stratification is similar (thick black line in fig. 3.20a). The characteristic buoyancy difference of both models roughly approximates the DNS data (thin black lines in fig. 3.20a), however, the models cannot reproduce the initial delay in the response of the buoyancy field and we note that Δb of the DNS data approaches its final steady state value (thin blue line in fig. 3.20a) at an earlier time than the time at which the modelled buoyancy difference is similarly close to the modelled steady state value (thick blue line in fig. 3.20a).

A step decrease of Γ results, according to in model 1b, in the formation of two new layers above and below the two layers of the initial steady state stratification. The intermediate layers, which correspond to the initial stratification, stay at their initial buoyancy values and decrease in depth over time, whereas the newly formed layers increase in depth (fig. 3.21b). The buoyancy of the top layer overshoots its asymptotic final steady state value (red horizontal line in fig. 3.21b) and approaches it from above; equivalently, the buoyancy of the bottom layer undershoots its respective final value. Numerically, we found from (3.46) that the initial buoyancy of the top (bottom) layer always exceeds (falls below) the top (bottom) layer's buoyancy in the asymptotic final state for $1 > \Gamma^B > \Gamma^A > 0$ and a constant total buoyancy flux on each boundary, $F_\ell + F_d = 1$.

As in the case of a step increase of Γ , the buoyancy field following a step decrease of Γ as described by the models 1 and 1b behaves similarly in terms of the characteristic buoyancy difference Δb (thick black lines in fig. 3.20b), although the modelled buoyancy values in the individual layers of the stratifications differ notably (fig. 3.21b). Indeed, since the buoyancies in each layer of the four-layer stratification of model 1b vary little with time compared to the buoyancy scale of the transition, the behaviour of the corresponding Δb is largely determined by the transient depth of the layers in the stratification. Both models roughly approximate the behaviour of the DNS buoyancy difference Δb (thin black line in fig. 3.20b), though the delay in the response of the DNS buoyancy field is not reproduced by the models.

A comparison between the characteristic buoyancy differences Δb from the DNS data and the model predictions of Δb (fig. 3.20) does not allow us to conclude that either the transient two-layer model 1 or the transient four-layer models 1a and 1b better reproduce the actual buoyancy field. Our observations in §3.4 suggest, that the buoyancy field following the simulated step increase of Γ (3.3) might be better represented by model 1, since the transient buoyancy field appears to be stratified into two layers at all times, while for modelling the buoyancy field following the step decrease (3.4) of Γ , model 1b may be preferable to reproduce the observed filling flow regime. In the latter case, it should be noted that the depth of the initial top and bottom layer in the DNS buoyancy field amounts to approximately 40% of half of the domain height, rather than being initially of infinitesimal depth as in model 1b, which may also justify modelling the transient that occurs following a step decrease of Γ as a two-layer stratification (model 1). The DNS data in this chapter, however, does not represent an exhaustive investigation of the possible transient states from unsteady combined localised and distributed sources. Intruding flow regimes may be observable following a step increase of Γ to a smaller final distributed source strength than the one chosen here ($\Gamma^B = 0.60$) and the transient that occurs following a step decrease of Γ may be better represented by a two-layer stratification, if Γ^B is sufficiently large. Whilst the two model types may be understood as bracketing extremal cases of the possible flow behaviour,

further work is needed to determine which transient stratification model more closely resembles the actual buoyancy field under given unsteady boundary conditions. However, our results suggest that, if a characteristic buoyancy difference between the upper and lower segment of the transient field is of interest, a two-layer stratification model (model 1) may be sufficient.

The models presented here show some disagreement with the DNS data. Firstly, the steady state values Δb , to which the transient models converge, correspond to the values predicted by the steady state model 1 of chapter 2, which were shown to increasingly differ from the DNS data with increasing Γ (cf. the thin and thick red and blue horizontal lines in fig. 3.20). Moreover, the transition timescale T^{AB} of model 1 in (3.53) is determined by the volume flux Q_p^{B} of the global circulation in the asymptotic final steady state, as predicted by the steady state model 1 (cf. §2.7.3):

$$T^{\text{AB}} = \frac{\Lambda}{4Q_p^{\text{B}}} . \quad (3.54)$$

Hence, the time scale for a transient described by model 1 increases with the value of the buoyancy flux ratio Γ^{B} after the step change. The DNS data in §3.4 showed an opposite scaling behaviour of the transition time with Γ^{B} : the transient that results from a step increase ($\Gamma^{\text{B}} = 0.60$) converged faster than the one from a step decrease ($\Gamma^{\text{B}} = 0$). Moreover, it would seem reasonable that the volume flux Q_p^{B} of the global circulation that is approached after the step change impacts the time scale of the transition. Since Q_p as predicted by the steady state model 1 does not scale correctly with Γ (see §2.7.3), this suggests that the transient model 1 cannot generally reproduce the time scale of the actual transient. In the case of the transitions simulated in this chapter, the resulting model time scales do not differ vastly, giving $T^{\text{AB}} \approx 4.0$ and $T^{\text{AB}} \approx 3.4$ for the step increase and decrease of Γ , respectively.

In chapter 2, we found that the scaling behaviour of the volume flux Q_p with Γ is predicted with good accuracy, if we allow for lateral buoyancy gradients in the layers (model 2, §2.6.2). Hence, a transient model in the manner of the steady state model 2, which describes the buoyancy field in each layer as a function of the horizontal position x , might return a more accurate transient time scale. Note, however, that the time required for a transition between two steady states is not solely dependent on the volume flux, but is also influenced by the amount of mixing that results from convection from distributed buoyancy flux sources.

Beyond the erroneous transition time scale as predicted by model 1, there are further indications that a spatially two-dimensional model would notably improve predictions of the transients. None of the spatially one-dimensional transient models 1, 1a or 1b can reproduce the initial delay observable in the response of the DNS value of Δb to the change of Γ (see fig. 3.20). The delay is a result of the lateral transport and mixing of fluid parcels within one layer on a finite time scale. In models 1, 1a and 1b, however, the mixing within a layer occurs instantaneously over the horizontal extent of the domain, since the layers are defined as homogenous. Note that, although a transient model in the manner of the steady state model 2 might be able to reproduce the observed delay, the latter would require a higher computational effort to solve than spatially one-dimensional models, since it corresponds to a non-linear partial differential equation, and the extension of model 2 to transient states is non-trivial (see remarks at the beginning of §3.5). Hence, the use of spatially one-dimensional models may be justifiable if the simplicity of the model takes priority over a detailed transient response and a precise time-dependence.

3.7 Conclusions

In this chapter, we studied the transient state following a step increase and decrease of the buoyancy flux ratio $\Gamma = \frac{F_d}{F_\ell}$ in a domain that is heated and cooled by a combination of localised sources (F_ℓ) and distributed sources (F_d). Before the step change of Γ , the system is statistically steady and the total buoyancy flux on each boundary, $F_\ell + F_d$, is constant at all times. The buoyancy flux ratios before and after the step change, Γ^A and Γ^B , respectively, are chosen such that both the initial steady state and the ‘final’ steady state that the system converges to after the step change correspond to a stable two-layer stratification of the buoyancy field in the bulk ($\Gamma^A, \Gamma^B < 1$). In the steady state at $\Gamma < 1$, the two-layer stratification of the buoyancy field is maintained by two plumes from the localised sources that entrain fluid from the ambient layer and shed fluid into the respective second layer, thus connecting both layers by a global circulation (see chapter 2).

We observe a difference in the character of the response of the system when the buoyancy flux ratio Γ is increased or decreased. After an increase of Γ , the transient buoyancy field remains stratified into two layers throughout its transition to the two-layer stratification of the ‘final’ steady state. In contrast, a decrease of Γ initially results in the formation of a hot and cold layer above and below the fluid of the initial stratification, similar to the stratification observed for plumes of increased source strength in confinement [20]. The two-layer stratification is then regained at a later time during the transient, as the volume of fluid from the original stratification becomes depleted by entrainment into the plumes. Following a decrease of Γ , the transition to the ‘final’ steady state takes approximately twice as long as the transition after the increase of Γ .

The cause for the difference in character between transients from an increase and decrease of Γ lies in the strength of the distributed sources after the step change. Distributed heating and cooling of the horizontal boundaries results in convection from the boundaries, which causes mixing in the bulk and suppresses the formation of additional layers from the plumes. The mixing of fluid in the bulk also impacts the time scale of the transition. Hence, we presume that the observed different characters of the transients are not associated with an increase versus a decrease of Γ , but with the size of the distributed source strength F_d^B after the step change, which is finite after the increase and zero after the decrease of Γ .

In this regard, we note that the buoyancy flux ratio Γ of the distributed to the localised source strength may not be a suitable parametrisation of the boundary conditions for transient states. Localised and distributed sources promote different dynamics and we presume that their impact on the transients is associated with different time scales, although we could not distinguish the temporal effect of the two source types in the system’s response. Hence, it may be necessary to account for the localised and the distributed source strength separately, instead of in terms of a buoyancy flux ratio Γ , when considering their effect on the transient state. To investigate the effect of unsteady localised and distributed sources further, it may be useful to consider transient states from localised and distributed sources that are varied independently of each other. In this case, the buoyancy fluxes cannot satisfy $F_\ell + F_d = 1$ at all times and the boundary conditions are described by two independent parameters, F_ℓ and F_d , instead of a by single parameter Γ .

Spatially dependent processes play a more prominent role in the transient states than in steady states, as changes of buoyancy in the fluid propagating across the domain can cause delays in the response of the system. In this context, we observe that the response of the volume flux of the global circulation to a step change of Γ consists of an immediate increase or decrease, followed by a reversal of

the previous behaviour which persists until the volume flux reaches its ‘final’ steady state value. The short-term response of the volume flux results from the plumes, whose source strength has undergone a step change, while the ambient fluid of the plumes is yet unchanged. The opposite trend of the long-term response sets in when the change of the buoyancy of fluid in the bulk has reached the ambient of the plumes and thereby affects the relative buoyancy of fluid parcels in the plumes.

In modelling the transient buoyancy field, we find that a stratification in two homogeneous layers at all times can serve as an approximation of the observed transient states both for a step increase and decrease of Γ . For a finite buoyancy flux Γ^B after the step change (increase of Γ), a two-layer stratification agrees with the observed transient. For $\Gamma^B = 0$ (decrease of Γ), the step change results in the formation of an additional hot and cold layer, however, the large initial depth of the newly formed layers relative to the layer depth of the previous stratification results in a transient stratification that is dominated by two layers. As an alternative to the transient two-layer models, we considered models that allow for the formation of a pair of additional homogeneous layers with the step change of Γ . Based on the DNS simulations performed in this chapter, we cannot state whether either of the two model types should generally be favoured to represent a transient buoyancy field produced by unsteady combined localised and distributed sources. However, our results suggest that transient two-layer models may be preferable if a characteristic buoyancy difference Δb of the stratification is of interest. The prediction of Δb is not improved by accounting for the formation of additional layers and modelling the transient as a four-layer stratification introduces more complexity, since such a model becomes invalid when a part of the stratification is destroyed by distributed heating or cooling.

Modelling the transient buoyancy field as a stratification of homogeneous layers, we neglect the horizontal buoyancy gradient in the layers already observed in the steady state (chapter 2). This simplification compromises the scaling of the transition time with Γ^B , since the modelled time scale is determined by the steady state volume flux at Γ^B , which is in conflict with observation (see §2.7.3). Behaviours that depend on the propagation of fluid parcels across the domain, such as the non-monotonic response of the transient volume flux, can therefore not be reproduced by a model of two homogeneous layers. However, neglecting the lateral buoyancy gradient significantly simplifies the model, since the inclusion of the gradient along the lines of chapter 2 results in a non-linear partial differential equation.

The configurations considered in this chapter are symmetric in the sense that the localised and distributed buoyancy fluxes on the top and bottom boundary are equal. Allowing for different buoyancy fluxes on the top and bottom boundary, we expect more complex behaviour in the transient state. Notably, the interface between the layers, which mainly changes in inclination for symmetric configurations, would be able to vary in elevation for asymmetric changes of the boundary conditions, corresponding to layers of changing depth.

In an asymmetric configuration, during a transition between an initial and final steady state with a stably stratified buoyancy field, the transient buoyancy field might not be stably stratified at all times. Asymmetric boundary conditions that allow for a steady state can be parametrised by the buoyancy flux ratios Γ_1 and Γ_2 of the bottom and top boundary, respectively, and the total buoyancy flux F on the top or bottom boundary, which is equal on both. If we were to approximate a step change of the boundary conditions in a symmetric configuration ($\Gamma = \Gamma_1 = \Gamma_2$) as an error function, we would find that the buoyancy flux ratio satisfies $\Gamma < 1$ at all times of the transition (thick black line in fig. 3.22), provided the initial and final steady state are stably stratified ($\Gamma^A, \Gamma^B < 1$). Thus, at all times of

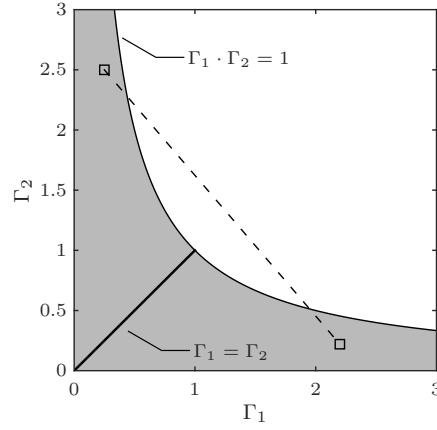


Figure 3.22: Condition for the stability of a steady state as predicted by the steady state models 1 and 2 (see §2.8). The buoyancy fluxes on the boundary can be parametrised by the buoyancy flux ratios $\Gamma_1 = F_{d1}/F_{\ell 1}$ and $\Gamma_2 = F_{d2}/F_{\ell 2}$ of the bottom and top boundary, respectively, and the total buoyancy flux $F = F_{\ell 1} + F_{d1} = F_{\ell 2} + F_{d2}$ on the top or bottom boundary. Configurations that lead to a stable stratification ($\Gamma_1 \cdot \Gamma_2 < 1$) are shaded grey, with cases where the buoyancy fluxes on the top and bottom are equal ($\Gamma_1 = \Gamma_2$) marked as a thick black line. The dashed line marks an example transition of Γ_1 and Γ_2 in the shape of an error function between two stable stratifications (square markers).

the transient the instantaneous value of Γ would allow for a stably stratified steady state. Indeed, we observe a stable stratification at all times in the two step changes of this type studied in this chapter.

In contrast, we can construct asymmetric changes of the boundary conditions that follow an error function, where the initial and final steady state correspond to a stable stratification (square markers in fig. 3.22), but Γ does not satisfy $\Gamma < 1$ at all times (dashed line in fig. 3.22). Such transients might display a breakdown of the stratification before re-establishing a stable stratification. However, the stability condition illustrated in fig. 3.22 is a condition for the steady state and we cannot necessarily use it to predict whether the two-layer stratification breaks down in the transient.

Chapter 4

Parameter estimation

4.1 Introduction

In the previous chapters, we examined the forward problem of the buoyancy field and flow arising from a combination of localised and distributed sources of buoyancy flux. In this chapter, we examine the reverse, or inverse problem, to the forward problem of chapter 2: we aim to determine the buoyancy fluxes on the boundary from a given buoyancy field in the steady state.

In building applications, simplified models of heat transport are commonly used for parameter estimation, since they are less computationally expensive than complex models and more reliable in their parameter estimate [54]. A commonly used type of physics-based simplified model are (multi-) zone models, where the physical properties of each zone, such as its temperature, are assumed to be homogeneous [7]. In this context, the simple buoyancy field models established in §2.6 are reasonable candidates for solving an inverse problem in a configuration of mixed localised and distributed heating and cooling and we base the parameter estimation in this chapter on said models.

We aim to utilise the DNS data of the steady states presented in chapter 2 as measurement data in the inverse problem. However, parameter estimation is typically based on a limited set of measurements, due to spatial and cost constraints on the placement of sensors. Hence, we will sample the buoyancy field at a discrete number of points. The aim of this chapter is to reconstruct the buoyancy fluxes on the boundary from samples of the DNS data of the buoyancy fields, utilising a simple two-layer stratification model.

In the present chapter, we approach the reconstruction of boundary buoyancy fluxes as follows. Section §4.2 serves as a background for our choice of numerical optimisation method and inverse model, giving a brief overview of numerical optimisation and considering the steady state models of chapter 2 in an inverse problem setting. Subsequently, we split the problem of reconstructing boundary buoyancy fluxes into two parts: the assignment of a buoyancy measurement to a layer of a distinct two-layer stratification and the estimation of boundary buoyancy fluxes from these measurements. The layer assignment of buoyancy measurements is the subject of §4.3, where we utilise k -means clustering. In §4.4, we give details of the parameter estimation and present the resulting estimates of the boundary buoyancy fluxes in §4.5. Conclusions on the contents of this chapter are drawn in §4.6.

Generally, our focus in the current chapter is on the feasibility of parameter estimation in configurations of combined localised and distributed buoyancy sources from simple models in connection

with properties of the models, rather than on the methodology of solving inverse problems. Hence, we chose to examine a time-independent problem in a low-dimensional parameter space and prioritise simplicity of approach over performance in our optimisation approach.

4.2 Pre-considerations to phrasing the inverse problem

Inverse problems can pose a variety of challenges, depending on the formulation of the problem, in particular the model used, and the methodology used to solve the problem. In this section, we examine such potential difficulties in order to enable us to phrase a simple inverse problem that can be solved with conceptually simple methods. First, we will give a brief introduction to concepts of numerical optimisation, in particular with respect to the challenges of optimisation that occur depending on characteristics of the optimisation problem. Subsequently, we examine the models introduced in chapter 2 analytically to determine their behaviour in an inverse problem setting.

4.2.1 Concepts of numerical optimisation

The problem of parameter estimation is an optimisation problem: we aim to determine the parameters $\boldsymbol{\xi}$ of a model such that the corresponding modelled state $\boldsymbol{\phi}(\boldsymbol{\xi})$ most closely resembles a given measured state $\tilde{\boldsymbol{\phi}}$ of a system. This is commonly phrased as a least-square problem, where we minimize a cost functional

$$\mathcal{J}(\boldsymbol{\xi}, \{\tilde{\boldsymbol{\phi}}_i\}) = \underbrace{\frac{1}{2} \sum_i \left\| \tilde{\boldsymbol{\phi}}_i - \boldsymbol{\phi}_i(\boldsymbol{\xi}) \right\|^2}_{\text{difference between model and measurement}} + \underbrace{\mathcal{J}_{\text{reg}}(\boldsymbol{\xi})}_{\text{regularization}} \quad , \quad (4.1)$$

which describes the discrepancy between the modelled and the measured state and may contain penalty or regularization terms $\mathcal{J}_{\text{reg}}$ to enforce requirements on the parameters. The operator $\|\cdot\|$ corresponds to the ℓ^2 -norm and the quantities $\boldsymbol{\phi}$ and $\boldsymbol{\xi}$ are vectors. Generally, the system state is described by a set of physical quantities, which we encapsulate as components of the vector $\boldsymbol{\phi}$, and the model depends on a set of parameters contained in $\boldsymbol{\xi}$. In the case of the models used in this chapter, the parameters $\boldsymbol{\xi}$ of the model are control parameters of the system with a clear physical meaning, such as the buoyancy fluxes on the boundaries. Hence, we can evaluate the results $\boldsymbol{\xi}$ of a parameter estimation by comparing them to the corresponding true parameter values $\tilde{\boldsymbol{\xi}}$ of the system causing the system state. Throughout this chapter, we will denote quantities of the observed system, i.e., measured states or true parameter values, with an overset tilde, $\tilde{\cdot}$. In estimating the parameters, our information on the system state is typically limited to a finite set of N_s measurements, $\{\tilde{\boldsymbol{\phi}}_i | i = 1, \dots, N_s\}$, which are summed over in (4.1). The set of measurements corresponds to the value of the state variable taken at a set $\{\mathbf{x}_i | i = 1, \dots, N_s\}$ of spatial measurement points or sampling points.

Minimizing a cost functional can pose a variety of challenges and the approach taken for minimization depends on the properties of the cost functional. Critical properties of the cost functional are for example the character of its curvature, i.e., whether it is convex or non-convex, its smoothness and how it scales with respect to changes of the different parameters. All of these criteria come into play for the inverse problem considered in this chapter and we will here briefly touch upon the issues they raise.

Most optimisation algorithms are only able to find local minima of the cost functional, which do

```

1 Choose a set of initial parameters  $\xi$ 
2 repeat
3   Calculate the gradient  $\frac{\partial \mathcal{J}}{\partial \xi}$  of the cost functional (4.1) with respect to the parameters
   (implicitly calculating the modelled system state  $\phi(\xi)$ )
4   Determine a step length  $k$ 
5   Update the parameter values:  $\xi = \xi - k \frac{\partial \mathcal{J}}{\partial \xi}$ 
6 until the gradient of the cost functional satisfies  $\left\| \frac{\partial \mathcal{J}}{\partial \xi} \right\| \leq \varepsilon_{\mathcal{J}}$ 

```

Algorithm 1: Pseudocode of the method of steepest descent to minimize a cost functional (4.1) with respect to the parameters ξ .

not necessarily correspond to the global minimum of $\mathcal{J}$ [80]. This does not pose a problem for convex cost functionals, since local minima are also global minima in this case. However, a solution found by such an algorithm for a non-convex cost functional may not correspond to its global minimum. Non-smooth cost functionals are difficult to minimize, because, in numerical optimisation, we do not have information on the entire cost functional available but use local information about $\mathcal{J}$ to infer its behaviour at neighbouring points. Such predictions are not possible at all points, if $\mathcal{J}$ contains a discontinuity and stochastic methods are required in these cases. In contrast to deterministic optimisation methods, stochastic algorithms employ random variables to determine the next iteration step towards the minimum. Lastly, the scaling of the cost functional with different parameters can be problematic if the cost functional is much more sensitive with respect to changes in one direction of the parameter space than with respect to another direction [80]. This can cause the optimisation algorithm to terminate prematurely [96], although there are optimisation algorithms that are unaffected by poor scaling [80].

A common optimisation algorithm for determining a local minimum is the method of steepest descent (alg. 1). In each iteration, this algorithm chooses a new parameter value by taking a step in the opposite direction of the gradient of the cost functional with respect to the parameters, $\frac{\partial \mathcal{J}}{\partial \xi}$. There exist several approaches to determine the step length k (alg. 1, l. 4): if k is too large, the algorithm will not converge, if it is too small, convergence may be extremely slow [80]. Commonly, the algorithm is terminated if the norm of the cost functional's gradient falls below a given tolerance $\varepsilon_{\mathcal{J}}$ (alg. 1, l. 6). Although the gradient descent method can be very slow for difficult problems, it is a globally convergent algorithm, that is, the norm of the gradient of the cost functional always converges to zero, independent of the starting point.

4.2.2 Inverting model 1 and 2

In this section, we examine the steady state models 1 and 2 introduced in chapter 2 with regard to their suitability to be used in the formulation of the inverse problem of determining buoyancy fluxes on the boundary from measurements of the buoyancy field. In this context, we consider the curvature of the models with respect to the buoyancy fluxes on the boundary, whether their inversion would result in an ill-posed problem and the implications on the number and position of measurement points required. As we focus on properties of the models, we consider the inverse problem under the assumption that the measured buoyancies are ideal, i.e., that the measured state is generated by the respective model.

Inverse problems are typically ill-posed in the sense of Hadamard [42]: a solution may not exist, may not be unique or may be unstable, due to its high sensitivity with respect to errors in the measurements of the considered state. To solve an inverse problem, it generally needs to be reformulated as a well-posed problem by including additional information, usually via a regularisation method [83]. However, if only a small number of constant parameters are to be estimated, the solution of the inverse problem can be stable [83].

In chapters 2 and 3, we utilised the models to obtain characteristic values of the buoyancy field, in particular the difference Δb between the peaks of the buoyancy field's PDF and the position z_1 of the interface between the two layers. In contrast, to estimate the boundary buoyancy fluxes from buoyancy measurements, we need to consider the entire modelled buoyancy field in the current chapter. Moreover, we consider the generalised models introduced in §2.8, since the boundary buoyancy fluxes behind a given measured buoyancy are unknown in an inverse problem setting. In the generalised model, the thermal boundary conditions determining a steady state can be expressed by three parameters: the ratio Γ_1 of the distributed to the localised buoyancy flux on the bottom boundary, the equivalent ratio Γ_2 of buoyancy fluxes on the top boundary and the total buoyancy flux F on each horizontal boundary, which is equal on the top and bottom boundary in the steady state (see §2.8).

As in the previous chapters, all quantities are non-dimensional, normalised with the height H of the domain and a characteristic buoyancy flux $\hat{F}$ (see §2.4). In the previous chapters, $\hat{F}$ was chosen as the total buoyancy flux on the boundaries, such that $F = 1$. However, in an inverse problem setting, the total buoyancy flux on the boundaries is generally unknown and we cannot assume $F = 1$ to hold. Hence, F appears explicitly in this chapter.

Model 1

In model 1, the buoyancy field generated by localised and distributed heating is assumed to consist of a lower and upper layer of homogeneous buoyancy, b_{a1} and b_{a2} , respectively, separated by a horizontal interface at elevation z_1 . It is convenient to describe the modelled buoyancy values of the layers via the buoyancy difference $\delta b = b_{a2} - b_{a1}$ between the layers and the sum $\Sigma b = b_{a2} + b_{a1}$ of buoyancies of both layers (cf. §2.8). The modelled buoyancy field described by δb , Σb and z_1 is determined by the buoyancy flux ratios Γ_1 and Γ_2 , the total buoyancy flux F on the boundaries and the volume integrated buoyancy B over the entire domain, excluding the plumes (cf. §2.8):

$$z_1 = \frac{1}{2} \frac{(1 + \Gamma_1)^{\frac{1}{3}} - (1 + \Gamma_2)^{\frac{1}{3}}}{(1 + \Gamma_1)^{\frac{1}{3}} + (1 + \Gamma_2)^{\frac{1}{3}}}, \quad (4.2a)$$

$$\delta b = \frac{F^{\frac{2}{3}}}{\alpha^{\frac{2}{3}}} \left[(1 + \Gamma_1)^{\frac{1}{3}} + (1 + \Gamma_2)^{\frac{1}{3}} \right] \frac{1 - \Gamma_1 \Gamma_2}{(1 + \Gamma_1)(1 + \Gamma_2)}, \quad (4.2b)$$

$$\Sigma b = \frac{F^{\frac{2}{3}}}{\alpha^{\frac{2}{3}}} \left[(1 + \Gamma_1)^{\frac{1}{3}} - (1 + \Gamma_2)^{\frac{1}{3}} \right] \frac{1 - \Gamma_1 \Gamma_2}{(1 + \Gamma_1)(1 + \Gamma_2)} + \frac{2B}{\Lambda}. \quad (4.2c)$$

It might appear counter-intuitive that a buoyancy value B appears as a parameter determining the buoyancy field. However, the buoyancy sum Σb is not determined by the buoyancy fluxes (cf. §2.8) and the volume integrated buoyancy B is an unknown quantity in the context of parameter estimation, where our information on the buoyancy field is limited to a (sparse) set of buoyancy measurements.

The state variables δb , Σb and z_1 in (4.2) are constants for a given set of parameters Γ_1 , Γ_2 , F and B . A set of four parameters cannot be determined from a set of three constant state variables,

i.e., a state described by model 1 is not unique to the set of parameters and the inverse problem is generally ill-posed. A problem may become well-posed if additional information is included, e.g. if we assume certain parameters or their relationship to each other as given. However, the problem cannot necessarily be made well-posed by reducing the number of free parameters to three. For example, in the symmetric case, $\Gamma \equiv \Gamma_1 = \Gamma_2$, the governing equations (4.2) become

$$z_1 = 0, \quad \delta b = 4 \frac{F^{\frac{2}{3}}}{\alpha^{\frac{2}{3}}} \frac{1 - \Gamma}{(1 + \Gamma)^{\frac{2}{3}}}, \quad \Sigma b = \frac{2B}{\Lambda}, \quad (4.3)$$

such that there exist three free parameters but only two independent state variables, δb and Σb .

In cases where model 1 results in a well-posed inverse problem and can be utilised in a parameter estimation, at what spatial positions should buoyancy measurements be taken? Generally, we require sampling points in both layers to estimate the parameters. This holds true for any model of stratified buoyancy fields, since to obtain information on the stratification, measurements in all layers are necessary. Hence, measurement points should be distributed vertically over the full height of the domain. Additionally distributing the measurement points in the horizontal has no effect on the capacity of model 1 to yield information on the parameters, since the state variables are modelled as constants in x . In practice, where the measured buoyancy field does not conform to the shape predicted by model 1, horizontally distributed points are practical for statistical accuracy.

Model 2

In model 2, the buoyancy in the layers is modelled with a horizontal gradient, such that the state variables δb , Σb and z_1 in the steady state depend on the parameters Γ_1 , Γ_2 , F , B and the horizontal position x (see §2.8.2):

$$z_1(x) = -\frac{1}{2} \left(\frac{1 - \frac{2x}{\Lambda}}{1 + \Gamma_1} + \frac{1 + \frac{2x}{\Lambda}}{1 + \Gamma_2} \right)^{-1} \left[\frac{1 + \frac{2x}{\Lambda} \Gamma_1}{1 + \Gamma_1} - \frac{1 - \frac{2x}{\Lambda} \Gamma_2}{1 + \Gamma_2} + 2 \frac{(1 + \Gamma_1)^{\frac{2}{3}} - (1 + \Gamma_2)^{\frac{2}{3}}}{(1 + \Gamma_1)^{\frac{2}{3}} + (1 + \Gamma_2)^{\frac{2}{3}}} \right], \quad (4.4a)$$

$$\delta b(x) = \frac{F^{\frac{2}{3}}}{2\alpha^{\frac{2}{3}}} \left(\frac{1}{(1 + \Gamma_1)^{\frac{2}{3}}} + \frac{1}{(1 + \Gamma_2)^{\frac{2}{3}}} \right) \left(\frac{1 + \frac{2x}{\Lambda} \Gamma_1}{1 + \Gamma_1} + \frac{1 - \frac{2x}{\Lambda} \Gamma_2}{1 + \Gamma_2} \right), \quad (4.4b)$$

$$\begin{aligned} \Sigma b(x) = -\frac{F^{\frac{2}{3}}}{2\alpha^{\frac{2}{3}}} \left[\left(\frac{1}{(1 + \Gamma_1)^{\frac{2}{3}}} + \frac{1}{(1 + \Gamma_2)^{\frac{2}{3}}} \right) \left(\frac{1 + \frac{2x}{\Lambda} \Gamma_1}{1 + \Gamma_1} - \frac{1 - \frac{2x}{\Lambda} \Gamma_2}{1 + \Gamma_2} \right) \right. \\ \left. - 2 \left(\frac{1}{(1 + \Gamma_1)^{\frac{2}{3}}} - \frac{1}{(1 + \Gamma_2)^{\frac{2}{3}}} \right) \right] + \frac{2B}{\Lambda}. \end{aligned} \quad (4.4c)$$

If, for parameter estimation, we rely on measurements at a single horizontal position x , we face the same problem as for model 1, i.e., the four parameters cannot be determined from three values of state variables. However, the state variables in model 2 differ from those in model 1 in their dependence on the horizontal position x . Hence, we may determine the parameters by utilising the gradients of the state variables, i.e., we require measurements at at least two positions x in the horizontal.

Indeed, an analytical inversion of (4.4) is possible in terms of δb and Σb and their respective gradients in x

$$\begin{aligned} \Gamma_1 &= \Gamma_1(x, \delta b, \partial_x \delta b, \partial_x \Sigma b), & F &= F(x, \delta b, \partial_x \delta b, \partial_x \Sigma b), \\ \Gamma_2 &= \Gamma_2(x, \delta b, \partial_x \delta b, \partial_x \Sigma b), & B &= B(x, \delta b, \partial_x \delta b, \Sigma b, \partial_x \Sigma b). \end{aligned} \quad (4.5)$$

Generally, an analytical inversion is not possible to solve an inverse problem and we will not employ the analytical inversion of model 2 to estimate the parameters Γ_1 , Γ_2 , F and B . However, (4.5) serves to demonstrate that the buoyancy values and horizontal gradients of model 2 at a position x are a bijective function of the parameters Γ_1 , Γ_2 , F and B . Hence, the inverse problem of estimating Γ_1 , Γ_2 , F and B from measurements of the buoyancy field $(x, \delta b, \Sigma b, \partial_x \delta b, \partial_x \Sigma b)$ is well-posed if the solution of the inverse problem is stable with respect to measurements of the buoyancy field. With regard to the curvature of (4.4), we cannot prove that δb and Σb in (4.4) are convex with respect to the parameters Γ_1 , Γ_2 , F and B and we have to assume that the equations are non-convex.

The expression (4.5) shows that the modelled buoyancies of the upper and lower layer are sufficient to obtain all parameters determining the state, without the exact interface height z_1 being required. It is preferable not to rely on z_1 , since determining the position of the interface from measurements at a single position in the horizontal would require a large number of measurement points in the vertical. If we utilise only δb and Σb to determine the parameters, we require at least four measurement points, provided there are two points in each layer and the points in the same layer are placed at different positions in x . Note, that while the interface height does not need to be known exactly in this case, information on the interface position is not redundant: as we model the buoyancies of different layers as separate state variables, a measured buoyancy needs to be assigned to either the upper or lower layer.

Model 2, in contrast to model 1, may result in a well-posed inverse problem for determining the parameters Γ_1 , Γ_2 , F and B from the buoyancy field. Hence, we choose to employ model 2 for the parameter estimation attempted in this chapter. In the following, all references to modelled buoyancies refer to model 2.

4.3 Assigning buoyancy layers

We choose to assign measured buoyancy values to the upper or lower buoyancy layer of a two-layer stratification model prior to the parameter estimation, due to challenges associated with the piecewise defined buoyancy model. We realize the layer assignment via a clustering algorithm and evaluate the assignment by comparison with a layer definition based on considerations of the steady state in chapter 2. The results of the layer assignment are given in §4.3.5.

4.3.1 Parameter estimation with a piecewise defined model

In the current chapter, we aim to estimate the thermal boundary conditions of the simulated enclosure from DNS data of the buoyancy field. In particular, we base the parameter estimation on a set of samples of the buoyancy field

$$\{\tilde{b}(x_i, y_i, z_i) \mid i \in \{1, \dots, N_s\}\}, \quad (4.6)$$

that corresponds to a set of buoyancy measurements at a number of N_s spatial positions. In an inverse problem setting, we typically work with a limited set of measurements, i.e., the sample size N_s is such that we do not have information about the entire buoyancy field.

As discussed in §4.2.1, the parameters are estimated by comparing a measured quantity to its model equivalent and minimizing a cost functional that quantifies the difference between model and measurement. We chose the generalised model 2 of §2.8 to represent the stratified steady state buoyancy

in the bulk of the enclosure. The model describes the buoyancy field as a piecewise defined function

$$b_a(x, z) = \begin{cases} b_{a1}(x) & \text{for } z < z_I(x), \\ b_{a2}(x) & \text{for } z \geq z_I(x), \end{cases} \quad (4.7)$$

which consists of a lower layer 1 at buoyancy b_{a1} and an upper layer 2 at buoyancy b_{a2} , separated by an interface at elevation z_I (model 1 likewise corresponds to a piecewise defined function).

Parameter estimation in the case considered here involves a comparison of the expressions (4.6) and (4.7). Thus, we aim for a parameter estimation from measurement values $\tilde{b}(x_i, y_i, z_i)$ that do not directly correspond to the state variables (z_I, b_{a1}, b_{a2}) of the models. The elevation of the interface z_I is not readily available from a (sparse) set of buoyancy measurements and assigning a measured buoyancy to layer 1 (b_{a1}) or 2 (b_{a2}) is non-trivial.

This problem can be solved by setting the elevation z_I of the interface dynamically as part of the minimization of the cost functional. Let us consider the cost functional $\mathcal{J}$ corresponding to such an approach (disregarding any regularisation terms, cf. (4.1)):

$$\mathcal{J}(\boldsymbol{\xi}, \{\tilde{b}(x_i, y_i, z_i)\}) = \frac{1}{2} \left\{ \sum_{k=1}^2 \sum_{i \in \Omega_k} [\tilde{b}(x_i, y_i, z_i) - b_{ak}(x_i, \boldsymbol{\xi})]^2 \right\}, \quad (4.8)$$

$$\text{with } i \in \{1, \dots, N_s\}, \quad (4.9)$$

$$i \in \Omega_1 \text{ for } z_i < z_I(x_i, \boldsymbol{\xi}), \quad (4.10)$$

$$i \in \Omega_2 \text{ for } z_i \geq z_I(x_i, \boldsymbol{\xi}). \quad (4.11)$$

As in (4.1), the parameters to be estimated are condensed in a vector $\boldsymbol{\xi}$; the parameters contain information on the boundary buoyancy fluxes and the volume integrated buoyancy that determine the modelled buoyancy field (see §4.2.2), but we do not specify their definition here. The sets Ω_1 and Ω_2 contain the indices of the buoyancy samples that belong to the lower layer (layer 1) or upper layer (layer 2), respectively. A sample i is assigned to layer 1 or 2 depending on the elevation z_i at which the buoyancy field was sampled relative to the parameter-dependent modelled interface height z_I . Since the parameters $\boldsymbol{\xi}$ can change with every iteration step of the optimization, so can the interface height. Depending on which layer a buoyancy sample $\tilde{b}(x_i, y_i, z_i)$ is assigned, the difference between measurement and model is expressed as a difference to the modelled buoyancy b_{a1} of the lower layer or the modelled buoyancy b_{a2} of the upper layer.

The modelled buoyancy field (4.7) contains a discontinuity at the position of the interface $z = z_I$. From (4.8), it is apparent that the cost functional inherits this discontinuity: $\mathcal{J}$ is discontinuous in the parameter space $\boldsymbol{\xi}$. Discontinuities occur whenever a change in $\boldsymbol{\xi}$ causes at least one sampling point (x_i, y_i, z_i) to be assigned to a different buoyancy layer than before the change in $\boldsymbol{\xi}$.

A discontinuous cost functional cannot generally be minimized with a deterministic optimisation method but typically requires stochastic methods. However, stochastic methods tend to be less accurate and more computationally expensive than deterministic methods [33], in particular, they typically scale poorly with the dimension of the parameter space [35]. Note that the problem of a discontinuous cost functional is not specific to the configuration considered in this thesis but will always occur in parameter estimation for a stratified buoyancy field modelled by a piecewise function, such as in filling box type models.

Let us consider utilising a deterministic method, such as a gradient based approach, to minimize the cost functional in (4.8). The cost functional $\mathcal{J}$ is piecewise continuous for each range of parameter values ξ that causes the set of buoyancy samples to be separated into the same sets Ω_1 and Ω_2 of indices. Hence, if there exist a finite number of N' possibilities to separate the set of buoyancy samples, $\mathcal{J}$ is continuous on the corresponding N' subdomains. The cost functional can then be minimized with a gradient-based approach over the N' piecewise continuous subdomains and the global minimum is found by choosing the smallest of the resulting set of N' minima. However, this approach would be computationally expensive since we need to perform N' minimizations. Instead, we choose a reduced version of the approach described above: we pick *one* separation of the set of samples, and thus one layer assignment for the sampling points, and minimize the single corresponding cost functional. In choosing a layer assignment, we solve the discontinuous part of the optimisation problem separately and retain the conceptual simplicity of a gradient-based approach in the minimisation of the cost functional. How to choose a meaningful layer assignment for the sample points will be addressed in the following section.

4.3.2 Method of layer assignment and evaluation

In §4.3.1, we showed that the cost functional $\mathcal{J}$ that describes the difference between a measured buoyancy field $\tilde{b}$ and a modelled buoyancy field b is discontinuous for the piecewise defined buoyancy fields described by model 1 and 2 (see §2.8 for the models' general definition). To avoid the complications associated with a discontinuous cost function, we chose to make $\mathcal{J}$ continuous by assigning the measured buoyancy values $\tilde{b}_i$ ($i \in \{1, \dots, N_s\}$) to layer 1 or 2 *before* minimizing the cost functional.

In chapter 2, the layers were defined based on our knowledge of the net heat flux $F(z = -\frac{1}{2}) - F(z = \frac{1}{2}) = 0$ and the time- and y -averaged temperature field at all spatial positions (x, z) . However, this information is generally not available in an inverse problem setting, where we aim to infer information about the system's forcing from a limited set of measurements. Instead, we utilise a clustering algorithm to assign samples of the buoyancy field to the upper or lower layer of the two-layer stratification. The details of this approach and the method of evaluating the clustering results are the subject of this section.

Clustering of points with the k -means algorithm

Generally, clustering aims to separate a data set such that each of the resulting subsets (clusters) contains data objects that are similar to each other, while objects in different clusters are dissimilar from each other [118]. The degree of similarity or dissimilarity between data objects or clusters is quantified through a proximity measure.

The types of information considered in clustering are termed features: features for assigning a sample point to a buoyancy layer could be its spatial position (x_i, z_i) and/or the buoyancy value $\tilde{b}(x_i, z_i)$ at the considered spatial position. A data object $\mathbf{s}_i$ is described by a set of d features and can be represented as a d -dimensional vector $\mathbf{s}_i = (s_{i1}, \dots, s_{id})$. In the context of this work, possible definitions of $\mathbf{s}_i$ for layer assignment include $\mathbf{s}_i = (x_i, z_i, \tilde{b}(x_i, z_i))$, where $d = 3$, and $\mathbf{s}_i = \tilde{b}(x_i, z_i)$, where $d = 1$. A common proximity measure to quantify the similarity of two such data objects $\mathbf{s}_i$ and


```

1 Choose an initial partition of the data set into  $k$  clusters  $C_1, \dots, C_k$ 
2 Calculate the cluster centroids  $\mathbf{c}_1, \dots, \mathbf{c}_k$  via (4.14)
3 repeat
4   Assign each data object to the nearest cluster  $C_j$ :
       $\mathbf{s}_i \in C_j$  if  $D(\mathbf{s}_i, \mathbf{c}_j) < D(\mathbf{s}_i, \mathbf{c}_\ell)$ , where  $i \in \{1, \dots, N_s\}$  and  $j \in \{1, \dots, k\} \setminus \{\ell\}$ 
5   Recalculate the cluster centroids  $\mathbf{c}_1, \dots, \mathbf{c}_k$  via (4.14)
6 until all cluster centroids  $\mathbf{c}_i$  remain unchanged

```

Algorithm 2: Pseudocode of the k -means algorithm, where $D(\cdot, \cdot)$ denotes the (weighted) Euclidean distance between two points in feature space (see (4.12), (4.13)).

s_j is the Euclidean distance between both objects in the d -dimensional feature space:

$$D(\mathbf{s}_i, \mathbf{s}_j) = \left[\sum_{\ell=1}^d (s_{i\ell} - s_{j\ell})^2 \right]^{\frac{1}{2}}. \quad (4.12)$$

Since a clustering algorithm aims to find structures in a set of data objects based on the proximity measure, it is apparent from (4.12) that the scale of the values of different features is crucial for the definition of clusters. Hence, it may be necessary to re-scale the data used for clustering by feature in order to find meaningful clusters. This is equivalent to weighting features in the proximity function, e.g. with a Euclidean distance defined as

$$D(\mathbf{s}_i, \mathbf{s}_j) = \left[\sum_{\ell=1}^d c_\ell^2 (s_{i\ell} - s_{j\ell})^2 \right]^{\frac{1}{2}}, \quad (4.13)$$

where c_ℓ represents a weight associated with the ℓ th dimension of the feature space.

To assign sample points to a buoyancy layer, we choose k -means clustering. The k -means algorithm separates a set $\mathcal{S}$ of N_s data objects, $\mathcal{S} = \{\mathbf{s}_i \mid i \in \{1, \dots, N_s\}\}$, into a pre-defined number of k clusters, $C_1, \dots, C_k$, which are characterised by their respective centroid

$$\mathbf{c}_j = \frac{1}{N_{sj}} \sum_{i \mid \mathbf{s}_i \in C_j} \mathbf{s}_i. \quad (4.14)$$

Here, N_{sj} is the number of data objects in cluster C_j . The k -means algorithm seeks a partition of the data set that minimizes the sum-of squared-errors J_e between the data objects of a cluster and the cluster centroid $\mathbf{c}_j$ [118]:

$$J_e = \sum_{j=1}^k \sum_{i \mid \mathbf{s}_i \in C_j} D(\mathbf{s}_i, \mathbf{c}_j)^2. \quad (4.15)$$

This is achieved by an iterative optimization procedure, as outlined in the pseudocode alg. 2. The iterative optimization converges to a local minimum of J_e but cannot guarantee a global minimum, i.e. k -means is sensitive to the initial partition of the data set (alg. 2, l. 1). However, there are strategies to choose the initial clusters such that poor clustering can be avoided.

Since k -means is based on the Euclidean distance, it tends to create hyperspherical clusters in

feature space and thus works well for identifying compact data structures. This emphasizes the need for suitably scaled data if we seek to cluster data objects that are described by more than one feature. Hyperspherical clusters can be separated by linear boundaries, i.e., flat planes in the feature space. Hence, if the feature space includes information on the spatial position of the sampling points, the cost functional of the k -means algorithm includes the requirement of a linear interface between the layers, although the weight of this condition depends on the scaling of the data in the data objects.

We assign sample points to buoyancy layers by employing the k -means implementation of the ‘Statistics and Machine Learning Toolbox’ in Matlab to split a set of N_s samples into $k = 2$ clusters. Calculating the mean buoyancy of each cluster, we classify the samples in the cluster with the lower mean buoyancy as belonging to layer 1 and the samples in the cluster of higher mean buoyancy as belonging to layer 2. Matlab’s k -means implementation mitigates the risk of poor clustering caused by the choice of initial clusters by employing the k -means++ algorithm for initialisation (see [6]).

Measures of clustering evaluation

To evaluate the layer assignment of sampling points detailed in the previous section, we require a definition of the buoyancy layers. For the steady states considered in the present chapter, we can refer

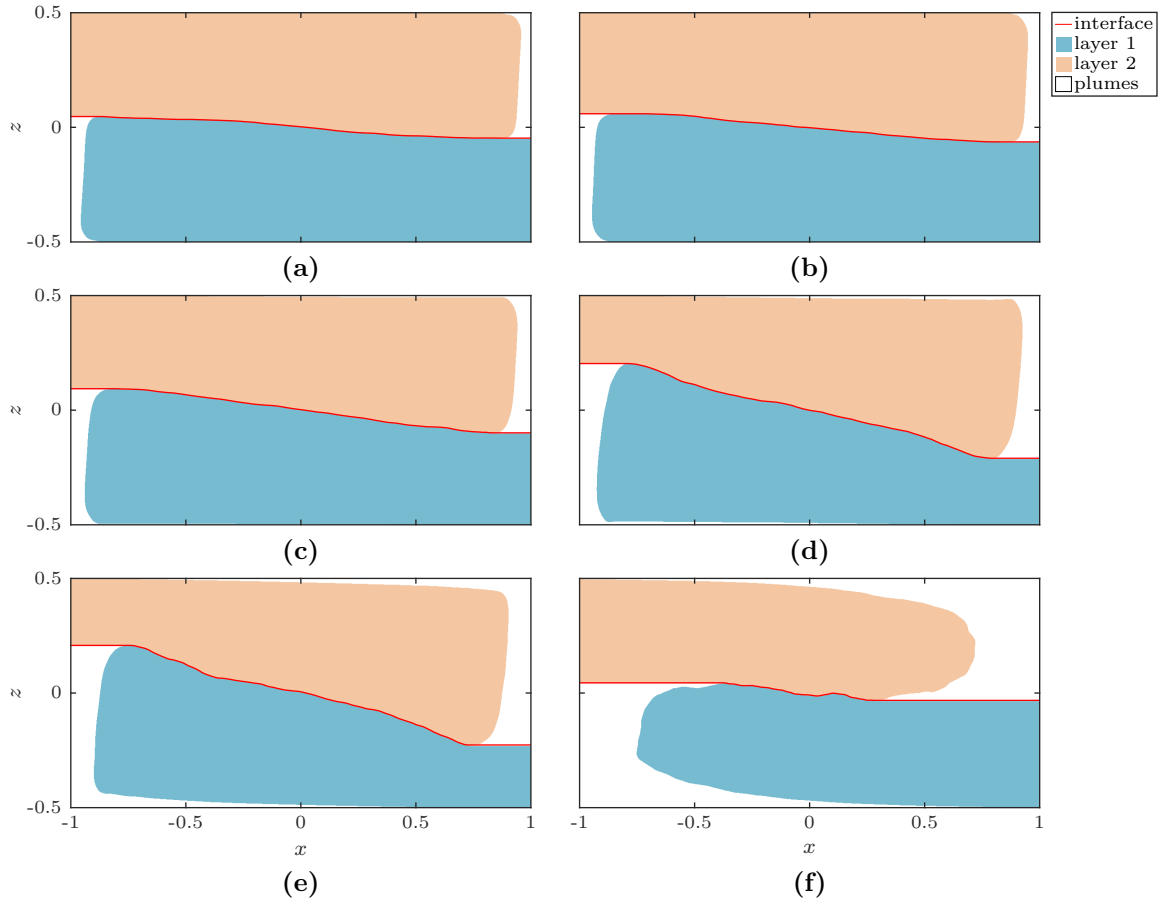


Figure 4.1: Definition of layer 1 and 2 in the steady state for (a) $\Gamma = 0$, (b) $\Gamma = 0.10$, (c) $\Gamma = 0.23$, (d) $\Gamma = 0.39$, (e) $\Gamma = 0.60$ and (f) $\Gamma = 1.29$. The layer definition is based on the values of the t - and y -averaged buoyancy field (cf. §2.5.2) and the interface between the layers (red line) defined in §2.5.3.

to the ‘extended’ interface between layer 1 and 2 as defined in chapter 2, where the interface separating the layers is extended to the horizontal boundaries (red line in fig. 2, cf. appendix B). Additionally, we consider the buoyancy field $\bar{b}$ averaged in time and the spatial y -direction, as defined in chapter 2 (see (2.10)), and require that the left-hand plume and (upper) layer 2 are at an average buoyancy $\bar{b} \geq 0$, while the average buoyancy in the right-hand plume and (lower) layer 2 satisfies $\bar{b} < 0$. The resulting definition of layer 1 and 2 is displayed in fig. 4.1. For further use of the layer definition given here, we define two mask functions m_{a1} and m_{a2} for layer 1 and 2, respectively:

$$m_{aj}(x, z, \Gamma) = \begin{cases} 1 & \text{if } (x, z) \text{ in layer } j, \\ 0 & \text{otherwise.} \end{cases} \quad (4.16)$$

The result of the layer assignment via k -means clustering is a classification of sampling points as belonging to layer 1 or 2. To evaluate the classification, we need to consider the possible outcomes of a prediction made by the classification scheme versus the true class of the considered data (tab. 4.1). Let us consider a point assigned to layer 1 by the classification scheme. The point might have been classified correctly, as it truly belongs to layer 1 (true positive, highlighted red in tab. 4.1). Alternatively, the point might truly be positioned in layer 2 or in one of the plumes, but is classified incorrectly as layer 1 (false positive, highlighted blue in tab. 4.1). Moreover, a point that is truly part of layer 1 might not have been recognized as such by our classification scheme and instead be assigned to layer 2 or, in theory, to one of the plumes (false negative, highlighted pale red in tab. 4.1).

If we classify a set of data points, the number of outcomes that are true positives, false positives or false negatives, N_{tp} , N_{fp} and N_{fn} , respectively, are collectively referred to as priors. Classifications schemes can be evaluated by considering ratios of priors, in particular precision and recall. With respect to the classification of data points to layer 1, precision and recall are defined as

$$\text{precision}_1 = \frac{N_{tp}}{N_{tp} + N_{fp}} \in [0, 1], \quad \text{recall}_1 = \frac{N_{tp}}{N_{tp} + N_{fn}} \in [0, 1]. \quad (4.17)$$

Precision quantifies what proportion of all the points predicted to belong to layer 1 (blue dashed frame in tab. 4.1) is truly positioned in layer 1. Recall answers the question what proportion of points actually positioned in layer 1 (blue dashed frame in tab. 4.1) is correctly classified. A classification scheme with a precision of one *only* classifies data objects as relevant that are truly relevant; if recall equals one, it is able to identify *all* relevant cases within a data set. Hence, high values of both quantities are

Table 4.1: Confusion matrix for assignment of points to layers or plumes. Note that the outcomes in the grey row are not an option for layer assignment based on k -means clustering, where $k = 2$ and the clusters are interpreted as belonging to layer 1 or 2.

		true class		
		layer 1	layer 2	plume 1 or 2
predicted class	layer 1	$\mathcal{C}_{11}$	$\mathcal{C}_{21}$	$\mathcal{C}_{31}$
	layer 2	$\mathcal{C}_{12}$	$\mathcal{C}_{22}$	$\mathcal{C}_{32}$
	plume 1 or 2	$\mathcal{C}_{13} = 0$	$\mathcal{C}_{23} = 0$	$\mathcal{C}_{33} = 0$

Example layer 1:

- N_{tp}
- N_{fn}
- N_{fp}
- belonging to layer 1
- classified as layer 1

desirable.

In the classification problem considered here, there exist three relevant classes: layer 1, layer 2 or neither layer 1 nor 2, which is equivalent to the plumes. The priors for all classes are contained in the 3×3 confusion matrix $\mathcal{C}$ (see tab. 4.1): each element $\mathcal{C}_{ij}$ of the confusion matrix gives the number of data points that truly belong to the class of index i and has been assigned to the class of index j by the classification algorithm. The sum over all elements of the confusion matrix corresponds to the total number of data points. The definition of precision and recall can be generalised in terms of the confusion matrix to

$$\text{precision}_i = \begin{cases} \frac{\mathcal{C}_{ii}}{\sum_{j=1}^3 \mathcal{C}_{ji}} & \text{for } \mathcal{C}_{ii} > 0 \text{ and } \sum_{j=1}^3 \mathcal{C}_{ji} > 0, \\ 1 & \text{otherwise,} \end{cases} \quad (4.18a)$$

$$\text{recall}_i = \begin{cases} \frac{\mathcal{C}_{ii}}{\sum_{j=1}^3 \mathcal{C}_{ij}} & \text{for } \mathcal{C}_{ii} > 0 \text{ and } \sum_{j=1}^3 \mathcal{C}_{ij} > 0, \\ 1 & \text{otherwise,} \end{cases} \quad (4.18b)$$

where $i \in \{1, 2, 3\}$ and $i = 1$ or 2 corresponds to layer 1 or 2, respectively. There exist different approaches to deal with division by zero in precision and recall; the definition given in (4.18) follows the approach used in [110], which is detailed in [93].

Precision and recall are often joined in one classifier, the F_1 -score, which corresponds to their harmonic mean

$$F_{1,i} = 2 \frac{\text{precision}_i \cdot \text{recall}_i}{\text{precision}_i + \text{recall}_i} \in [0, 1]. \quad (4.19)$$

To evaluate the classification to all classes with one measure, we define a weighted-average F_1 -score

$$F_1 = \frac{1}{\sum_{i=1}^3 \sum_{j=1}^3 \mathcal{C}_{ji}} \sum_{i=1}^3 \left[F_{1,i} \cdot \sum_{j=1}^3 \mathcal{C}_{ij} \right], \quad (4.20)$$

where the per-class $F_{1,i}$ -scores are weighted with the number of data points $\sum_{j=1}^3 \mathcal{C}_{ij}$ truly belonging to the corresponding class i . Since the layers account for the majority of the volume in the simulated domain, we emphasize the classification to layer 1 and 2 by employing a weighted-average F_1 -score, as opposed to, for example, considering classification to all three classes as equally important.

For sake of simplicity, we chose a classification method that considers all points as relevant, i.e. either belonging to layer 1 or 2. Hence, the number of points classified as belonging to the plumes is fixed to zero, $\mathcal{C}_{i3} = 0 \forall i$. If there exist any points in the considered data sets that are truly part of the plumes ($\sum_j \mathcal{C}_{3j} > 0$), they will be assigned to one of the layers and decrease precision for classification

Table 4.2: Probability of a sampling point being placed in one of the plumes, $P(p1 \cap p2)$, or in one of the layers, $P(a1 \cap a2)$, for different buoyancy flux ratios Γ on the domain boundaries (see (4.21)).

Γ	0.00	0.10	0.23	0.39	0.60	1.29
$P(a1 \cap a2)$	0.97	0.96	0.94	0.91	0.87	0.75
$P(p1 \cap p2)$	0.03	0.04	0.06	0.09	0.13	0.25

to the respective layer. Thus, the performance of the classification scheme is tied to the probability of a sampling point being placed in the plumes. If the sampling points are placed randomly, this probability $P(p1 \cap p2)$, as well as the probability $P(a1 \cap a2)$ of the complementary case where a sampling point is placed in layer 1 or 2, can be calculated from the area aspect ratio of the regions defined as plumes or layers shown in fig. 4.1

$$P(a1 \cap a2)(\Gamma) = \frac{1}{\Lambda} \int_{-\frac{\Lambda}{2}}^{\frac{\Lambda}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} (m_{a1}(x, z, \Gamma) + m_{a2}(x, z, \Gamma)) dy dt, \quad (4.21a)$$

$$P(p1 \cap p2)(\Gamma) = 1 - P(a1 \cap a2)(\Gamma). \quad (4.21b)$$

The corresponding values for the simulated buoyancy flux ratios Γ are given in tab. 4.2.

4.3.3 Evaluation details

In the following section, we consider the classification of sample points $\mathbf{s}_i$ within a set $\mathcal{S}$ of size N_s .

$$\mathcal{S} = \{\mathbf{s}_i \mid i \in \{1, \dots, N_s\}\}. \quad (4.22)$$

The result of a classification via k -means is an assignment of sample points to layer 1 ($i \in \Omega_1$) or layer 2 ($i \in \Omega_2$), where Ω_1 contains N_{s1} elements and Ω_2 contains N_{s2} elements.

The data of the sample points is based on the DNS data of steady states at buoyancy flux ratios $\Gamma \in \{0, 0.10, 0.23, 0.39, 0.60, 1.29\}$, as presented in chapter 2. In the following section, a buoyancy sample $\tilde{b}_i$ corresponds to the buoyancy field at the position of the sampling points (x_i, z_i) averaged over $T = 10$ dimensionless turnover times (cf. §2.4):

$$\tilde{b}_i = \frac{1}{T} \int_0^T \tilde{b}(t, x_i, y = 0, z_i) dt. \quad (4.23)$$

A DNS buoyancy value averaged over a duration T and over the statistically homogeneous spatial direction y is denoted as $\tilde{\tilde{b}}$ (cf. (2.10)). As in chapter 2, all quantities are non-dimensionalised (see §2.4).

A set $\mathcal{S}$ of samples is generated by evaluating the DNS data at a corresponding set of spatial positions $\{(x_i, y_i, z_i) \mid i \in \{1, \dots, N_s\}\}$, which we refer to as a sampling grid. The positions of the points of the sampling grid determine the values of the samples in $\mathcal{S}$ and thus impact the outcome of the layer assignment and later parameter estimation. There is limited value in considering the *optimal* placement of the points of the sampling grid for the most accurate parameter estimation, since such statements tend to be relative to the investigated unknown stratification. Instead, we evaluate the layer assignment statistically by considering an ensemble of N_e sample sets

$$\{\mathcal{S}_k \mid k \in \{1, \dots, N_e\}\}, \quad (4.24)$$

i.e., we run the layer assignment N_e times for different sets of samples $\mathcal{S}_k$ and evaluate the set of N_e outcomes. The ensemble is generated by varying the positions of the points in the sampling grid, where we consider an ensemble of $N_e = 1000$ different sampling grids. For an ensemble of sampling grids, each entry $\mathcal{C}_{ij}$, $i, j \in \{1, 2, 3\}$, in the confusion matrix corresponds to the number of matching

outcomes from all sample sets $\mathcal{S}_k$, i.e., the entries of the confusion matrix satisfy

$$\sum_{i=1}^3 \sum_{j=1}^3 c_{ji} = N_s \cdot N_e. \quad (4.25)$$

Lastly, we require a set of N_e sampling grids, which should satisfy certain conditions. Note that, since we consider data statistically homogeneous in y , the y -coordinate is neglected in our description of the sampling grid. The buoyancy field in the considered configurations is statistically antisymmetric to the central point $(x, z) = (0, 0)$: $\tilde{b}(x, z) = -\tilde{b}(-x, -z)$ (cf. fig. 2.7). Hence, we require sampling grids that break this symmetry, otherwise, we risk results that are only valid for similarly symmetric data sets. Moreover, all points of the DNS data in the considered domain should be sampled with equal probability by the sampling grid. Hence, we choose sampling ‘grids’ of points randomly distributed in x and z with uniform probability.

An advantage of random sampling grids is their simplicity of description, as they are determined by a single parameter: the number of sample points N_s . In considering parameter estimation, we would like to make a statement about the relationship between the available information, such as N_s , and the thermal boundary conditions we can infer from this information. A sampling grid that is solely dependent on N_s simplifies conclusions with respect to this connection.

4.3.4 Layer assignment results

In this section, we evaluate the performance of the chosen k -means classification scheme for different types of data sets. In particular, we consider different sizes of sampling grids and different feature spaces for clustering.

Sample size N_s

The task of assigning sample points to layers is straightforward if the buoyancy field is known at all points in the considered enclosure. However, in the context of inverse problems we typically aim to establish the boundary conditions to a given state based on limited information of the said state and there is usually a cost associated with an increase of the number of sample points. Thus, key points of interest are the minimal amount of information that enables us to draw conclusions on the boundary conditions and the pay-off in terms of accuracy for an increase of data on the state. To allow us to make a statement about the impact of the available buoyancy information, we consider the outcome of the k -means classification scheme for data sets of different size N_s .

To this end, we consider the clustering of time-averaged buoyancy values $\tilde{b}$, i.e., clustering in a one-dimensional feature-space. Each data set $\mathcal{S}$ to be clustered consists of N_s buoyancy values determined by the position of the spatial sampling points (cf. (4.23))

$$\mathcal{S} = \{\tilde{b}_i \mid i \in \{1, \dots, N_s\}\}. \quad (4.26)$$

For $\Gamma < 1$, it is apparent from the weighted F_1 -score in fig. 4.2 that the k -means classification scheme performs better as the sample size is increased from the minimum value $N_s = 2$ to $N_s \approx 6$. The F_1 -score then stays approximately constant as the sample size is increased further and eventually slightly decreases with N_s from $N_s \approx 11$ onwards. The increase of F_1 with N_s for small sample sizes is

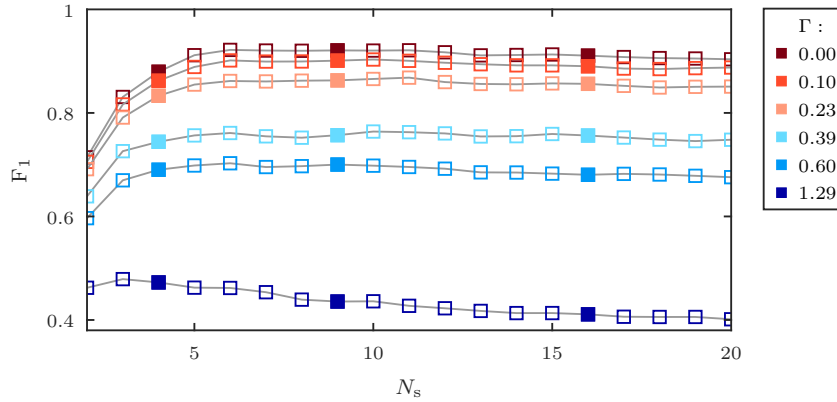


Figure 4.2: The dependence of the F_1 -score on the number N_s of sample points for steady states at different values of the buoyancy flux ratio $\Gamma \in \{0, 0.10, 0.23, 0.39, 0.60, 1.29\}$. The filled squares mark the results corresponding to the values of N_s we picked for further consideration ($N_s \in \{4, 9, 16\}$). Clustering is based on the time-averaged buoyancy values $\tilde{b}_i$ at the sampling points.

intuitive: as the sample size increases, the set of buoyancy values $\{\tilde{b}_i | i \in \{1, \dots, N_s\}\}$ becomes more representative of the buoyancy of the layers and the set become more clearly structured into two main clusters of buoyancy that can be recognized by k -means. We expected F_1 to approach a maximum value smaller than one for increasing N_s : as the k -means classification scheme defined by us cannot assign sample points to the plumes, a perfect classification of any set of sample points is not possible. The behaviour shown in fig. 4.2 approximately satisfies this expectation but for the slight decrease of F_1 with N_s for large sample sizes. This effect might be due to the k -means algorithm's preference for compact clusters, in the sense of clusters that are close to hyperspherical in shape: with larger sample sizes, the probability for the set of sample buoyancy values to represent the full range of the sampled buoyancy field increases and thus buoyancy values belonging to the sample layer are less likely to form compact clusters.

As the buoyancy flux ratio Γ on the boundaries increases, the F_1 -score in fig. 4.2 decreases. This is to be expected, since the buoyancy field within the layers grows more heterogeneous with increasing Γ and the buoyancy difference between the layers decreases (see chapter 2). The gap between the F_1 values for $\Gamma = 0.23$ and 0.39 coincides with the marked decrease of the buoyancy difference between the layers observed in chapter 2 between these two values of the buoyancy flux ratio (see fig. 2.4). The F_1 -score for $\Gamma = 1.29$ differs in its behaviour from the curves at $\Gamma < 1$: the F_1 value significantly lower than for $\Gamma < 1$ and decreases with N_s over nearly the full range of considered sample sizes. This is not surprising, as the buoyancy field at $\Gamma = 1.29$ can no longer be clearly separated into two layers (see chapter 2). It is therefore questionable whether the layer definition shown in fig. 4.1 carries any physical meaning for $\Gamma = 1.29$, so we cannot expect the k -means algorithm to identify clusters that fit this definition.

Prior ratios are a useful tool to compare the performance of a classification scheme for different data sets (or to compare different classification schemes), and we use the F_1 -score here for this purpose. However, a ratio of priors does not intrinsically hold information about the quality of the classification result: what constitutes a 'good' classification crucially depends on the intended purpose to which the classification result will be put. Hence, in evaluating a classification scheme, it is essential to choose an evaluation measure that aligns with the planned application of our classification results.

We aim to estimate the thermal boundary conditions from samples of the buoyancy field. Hence, the key information from the clustered data for our purpose is the buoyancy of the layers. In the following we consider the mean buoyancy of the layers as defined by our k -means classification scheme to appraise the quality of the classification results and ascertain whether the weighted F_1 -score is a suitable evaluation measure.

The mean buoyancy $\mu_{ak}(\tilde{b})$ of layer k , $k \in \{1, 2\}$, as assigned by the k -means classification scheme, is defined as

$$\mu_{ak}(\tilde{b}) = \frac{1}{N_{sk}} \sum_{i \in \Omega_k} \tilde{b}_i. \quad (4.27)$$

To evaluate this mean layer buoyancy, we require reference values. One option is to consider the layer definition shown in fig. 4.1 and to calculate a corresponding ‘true’ mean layer buoyancy by integrating over the buoyancy field of the entire layer

$$\mu_{ak}(\tilde{b}) = \frac{1}{\Lambda} \int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{\Lambda}{2}}^{\frac{\Lambda}{2}} m_{ak}(x, z, \Gamma) \tilde{b}(x, z) dx dz, \quad (4.28)$$

where we employ the time- and y -averaged buoyancy field $\tilde{b}$ (cf.(2.10) in chapter 2) and m_a denotes the mask function for each layer (4.16) displayed in fig. 4.1. However, the reference mean buoyancy of the above expression is based on a much larger data set than the mean buoyancies resulting from the k -means classification scheme. What is the best mean buoyancy value that can be achieved from a grid of N_s sample points? We can answer this question by considering a fictitious ideal classification scheme that assigns every sample point to the correct layer or plume as per our definition. The confusion matrix of such a classification scheme only holds non-zero values on the diagonal (only true positives) and the corresponding mean layer buoyancy can be expressed by

$$\mu_{ak}(\tilde{b}) = \left[\sum_{i=1}^{N_s} m_{ak}(x_i, z_i, \Gamma) \right]^{-1} \sum_{i=1}^{N_s} m_{ak}(x_i, z_i, \Gamma) \tilde{b}_i. \quad (4.29)$$

For comparison of the mean layer buoyancy, we consider the classification results for sampling grids of size $N_s \in \{4, 9, 16\}$ at different values of the buoyancy flux ratio Γ . Fig. 4.3 shows the PDFs of the mean buoyancy of layer 1 and 2 for the k -means classification scheme (solid-coloured PDFs, (4.27)) and an ideal classification scheme (PDF outlines, (4.29)), as well as the ‘true’ mean buoyancy of the layers according to our layer definition (dashed lines, (4.28)). In the plot, the mean buoyancy values $\mu_a(\tilde{b})$ are normalized with one half of the characteristic DNS buoyancy difference $\Delta\tilde{b}$ between the layers, which corresponds to the difference between the peaks of the entire buoyancy field’s PDF (cf. 2.5.1). The values $2\mu_a(\tilde{b})/\Delta\tilde{b} = \pm 1$ thus correspond to the position of the peaks of the buoyancy field’s PDF.

Fig. 4.3 shows that, apart from $\Gamma > 1$, there is generally good agreement between the PDFs resulting from the k -means classification scheme and from an ideal classification scheme. Moreover, the peaks of the PDFs coincide with the ‘true’ mean buoyancy of the layers. Thus, despite the in-built limitation of the k -means classification scheme that samples of the plumes cannot be recognized as such, an improvement of the classification scheme would have only little effect on the resulting mean buoyancies of the layers.

In fig. 4.3, the discrepancy between the ideal and the k -means classification results increases for increasing Γ , as is also reflected in the F_1 -score in fig. 4.2. Indeed, the difference between the PDFs of

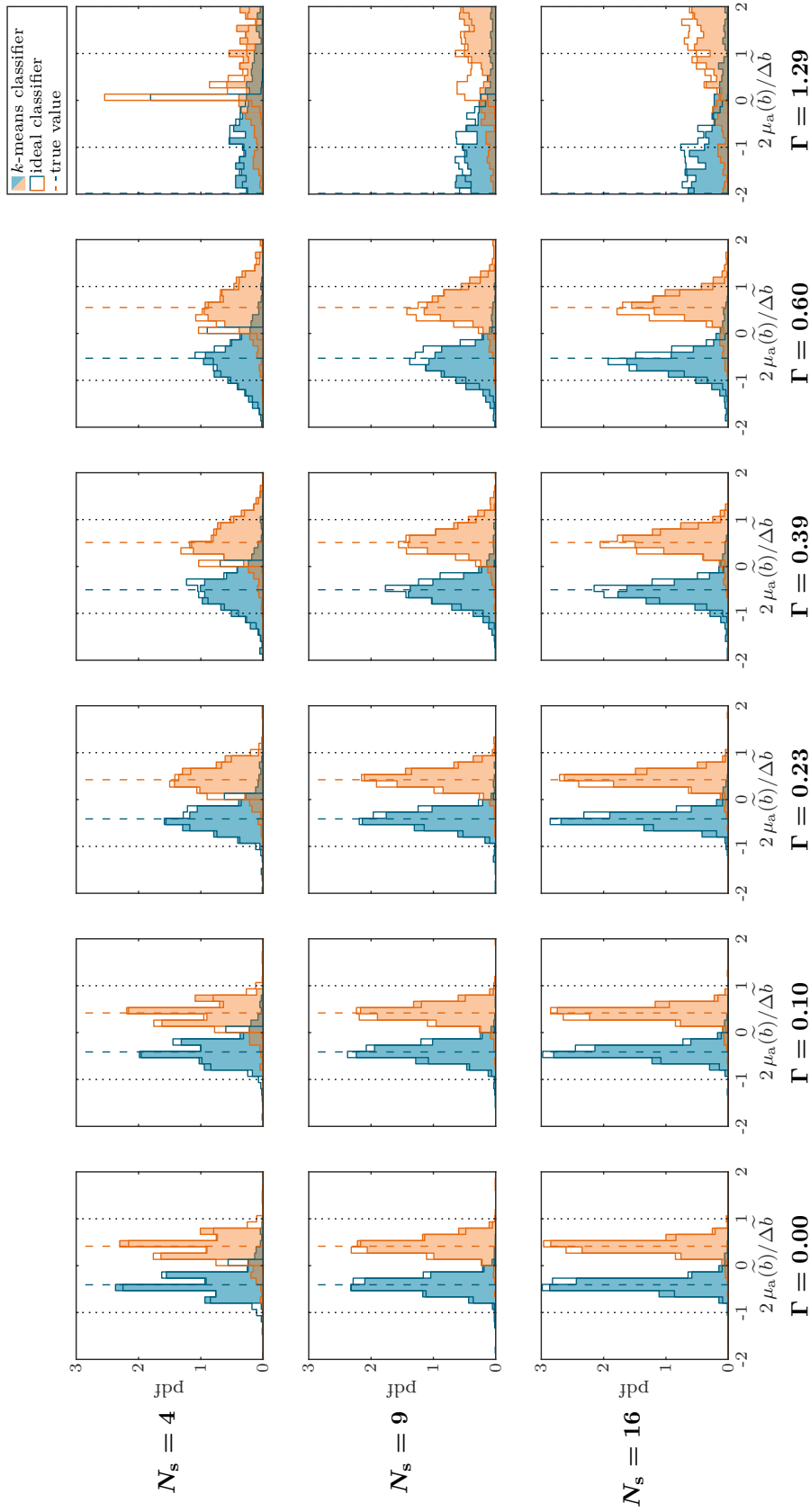


Figure 4.3: PDFs of the mean buoyancy of layer 1 (blue) and layer 2 (red) in the steady state for different numbers of sample points $N_s \in \{4, 9, 16\}$ (rows) and different values of the buoyancy flux ratio $\Gamma \in \{0, 0.10, 0.23, 0.39, 0.60, 1.29\}$ (columns). Displayed are the mean buoyancies for the k -means classification scheme (solid-coloured PDFs), see (4.27), for an ideal classification scheme (PDF outlines), see (4.29) and the true mean buoyancy of the layers according to the layer definition shown in fig. 4.1 (dashed lines), see (4.28).

The mean buoyancy values $\mu_a(\tilde{b})$ of the layers are normalized with one half of the characteristic buoyancy difference $\Delta\tilde{b}$ between the layers, where $\Delta\tilde{b}$ is the difference between the peaks of the entire buoyancy field's PDF (cf. §2.5.1). Clustering is based on the time-averaged buoyancy values at the sampling points.

the ideal and the k -means is closely connected to the F_1 -score and the ideal classification corresponds to a F_1 -score of one. However, the mean layer buoyancies contain information that is not included in the F_1 -score: the PDFs' widths increase with the buoyancy flux ratio Γ and decrease with the sample size N_s . The former behaviour is connected to the increasing heterogeneity of the buoyancy field in the layers with increasing Γ , as was observed in chapter 2. Narrower PDFs for an increasing sample size N_s occur because the sample of buoyancy values becomes more representative of the layers' true buoyancy average with increasing N_s . In particular, the latter is not an effect connected with the performance of the k -means classification scheme but can also be observed in the result of the ideal classifier. A narrower PDF of mean buoyancy values should improve the accuracy of a later parameter estimation. Thus, while we find that $N_s = 9$ and $N_s = 16$ give similar F_1 -values, the character of the corresponding clusters implies that they will not be equally well-suited for parameter estimation.

With respect to the width of the mean layer buoyancy PDFs, it should be noted that the distributions of buoyancy values are only narrower for small Γ if we consider buoyancies normalized with the characteristic buoyancy difference of the layers, $2\mu_a(\tilde{b})/\Delta\tilde{b}$. Since the characteristic buoyancy difference $\Delta\tilde{b}$ is larger at small Γ , the distribution of mean buoyancy values $\mu_a(\tilde{b})$ increases in width with *decreasing* Γ : because the total range of buoyancy values is larger at low values of Γ , the absolute error introduced by the spread of the distribution is larger as well. Thus, large sample sizes N_s might be of particular interest for buoyancy fields with a stratification in layers of vastly different buoyancy values.

It can be seen from fig. 4.3 that the mean buoyancy of the layers as per our definition (dashed lines) does differ significantly from the buoyancy value corresponding to the peaks of the entire buoyancy field's PDFs ($2\mu_a(\tilde{b})/\Delta\tilde{b} = \pm 1$, dotted lines in fig. 4.3). This is partly due to the skewed buoyancy distribution in the layers (see fig. 2.4). Additionally, fluid parcels that envelope the plumes and, in case of distributed heating and cooling, the boundary layers at the top and bottom boundary contribute to the peaks of the PDFs in fig. 2.4 (cf. fig. 3.14c and 3.14d). These fluid parcels are not necessarily included in our definitions of the layers: their position fluctuates with time and is close to the boundary between the sections considered as plumes and as layers in fig. 4.1.

So far, we considered the ability of the k -means classification scheme to correctly assign sample points to their corresponding layer. There is, however, a further point of interest connected to the sample size: to estimate the thermal boundary conditions from a sample of the buoyancy field, we require sample points in *both* layers (cf. §4.2.2). What is the probability for both layers being sampled by a set of sample points of size N_s ? Fig. 4.4(a) shows the probability $P(A)$ for this event 'A', which can be described via the confusion matrix

$$A = \left(\sum_j \mathcal{C}_{1j} > 0 \right) \wedge \left(\sum_j \mathcal{C}_{2j} > 0 \right). \quad (4.30)$$

It can be seen that $P(A)$ increases rapidly with the sample size and is approximately one for $N_s \geq 9$. The value of $P(A)$ is lower for higher buoyancy flux ratios, since the probability for points being placed in the plumes increases with Γ (see tab. 4.2).

For parameter estimation, we not only require both layers to be sampled but also at least one point per layer that is correctly classified by the k -means classification scheme. The probability $P(B)$ for this event

$$B = (\mathcal{C}_{11} > 0) \wedge (\mathcal{C}_{22} > 0) \quad (4.31)$$

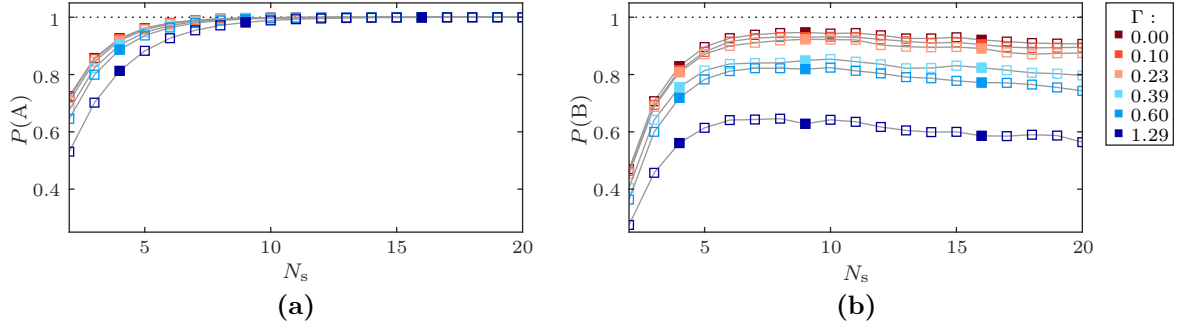


Figure 4.4: Probability for (a) at least one sample point being placed in layer 1 and 2, respectively, (event ‘A’) and (b) at least one sample point in each layer being classified correctly by the k -means classification scheme (event ‘B’). See (4.30) and (4.31) for a formal definition of events A and B, respectively. The filled squares mark the results corresponding to the values of N_s we picked for further consideration ($N_s \in \{4, 9, 16\}$). Clustering is based on the time-averaged buoyancy values $\tilde{b}_i$ at the sampling points for steady states at buoyancy flux ratios $\Gamma \in \{0, 0.10, 0.23, 0.39, 0.60, 1.29\}$.

is shown in fig. 4.4(b). The probability $P(B)$ shows a similar behaviour as the F_1 -score in fig. 4.2 and is at least at a value of ~ 0.7 for $N_s \geq 4$ and $\Gamma < 1$.

The values of the probabilities $P(A)$ and $P(B)$ also justify a posteriori our choice of randomly placed sample points, since we consider the probabilities as sufficiently high to abate any concerns that we might have introduced a significant source of error by our choice of sampling. Note, however, that the issue of not sampling all relevant buoyancy layers is generally not one artificially introduced by placing the sample points randomly. Since the structure of a stratification cannot be known before sampling the buoyancy field, it is always possible that buoyancy layers are not represented in the sample, particularly when the number of relevant layers is unknown.

In the parameter estimation that follows, we restrict our considerations of different sample sizes to $N_s \in \{4, 9, 16\}$.

Feature space

In the previous section, we considered the classification of samples as belonging to layer 1 or 2 purely based on their associated buoyancy value, i.e., by clustering in a one-dimensional feature space. However, the stratification in an enclosure is described by the spatial distribution of buoyancy. Hence, we consider the clustering of datasets

$$\mathcal{S} = \{(x_i, z_i, \tilde{b}_i) \mid i \in \{1, \dots, N_s\}\}, \quad (4.32)$$

where $\tilde{b}_i$ is the buoyancy value corresponding to the sampling point (x_i, z_i) . Results from clustering in this three-dimensional feature space are compared with the clustering of data sets as described by (4.26), corresponding to a one-dimensional feature space.

For a feature space with more than one dimension, the scaling of the features is crucial for the clustering outcome. Since the relative scale of $x \in \{-\frac{\Lambda}{2}, \frac{\Lambda}{2}\}$ to $z \in \{-\frac{1}{2}, \frac{1}{2}\}$ has a physical meaning, we only consider the scale of the buoyancy values relative to the spatial dimensions. We perform clustering with re-scaled buoyancy values, which is equivalent to a k -means algorithm with a weighted

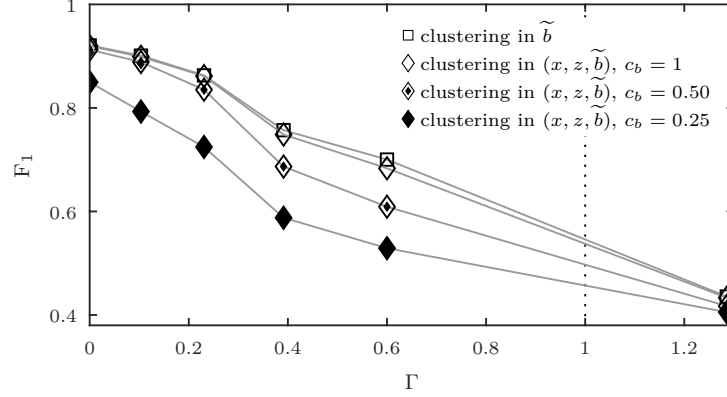


Figure 4.5: The dependence of the F_1 -score on the buoyancy flux ratio Γ : comparing clustering based on data objects of type $s_i = \tilde{b}_i$ and $\mathbf{s}_i = (x_i, z_i, \tilde{b}_i)$, $i \in \{1, \dots, N_s\}$, the latter under different weights c_b of the buoyancy value in a weighted Euclidean distance (4.33). The buoyancy values are time-averaged values from the steady states at $\Gamma \in \{0, 0.10, 0.23, 0.39, 0.60, 1.29\}$; the number of sample points is $N_s = 9$.

Euclidean distance (cf. (4.13)):

$$D(\mathbf{s}_i, \mathbf{s}_j) = \left[(x_i - x_j)^2 + (z_i - z_j)^2 + c_b (\tilde{b}_i - \tilde{b}_j)^2 \right]^{\frac{1}{2}}. \quad (4.33)$$

Fig. 4.5 shows the F_1 -score for clustering based on data objects of type $s_i = \tilde{b}_i$ and $\mathbf{s}_i = (x_i, z_i, \tilde{b}_i)$, with a sample size $N_s = 9$. If the buoyancy in the data objects of type $(x_i, z_i, \tilde{b}_i)$ is not re-scaled ($c_b = 1$), the clustering for $s_i = \tilde{b}_i$ and $\mathbf{s}_i = (x_i, z_i, \tilde{b}_i)$ gives similar results. However, if we emphasize the spatial data in $(x_i, z_i, \tilde{b}_i)$ by weighting the buoyancy with $c_b < 1$, the F_1 -score decreases for $\Gamma < 1$ with decreasing c_b (fig. 4.5). Conversely, emphasizing the buoyancy information in data objects of type $(x_i, z_i, \tilde{b}_i)$ by choosing a weight $c_b > 1$ does not improve the clustering results beyond that obtained purely with buoyancy information, $s_i = \tilde{b}_i$. Thus, the stratification is best described by solely considering the buoyancy values $\tilde{b}_i$ when clustering with a k -means algorithm.

The F_1 -score at $\Gamma = 1.29$ forms an exception in that we obtain similar results for all considered types of feature spaces and weights. However, the F_1 -score at $\Gamma = 1.29$ is at a low value and we do not expect k -means to be able to identify clusters that correspond to our layer definition (fig. 4.1). Hence, we assume that the classification at $\Gamma = 1.29$ does not give meaningful results in any of the considered cases.

4.3.5 Summary

In this section, we assigned samples of the buoyancy field to an upper or lower layer of a two-layer stratification, thereby solving the non-smooth aspect of the parameter estimation without reference to the specific buoyancy model used, apart from its character as a two-layer model.

The layer assignment was realised with k -means clustering, where all sample points were assigned to either layer, i.e., none of the samples was excluded as belonging to the plumes. Hence, the classification resulting from this approach cannot be ideal, however, the mean buoyancy values resulting from the k -means classification scheme showed a good agreement with those from an ‘ideal’ classification.

Classification based purely on buoyancy values gave similar or better results to classifications that additionally included spatial information of the samples. Hence, we will use results from the former approach in the following sections. Note, that these layer assignments have been obtained without constraints on the position of the interface between the layers. Based on the results of this section, we pick sample sizes $N_s \in \{4, 9, 16\}$ for further consideration.

Having fixed the assignment of sample points to the upper or lower layer, we can now proceed to estimate the buoyancy fluxes of the boundary by minimizing a smooth cost functional, which compares the sample buoyancies to model values.

4.4 Parameter estimation details

In this section, we give details on how we estimate buoyancy fluxes on the boundary via the minimisation of a cost functional. We utilise model 2 for parameter estimation and all references to modelled buoyancies in the following refer to model 2.

In §4.2.2, we showed that the modelled steady state buoyancy field is determined by four parameters: the ratio Γ_1 of the distributed to the localised buoyancy flux on the bottom boundary, its equivalent Γ_2 on the top boundary, the total buoyancy flux F on each horizontal boundary, which is equal at the top and bottom, and the volume integrated buoyancy B over the bulk of the domain. In general, each of these causal characteristics behind the observed buoyancy field is unknown.

Here, we simplify the inverse problem by restricting the generally four-dimensional parameter space of Γ_1, Γ_2, F and B to the two dimensions spanned by the buoyancy flux ratios Γ_1 and Γ_2 . The total buoyancy flux on the boundaries and the volume integrated buoyancy are fixed to their respective true value, $F = \tilde{F}$ and $B = \tilde{B}$. Note, that an optimisation problem in the two-dimension parameter space (Γ_1, Γ_2) avoids scaling problems that might occur for optimisation in the general parameter space $(\Gamma_1, \Gamma_2, F, B)$, particularly because it would be difficult to choose a suitable characteristic dimensional buoyancy flux $\hat{F}$ for normalisation in a system where the true buoyancy fluxes are unknown (cf. §4.2). The buoyancy flux ratios Γ_1 and Γ_2 fulfil equivalent roles in determining the modelled buoyancy field (4.4), hence the cost functional to be minimized should scale similarly with respect to these parameters.

In order for the modelled buoyancy field to be physical, the buoyancy fluxes should satisfy (see §2.8)

$$0 \leq \Gamma_1, \quad 0 \leq \Gamma_2, \quad \Gamma_1 \cdot \Gamma_2 < 1. \quad (4.34)$$

We realise the first two constraints by phrasing the optimisation problem in terms of parameters ξ_1 and ξ_2 , defined as

$$\xi_1^2 \equiv \Gamma_1, \quad \xi_2^2 \equiv \Gamma_2. \quad (4.35)$$

For $\xi_i \in \mathbb{R} \forall i$, the limits $0 \leq \Gamma_1$ and $0 \leq \Gamma_2$ are intrinsically satisfied. We do not enforce the limit $\Gamma_1 \cdot \Gamma_2 < 1$, such that within the optimization routine, values beyond the limit of the model may still occur. This does not pose a problem for the optimisation, since $\Gamma_1 \geq 1$ and $\Gamma_2 \geq 1$ result in real values of the model and non-zero sensitivities. A similar methodology could be extended to F for the constraint $F > 0$.

We aim to determine the buoyancy fluxes Γ_1 and Γ_2 by minimizing the cost functional

$$\mathcal{J}(\xi_1, \xi_2, \{\tilde{b}_i\}) = \frac{1}{2} \sum_{k=1}^2 \sum_{i \in \Omega_k} \left[\tilde{b}(x_i, y_i, z_i) - b_{ak}(x_i, (\xi_1)^2, (\xi_2)^2, \tilde{F}, \tilde{B}) \right]^2, \quad i \in \{1, \dots, N_s\}, \quad (4.36)$$

with respect to the parameters ξ_1 and ξ_2 . The modelled buoyancies correspond to $b_{a1} = \frac{1}{2} (\Sigma b - \delta b)$ and $b_{a2} = \frac{1}{2} (\Sigma b + \delta b)$ (cf. §2.8), with Σb and δb being given in (4.4). By minimizing $\mathcal{J}$, we minimize the difference between the modelled and the measured buoyancies at a set of N_s sampling points. The sampling points have been assigned to layer 1 (Ω_1) and layer 2 (Ω_2) prior to the minimisation of $\mathcal{J}$ via clustering (§4.3).

Though we have not rigorously analysed whether the inverse problem considered here is ill- or well-posed, we proceed without regularisation terms in the cost functional (4.36). Regularisation terms typically restrict the space of possible solutions, for example to reduce the number of large coefficients in a polynomial or to favour a specific shape of spatial- or time-dependence. In this context, we note that the optimisation problem (4.36) is already very restricted, allowing for only two parameters that are constant in space and time. Instead of such a simplified problem, we could have used, for example, Tikhonov regularisation to favour steady state solutions in an optimisation of time-dependent parameters and require the total buoyancy flux F and the volume integrated buoyancy B to be close to their true values, $\tilde{F}$ and $\tilde{B}$, respectively.

We minimize the cost functional (4.36) with the method of steepest descent (see alg. 1). For the sake of simplicity, we choose a constant step size k . We found that a step size $k = 4 \times 10^{-3}$ appears to be sufficiently small for the cost functional to converge under the measurement data employed in the following section. However, such a small constant step size results in very slow convergence and is not generally recommended (see e.g. Nocedal [80] for determining a suitable k in terms of the cost functional). The parameters ξ_1 and ξ_2 are initialised with random values in the range $\xi_1, \xi_2 \in [\varepsilon_\xi, 1 - \varepsilon_\xi]$, with $\varepsilon_\xi = 10^{-5}$. We terminate the optimisation if the norm of the cost functional's gradient, $\|\frac{\partial \mathcal{J}}{\partial \xi}\|$, is less than $\varepsilon_{\mathcal{J}} = 10^{-3}$.

The optimisation algorithm was tested with manufactured measurement data corresponding to the model buoyancy values at sets of $N_s = 9$ sampling points. The results from an ensemble of $N_e = 1000$ sets of sampling points differed from the true buoyancy flux ratio $\tilde{\Gamma}$ at an order of magnitude of 10^{-4} , where we tested for the values $\tilde{\Gamma} < 1$ used in the DNS simulations of chapter 2. Note that the method of steepest descent converges to a local minimum of the cost functional, which is not guaranteed to be its global minimum, since the buoyancy model and thus the cost functional is not convex with respect to the parameters (see §4.2.2). However, it is indicated that the cost functional contains only one physically relevant minimum in the parameter range in which we obtain the optimisation results presented in the following section, such that an optimisation algorithm searching for a local solution is likely sufficient. The method of steepest descent is sensitive to poor scaling, which should be acceptable in a parameter space corresponding to (Γ_1, Γ_2) , as outlined earlier. However, in similar problems where poor scaling can be expected, such as for optimisation in the general parameter space $(\Gamma_1, \Gamma_2, F, B)$, an algorithm that is unaffected by scaling should be considered, e.g. Newton's method [80].

We evaluate the results of the parameter estimation statistically, i.e., for each considered configuration $(\tilde{\Gamma}_1, \tilde{\Gamma}_2)$, we perform $N_e = 1000$ parameter estimations based on an ensemble of N_e sets of sampling points (cf. §4.3.3). Not all sets of samples $\{\tilde{b}_i | i = 1, \dots, N_s\}$ of the buoyancy field allow for the cost functional to converge in a realistic time frame such that $\|\frac{\partial \mathcal{J}}{\partial \xi}\| < \varepsilon_{\mathcal{J}}$. Hence, we run the

optimisation for a sufficiently long time to collect $N'_e > 600$ results that satisfy the tolerance $\varepsilon_{\mathcal{J}}$ and base statistics on the corresponding set of N'_e results.

The iteration steps of the steepest descent algorithm in the parameter space are determined by the sensitivity of the cost functional with respect to ξ_1 and ξ_2

$$\frac{\partial \mathcal{J}}{\partial \xi_j} = - \sum_{k=1}^2 \sum_{i \in \Omega_k} \left[\tilde{b}(x_i, y_i, z_i) - b_{ak}(x_i) \right] 2 \xi_j \frac{\partial b_{ak}}{\partial \Gamma_j}, \quad i \in \{1, \dots, N_s\}, j \in \{1, 2\}, \quad (4.37)$$

where we dropped the parameter dependencies for better readability. Let us consider the sensitivity of the modelled buoyancy of the lower layer with respect to the buoyancy fluxes Γ_1 and Γ_2 (the sensitivity of b_{a2} is similar):

$$\frac{\partial b_{a1}}{\partial \Gamma_1} = \frac{F^{\frac{2}{3}}}{2 \alpha^{\frac{2}{3}}} \frac{1 - \frac{2x}{\Lambda}}{(1 + \Gamma_1)^2} \left[\frac{1 - \frac{2}{3} \Gamma_1}{(1 + \Gamma_1)^{\frac{2}{3}}} + \frac{1}{(1 + \Gamma_2)^{\frac{2}{3}}} \right], \quad (4.38a)$$

$$\frac{\partial b_{a1}}{\partial \Gamma_2} = \frac{F^{\frac{2}{3}}}{3 \alpha^{\frac{2}{3}}} \frac{1}{(1 + \Gamma_2)^{\frac{5}{3}}} \left[1 + \frac{1 + \frac{2x}{\Lambda} \Gamma_1}{1 + \Gamma_1} \right]. \quad (4.38b)$$

The derivative of the cost functional (4.37) with respect to ξ_1 or ξ_2 is zero at $\xi_1 = 0$ and $\xi_2 = 0$, respectively, due to a factor ξ_1 or ξ_2 . However, these points of zero sensitivity arise from the parametrisation with ξ_1 and ξ_2 rather than from the model, since the derivatives of the buoyancy in (4.38) are not equal to zero at the buoyancy flux ratios $\Gamma_1 = 0$ and $\Gamma_2 = 0$ that correspond to $\xi_1 = 0$ and $\xi_2 = 0$. Potential minima of the cost functional that are artefacts of the parametrisation might pose a problem for the parameter estimation. However, the additional extrema or saddle points correspond to the limits $0 \leq \Gamma_1$ and $0 \leq \Gamma_2$, where an optimisation routine would necessarily have to terminate. The only precaution necessary in this context is to avoid initialising ξ_1 and ξ_2 at zero, in order to prevent the optimisation becoming stuck at an extremum corresponding to $\Gamma_1 = 0$ or $\Gamma_2 = 0$.

4.5 Results

In this section, we consider the results of parameter estimation based on model 2. The measurement data used in the parameter estimation either corresponds to the DNS data of chapter 2 or to buoyancy fields generated from model 2. To avoid confusion, we denote modelled buoyancies that are not determined by the parameter estimate with an overset asterisk, b^* .

4.5.1 Parameter estimation from DNS data

In this section, we attempt to estimate the buoyancy flux ratios Γ_1 and Γ_2 on the top and bottom boundary, respectively, from samples of the DNS buoyancy field. In particular, the measured buoyancies $\tilde{b}$ in this section correspond to samples of the time-averaged DNS buoyancy field in the steady state, where we take the average over $T = 10$ dimensionless turnover times (see (4.23)). The DNS simulations were run with equal buoyancy flux ratios on the top and bottom boundary, $\tilde{\Gamma} \equiv \tilde{\Gamma}_1 = \tilde{\Gamma}_2$, at $\tilde{\Gamma} \in \{0, 0.10, 0.23, 0.39, 0.60\}$, as presented in chapter 2. The parameter estimation is based on $N_s = 9$ samples of the time-averaged buoyancy field at sampling points in the plane $y = 0$ (see §4.3.3). The samples have been assigned to layer 1 or 2 by the clustering algorithm detailed in §4.3.

Fig. 4.6 shows the two-dimensional PDF of the buoyancy flux ratios Γ_1 and Γ_2 resulting from the minimization of the cost functional (4.36). The true value $\tilde{\Gamma}$ of the buoyancy flux ratio is marked by

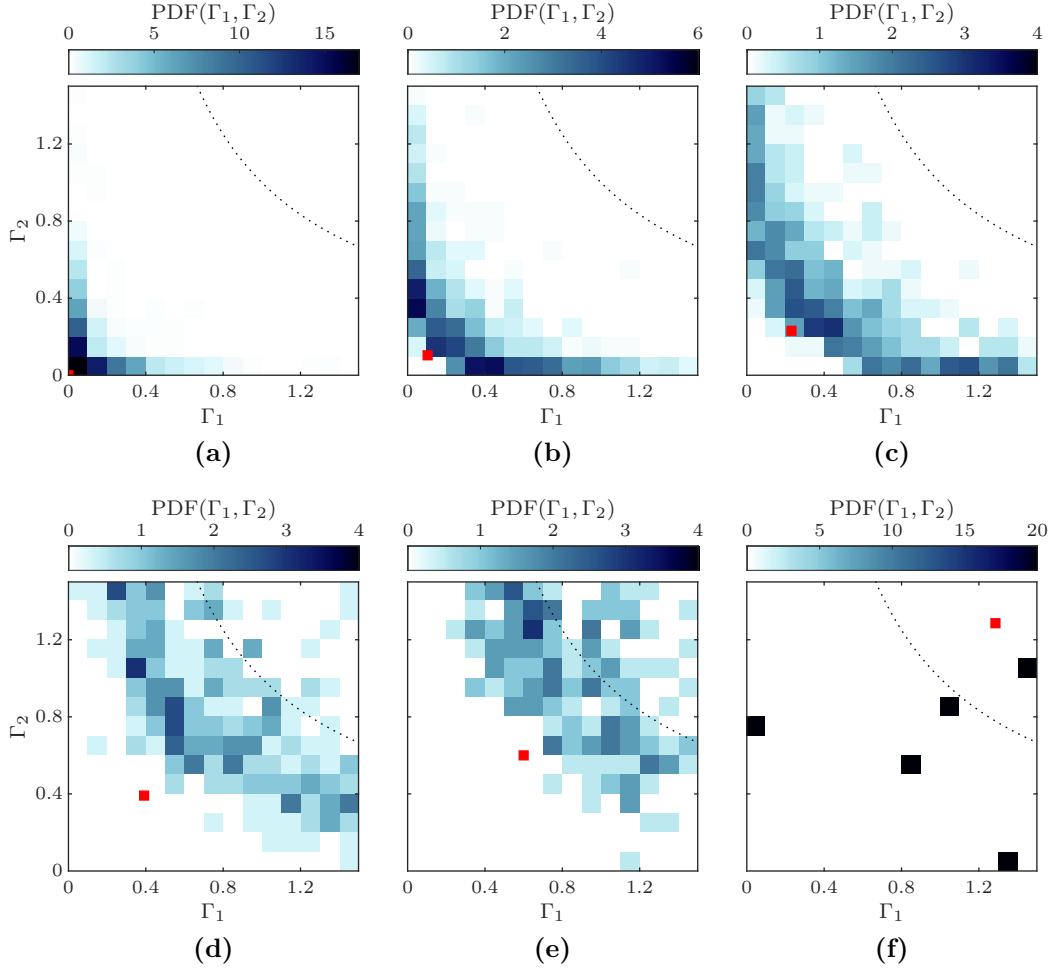


Figure 4.6: Two-dimensional PDFs of the buoyancy flux ratios Γ_1 and Γ_2 estimated from DNS data at true buoyancy flux ratios (a) $\tilde{\Gamma} = 0$, (b) $\tilde{\Gamma} = 0.10$, (c) $\tilde{\Gamma} = 0.23$, (d) $\tilde{\Gamma} = 0.39$, (e) $\tilde{\Gamma} = 0.60$ and (f) $\tilde{\Gamma} = 1.29$. The position of the true value in the parameter space is indicated by a red square. The black dotted lines indicate the limit of the model $\Gamma_1 \cdot \Gamma_2 < 1$. The number of sample points is $N_s = 9$.

a red square. Since the upper limit $\Gamma_1 \cdot \Gamma_2 < 1$ is not enforced in the optimisation routine, results beyond this limit are possible; the corresponding boundary $\Gamma_1 \cdot \Gamma_2 = 1$ is marked by a dotted black line.

Evidently, the parameter estimation does not produce satisfactory results, since the results are widely spread over the space of values (Γ_1, Γ_2) and show multiple peaks in several of the considered cases. The only case in which we observe a single peak, which is close to the true buoyancy flux ratio, is $\tilde{\Gamma} = 0$ (fig. 4.6a) and the optimisation results become more distributed in (Γ_1, Γ_2) as the true buoyancy flux ratio is increased. For true buoyancy flux ratios $\tilde{\Gamma} \leq 0.23$ (fig. 4.6a-c), we find that the results are distributed primarily along the direction that preserves the product $\Gamma_1 \cdot \Gamma_2$, which can be seen by comparison of the two-dimensional PDFs with the upper boundary of the buoyancy flux ratios, $\Gamma_1 \cdot \Gamma_2 = 1$, plotted as a dotted black line. Hence, the product $\Gamma_1 \cdot \Gamma_2$ appears to be robust under a parameter estimation with model 2, while its orthogonal $(\Gamma_1)^2 - (\Gamma_2)^2$ is estimated very inaccurately by our approach. Since the information about the symmetry of the true configuration, $\tilde{\Gamma}_1 = \tilde{\Gamma}_2$, is contained in $(\Gamma_1)^2 - (\Gamma_2)^2$, this information is lost in the parameter estimation.

For $\tilde{\Gamma} = 0.39$ and $\tilde{\Gamma} = 0.60$ (fig. 4.6d and 4.6e), the spread of the optimization results still occurs mainly in a direction that preserve $\Gamma_1 \cdot \Gamma_2$, however, the spread in the orthogonal direction has grown noticeably, i.e., we can no longer consider $\Gamma_1 \cdot \Gamma_2$ robust under the parameter estimation. Note, that this increased distribution of the optimization results with the change of $\tilde{\Gamma}$ from $\tilde{\Gamma} = 0.23$ to 0.39 correlates with a significant increase of the buoyancy fields heterogeneity in each layer, as observed in chapter 2. At $\tilde{\Gamma} \leq 0.23$, the PDFs of the optimisation results contain peaks at or in close vicinity to the true buoyancy flux ratios $(\tilde{\Gamma}, \tilde{\Gamma})$. In contrast, the distributions of results at $\tilde{\Gamma} = 0.39$ and $\tilde{\Gamma} = 0.60$ do no longer include the true value of the buoyancy flux ratio to any significant extent.

At $\tilde{\Gamma} = 1.29$ (fig. 4.6f), we no longer observe a continuous distribution but a small set of distinct peaks. Since model 2 is not valid for $\Gamma_1 \cdot \Gamma_2 \geq 1$, giving non-physical results in these cases, we expected that the results of the parameter estimation would not be correlated with each other in this case. It is, however, surprising that all the optimisation results obtained lie within a such small set of points in the parameter space.

As noted earlier, we observe peaks close to the true buoyancy flux value for $\tilde{\Gamma} = 0.10$ and $\tilde{\Gamma} = 0.23$ (fig. 4.6b and 4.6c). However, we also observe peaks at the boundaries $\Gamma_1 = 0$ and $\Gamma_2 = 0$ of the parameter space; for $\tilde{\Gamma} = 0.10$, the peaks at the boundary exceed the peak close to $\tilde{\Gamma}$ in magnitude. The peaks of the PDFs at $\Gamma_1 = 0$ and $\Gamma_2 = 0$ appear to correspond to the points where the observed spread along an isoline of $\Gamma_1 \cdot \Gamma_2$ approaches the boundaries, hence, we consider the appearance of the boundary peaks as an extremal case of the spread along an isoline of $\Gamma_1 \cdot \Gamma_2$. To investigate this behaviour, we consider the path of the optimization routine in the parameter space, that is, the values of (Γ_1, Γ_2) that are assumed at each iteration of the optimisation.

Fig. 4.7 shows the contour plot of the cost functional and the path of the optimization routine at $\tilde{\Gamma} = 0.23$ for two types of outcomes: a successful parameter estimation with a result close to the true parameter value (fig. 4.7a) and a parameter estimation that produces a result corresponding to the boundary peaks observed in fig. 4.6b and 4.6c, in this case at $\Gamma_2 = 0$ (fig. 4.7b). The parameter space depicted in fig. 4.7 is spanned by ξ_1 and ξ_2 : the lower boundaries of the buoyancy flux ratios, $\Gamma_1 = 0$ and $\Gamma_2 = 0$, correspond to $\xi_1 = 0$ and $\xi_2 = 0$. Each quadrant in (ξ_1, ξ_2) corresponds to the same space of buoyancy flux ratios (Γ_1, Γ_2) , hence, fig. 4.7 displays mainly the first quadrant; the second to fourth quadrant are shaded in grey. The two optimisation problems of fig. 4.7a and 4.7b are identical but for the positions of the spatial sampling points $\{(x, z_i) \mid i = 1, \dots, N_s\}$ that determine the set of buoyancy values on which the optimisation is based. The initial parameter value (red framed diamond in fig. 4.7) and the true parameter value (red square in fig. 4.7) are the same in both cases.

The cost functional is shown as a contour plot in fig. 4.7, where lighter contour lines correspond to higher values of the cost functional. To better visualize the extrema of the cost functional, we marked positions where the derivative of the cost functional with respect to ξ_1 or ξ_2 changes sign: we refer to points with sign changes from positive to negative as ‘ridges’ in ξ_1 or ξ_2 , depending on the direction of the derivative; sign changes from negative to positive are termed ‘valleys’. Note, that these definitions do not correspond to valleys or ridges in a topological sense.

As noted in §4.4, the derivative $\partial\mathcal{J}/\partial\xi_1$ is always zero at $\xi_1 = 0$, as is $\partial\mathcal{J}/\partial\xi_2$ at $\xi_2 = 0$. This results in a maximum of the cost functionals at the origin $((\Gamma_1, \Gamma_2) = (0, 0))$, corresponding to a crossing of two ‘ridges’ in fig. 4.7, and saddle points where a ‘ridge’ and a ‘valley’ meet. A minimum in the cost functional is marked by a crossing of two ‘valleys’: the cost functionals in fig. 4.7 contain at most one minimum per quadrant in a range $\xi_1, \xi_2 \in [-10^2, 10^2]$ and thus only a single minimum in the

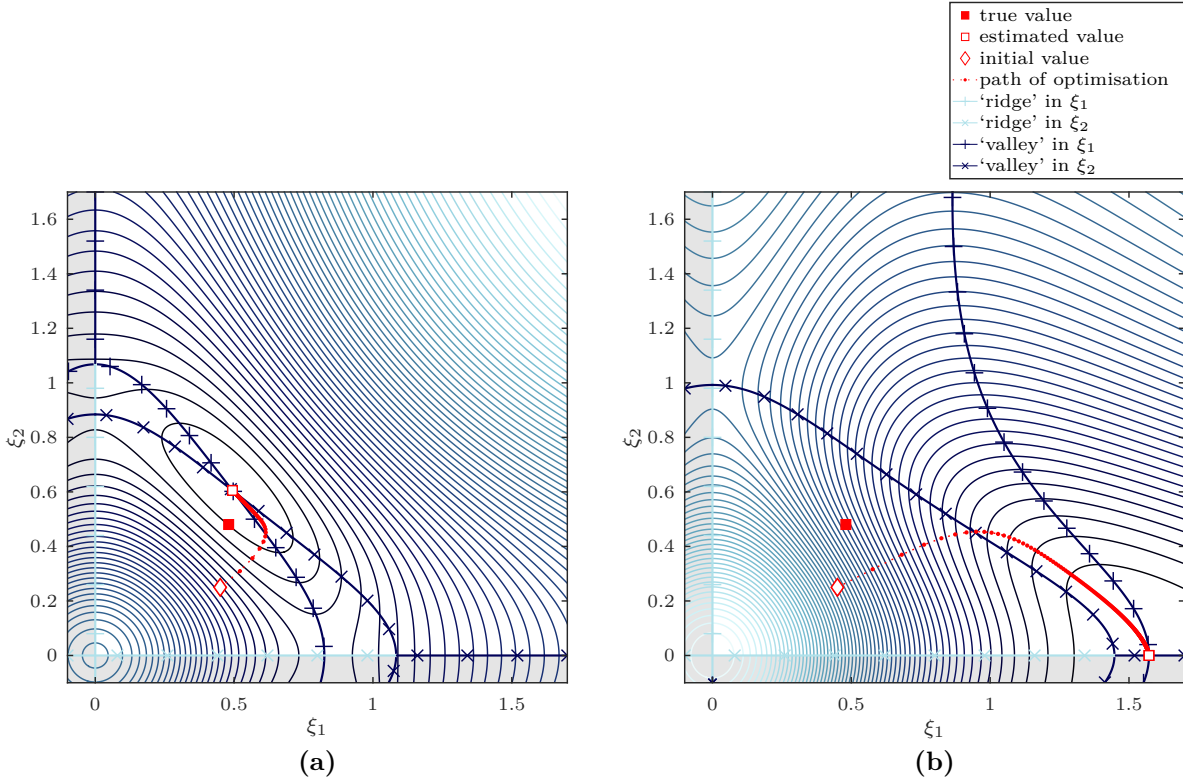


Figure 4.7: Contour plot of the cost functional and the path of the optimisation routine in the parameter space at $\bar{\Gamma} = 0.23$ for two different sets of sample points, producing (a) a result close to the true parameter value and (b) a result at $\Gamma_2 = 0$. Lighter contour lines correspond to higher values of the cost functional. The true parameter value and the initial parameter value in the optimization routine are the same in (a) and (b) and marked by a red square and a red framed diamond, respectively; the optimisation result is marked by a red framed square. ‘Ridges’ correspond to points where the derivative of the cost functional with respect to parameter ξ_1 or ξ_2 changes its sign from positive to negative; ‘valleys’ mark positions where the sign changes from negative to positive. Negative values of ξ_1 or ξ_2 are physically equivalent to their positive counterpart (see text), corresponding areas are shaded in grey.

corresponding space of (Γ_1, Γ_2) of buoyancy flux ratios. As there exists only a single minimum in the neighbourhood of the true parameter value $\tilde{\Gamma}$, we assume that this is a global minimum. Generally, we calculated the cost functional for ten sets of buoyancy samples per DNS simulation and found at most one minimum per quadrant in the parameter range displayed in fig. 4.6.

It is apparent from fig. 4.7 that the optimisation routine successfully locates the minimum of the cost functional in both cases: the path of the optimisation leads to a result (red framed square) at the respective minimum. Thus, the peaks at $\Gamma_1 = 0$ and $\Gamma_2 = 0$ in fig. 4.6b and 4.6c are not caused by a failure of the optimisation routine, but by the shape of the cost functional. By extension, we expect the spread of the optimisation results along isolines of $\Gamma_1 \cdot \Gamma_2$ to be caused by the same process.

In this context, we note that the minima in fig. 4.7a and 4.7b are different in character. The cost functionals in both plots show a ‘valley’ in ξ_1 and ξ_2 for values $\xi_1, \xi_2 > 0$. In fig. 4.7a, both ‘valleys’ cross, which corresponds to the minimum of the cost functional. In contrast, the equivalent ‘valleys’ in fig. 4.7b do not cross, and the minimum of the cost functional corresponds to an intersection with the boundary $\Gamma_2 = 0$. Thus, the optimisation in fig. 4.7b is terminated because the estimated parameters

reach the limit of permissible values for $\Gamma_2 \geq 0$. In contrast, an ideal cost functional for a true value $\tilde{\Gamma}_2 = 0$ would produce an intersection of three ‘valleys’: a ‘valley’ in ξ_1 and ξ_2 , which continue beyond $\xi_2 = 0$, and the boundary ‘valley’ at $\xi_2 = 0$ ($\Gamma_2 = 0$).

We found that while the optimisation routine is adequate for the considered minimisation problem, the cost functional is ill-suited to produce meaningful estimates of the buoyancy flux ratio. What could be the cause for the disagreement between the cost functional’s minimum and the true parameter value? A possible candidate is the structure of the cost functional, i.e., the norm employed to measure the difference between the measured and the modelled buoyancy field and/or the lack of regularisation terms. Other possible sources of error are the ability of the employed model to approximate the DNS data with sufficient accuracy and the assignment of sample points to layer 1 or 2.

To investigate the behaviour of the cost functional, we first focus on one aspect in which the model and the DNS data differ: the modelled buoyancy field in each layer is more homogeneous than it is the case for the DNS data, partly because the buoyancy of each layer was assumed to be homogeneous in the vertical in the construction of model 2 (see §2.6.2). We model this difference between the DNS data and model 2 as Gaussian noise and study its impact on the results of the parameter estimation.

4.5.2 Impact of the modelling error amplitude on the parameter estimation

In this section, we generate the ‘measured’ buoyancy data $\tilde{b}$ by superposing buoyancy values b_a^* derived from model 2 (see (4.4)) with a random error ε_b

$$\tilde{b}_{ai}(x, \tilde{\Gamma}_1, \tilde{\Gamma}_2, \tilde{F}, \tilde{B}, \varepsilon_b) = b_{ai}^*(x, \tilde{\Gamma}_1, \tilde{\Gamma}_2, \tilde{F}, \tilde{B}) + \varepsilon_b, \quad i \in \{1, 2\}, \quad (4.39)$$

where ε_b is normally distributed with a variance $\tilde{\sigma}_b$,

$$\text{PDF}(\varepsilon_b, \tilde{\sigma}_b) = \frac{1}{\sqrt{2\pi}\tilde{\sigma}_b} \exp\left(-\frac{1}{2}\left(\frac{\varepsilon_b}{\tilde{\sigma}_b}\right)^2\right). \quad (4.40)$$

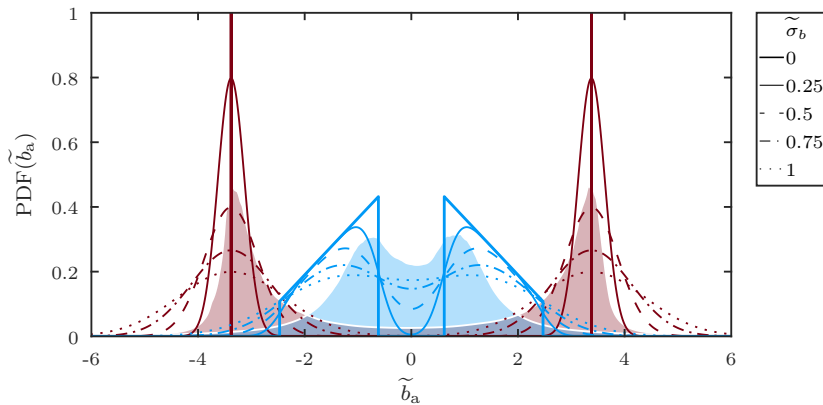


Figure 4.8: PDFs of the buoyancy fields $\tilde{b}$ generated from model 2 and Gaussian noise at $\tilde{\Gamma}_1 = \tilde{\Gamma}_2 = 0$ (red) and $\tilde{\Gamma}_1 = \tilde{\Gamma}_2 = 0.60$ (blue) for different values of the standard deviation $\tilde{\sigma}_b$ of the Gaussian noise (see (4.40)). The PDFs of the generated buoyancy fields are plotted as outlines, the corresponding PDFs of the buoyancy field from DNS data are given as shaded areas for reference.

Generating a measured buoyancy allows us to simulate a known and variable difference between the measured and the modelled buoyancy, where the modelling error is quantified by the standard deviation $\tilde{\sigma}_b$. The introduced Gaussian noise is not to be understood as measurement noise, which is indeed small in the time-averaged DNS data considered in the previous section, but as a representation of the difference between the modelled and measured buoyancy due to simplifications in the model. References to ‘noise’ in the current section correspond to this modelled difference. It should be noted, however, that a normally distributed modelling error is an idealisation and we do not assume that the difference between the DNS data and model 2 is Gaussian.

The generated measured buoyancy field is sampled at the same positions (x, z) as in §4.5.1, using a set of $N_s = 9$ sampling points. The buoyancy samples are assigned ideally to layer 1 or 2, that is, we calculate the corresponding buoyancy as b_{a1}^* or b_{a2}^* depending on the location of the sampling point relative to the modelled true interface elevation $\tilde{z}_1^*$, as calculated from x , $\tilde{\Gamma}_1$, $\tilde{\Gamma}_2$, $\tilde{F}$ and $\tilde{B}$ via model 2 (4.4a). As in §4.5.1, we restrict the true buoyancy flux ratios to $\tilde{\Gamma}_1 = \tilde{\Gamma}_2 \equiv \tilde{\Gamma}$ and consider the minimisation of the cost functional (4.36) in the two-dimensional parameter space (ξ_1, ξ_2) .

Fig. 4.8 shows the PDFs of the generated buoyancy field $\tilde{b}_a$ for $\tilde{\Gamma} = 0$ and 0.60, plotted as outlines, to illustrate different magnitudes of the noise level $\tilde{\sigma}_b$. The PDFs of the buoyancy field from the DNS data are added as scale reference, shown as shaded areas (cf. fig. 2.4).

Fig. 4.9 shows the results of the parameter estimation for an increasing noise level at $\tilde{\Gamma} = 0.20$ in terms of the two-dimensional PDFs, where the standard deviation $\tilde{\sigma}_b$ of the Gaussian noise is chosen as $\tilde{\sigma}_b \in \{0, 0.15, 0.30, 0.45, 0.60, 0.75\}$. As the noise is increased, it can be observed that the distribution of the results spreads primarily along the isoline $\Gamma_1 \cdot \Gamma_2 = \tilde{\Gamma}^2$ (red dashed line in fig. 4.9), reminiscent of the distributions observed in fig. 4.6 for the DNS data. As the distribution of the results in fig. 4.9 approaches the boundaries $\Gamma_1 = 0$ and $\Gamma_2 = 0$ for $\tilde{\sigma}_b \geq 0.60$, peaks occur at these boundaries.

In contrast to the DNS data in fig. 4.6, the results for the generated buoyancy fields shown in fig. 4.9 display only little spread in $\Gamma_1 \cdot \Gamma_2$, i.e., orthogonal to the isolines in $\Gamma_1 \cdot \Gamma_2$. However, fig. 4.9 presents results at a constant value of the true buoyancy flux ratio $\tilde{\Gamma} = 0.20$, whereas the DNS data was obtained for different values of $\tilde{\Gamma}$. Consequently, we consider a set of generated buoyancy fields at a constant noise level $\tilde{\sigma}_b = 0.60$ for a range of true buoyancy flux ratios $\tilde{\Gamma} \in \{0, 0.20, 0.40, 0.60, 0.80\}$; the corresponding PDFs of the results are shown in fig. 4.10.

It is evident from fig. 4.10 that the spread of the results in $\Gamma_1 \cdot \Gamma_2$ increases with an increasing value of the true buoyancy flux ratio $\tilde{\Gamma}$. In addition, we observe a larger spread in $\Gamma_1 \cdot \Gamma_2$ for buoyancy flux ratios estimated above the limit $\Gamma_1 \cdot \Gamma_2 < 1$ of the model (black dotted line in fig. 4.10) than for results that satisfy $\Gamma_1 \cdot \Gamma_2 < 1$, as can be seen for $\tilde{\Gamma} = 0.80$ in fig. 4.10. As the model does not produce physical results above $\Gamma_1 \cdot \Gamma_2 = 1$, we presume that optimisation results above this level do not show a consistent trend and thus occur over a wide range of values. Indeed, a comparatively large spread of results above $\Gamma_1 \cdot \Gamma_2 = 1$ also seems to occur for the DNS data at $\tilde{\Gamma} = 0.39$ and 0.60 (fig. 4.6d and 4.6e), although the general distribution of the optimisation results in these cases makes it difficult to determine this clearly.

Comparing the behaviour of the optimisation results shown in fig. 4.9 and 4.10 with the results from the DNS data in fig. 4.6, we conclude that the distributions of the results we observe in the DNS data can mainly be attributed to the spatial inhomogeneity of the DNS buoyancy field compared with the modelled buoyancy. In this section, the standard deviation $\tilde{\sigma}_b$ of the Gaussian noise is used as a measure of this relative inhomogeneity, and we will later attempt to quantify $\tilde{\sigma}_b$ for the DNS buoyancy

fields used in §4.5.1. However, the results from the DNS data in fig. 4.6 show a behaviour that is not present in the results from the generated buoyancy fields. The latter appear to be spread approximately evenly in $\Gamma_1 \cdot \Gamma_2$ around the isolines corresponding to the true buoyancy flux ratios, $\Gamma_1 \cdot \Gamma_2 = \tilde{\Gamma}^2$. In contrast, the distributions of results from the DNS data are shifted from the isoline $\Gamma_1 \cdot \Gamma_2 = \tilde{\Gamma}^2$ towards higher values of $\Gamma_1 \cdot \Gamma_2$. This corresponds to a systematic error in the modelled buoyancy field, which distorts the results of the parameter estimation in addition to the inhomogeneity of the DNS data relative to the model. We will address the cause of this systematic error later.

Modelling the inhomogeneity of the DNS buoyancy field relative to the model as Gaussian noise, we can investigate the connection between the parameter estimation results and the magnitude of the modelling error, expressed by the standard deviation $\tilde{\sigma}_b$ of the noise. This standard deviation could be reduced by obtaining the measured buoyancy data from a larger sample or by improving the model, e.g. by modelling the upper and lower layer as stratified. However, a more complex model or additional measurements raise the (computational) cost of the parameter estimation and it would be desirable to

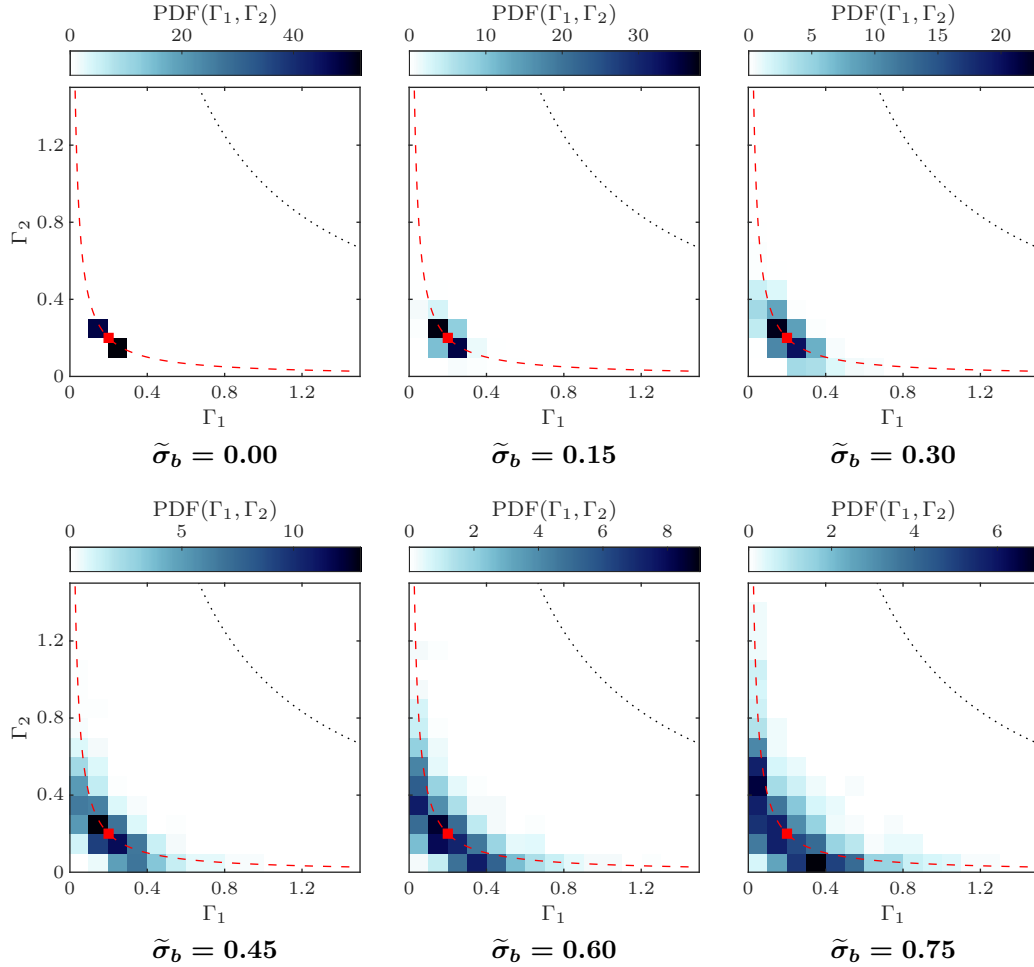


Figure 4.9: Two-dimensional PDFs of the estimated buoyancy flux ratios Γ_1 and Γ_2 for different noise levels $\tilde{\sigma}_b \in \{0, 0.20, 0.40, 0.60, 0.80, 1.00\}$ of the generated measured buoyancy at $\tilde{\Gamma}_1 = \tilde{\Gamma}_2 = 0.20$. The position of the true value in the parameter space is indicated by a red square. The black dotted lines indicate the limit of the model $\Gamma_1 \cdot \Gamma_2 < 1$; the red dashed lines correspond to the isoline $\Gamma_1 \cdot \Gamma_2 = \tilde{\Gamma}^2$. The number of sample points is $N_s = 9$.

improve the results with the least possible effort. How large a standard deviation would be permissible to obtain parameter estimation results of acceptable accuracy? To address this question, we consider the accuracy of parameter estimation results for a range of standard deviations $\tilde{\sigma}_b$ and true buoyancy flux values $\tilde{\Gamma}$.

Fig. 4.11 shows parameter estimation results in dependence of the level of Gaussian noise, $\tilde{\sigma}_b$, at different values of the true buoyancy flux ratio $\tilde{\Gamma} \in \{0, 0.20, 0.40, 0.60, 0.80\}$. The ensemble of estimated buoyancy fluxes ratios Γ_1 and Γ_2 , fig. 4.11a and 4.11b, respectively, is displayed in terms of the ensemble mean $\mu(\Gamma)$ (solid lines), and the standard deviation with respect to the true buoyancy flux ratio

$$\sigma(\Gamma_j) = \sqrt{\frac{1}{N'_e} \sum_{i=1}^{N'_e} (\Gamma_{ji} - \tilde{\Gamma})^2} \quad j \in \{1, 2\}. \quad (4.41)$$

In fig. 4.11, the ranges $[\mu(\Gamma) - \sigma(\Gamma), \mu(\Gamma) + \sigma(\Gamma)]$ are shown as shaded areas, where we collectively refer to $\sigma(\Gamma_1)$ and $\sigma(\Gamma_2)$ as $\sigma(\Gamma)$. The true values of the buoyancy flux ratio are given as dashed lines.

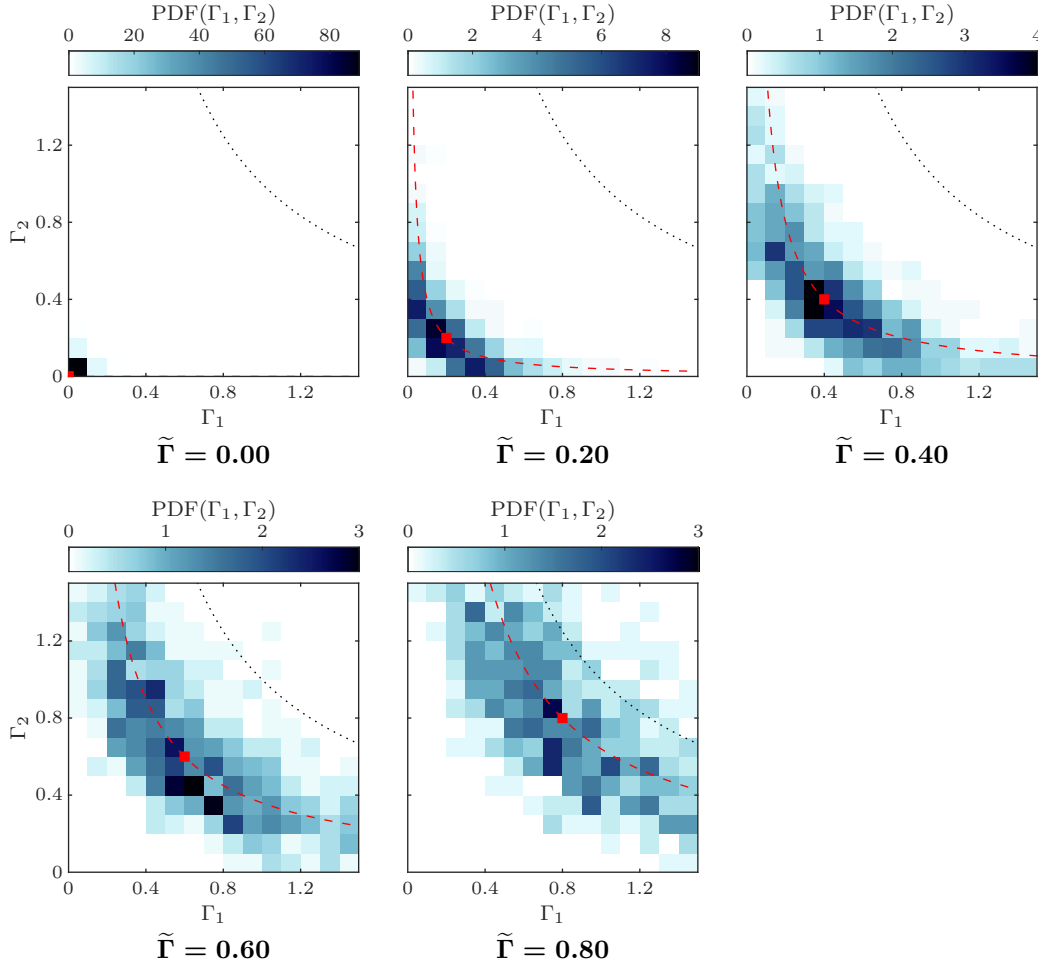


Figure 4.10: Two-dimensional PDFs of the estimated buoyancy flux ratios Γ_1 and Γ_2 for different true buoyancy flux ratios $\tilde{\Gamma} \in \{0, 0.20, 0.40, 0.60, 0.80\}$ at noise level $\tilde{\sigma}_b = 0.60$ of the generated measured buoyancy. The position of the true value in the parameter space is indicated by a red square. The black dotted lines indicate the limit of the model $\Gamma_1 \cdot \Gamma_2 < 1$; the red dashed lines correspond to the isoline $\Gamma_1 \cdot \Gamma_2 = \tilde{\Gamma}^2$. The number of sample points is $N_s = 9$.

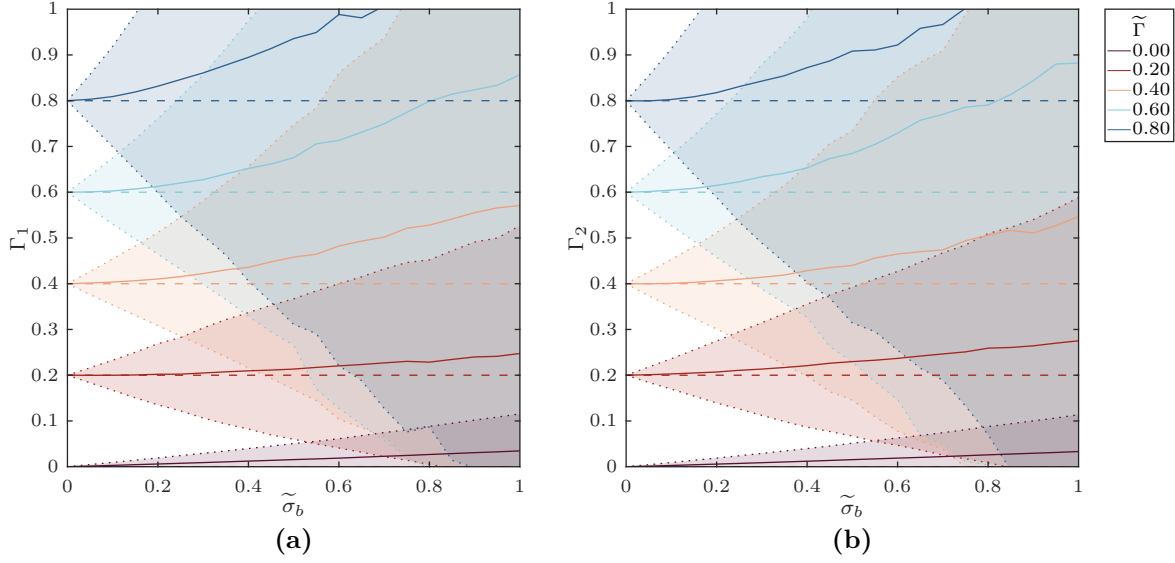


Figure 4.11: Parameter estimation results **(a)** Γ_1 and **(b)** Γ_2 , in terms of their ensemble mean (solid line) and standard deviation (shaded area), as a function of the noise level $\tilde{\sigma}_b$ of the generated measured buoyancy for true buoyancy flux ratios $\tilde{\Gamma} \in \{0, 0.2, 0.4, 0.6, 0.8\}$, where $\tilde{\Gamma} = \tilde{\Gamma}_1 = \tilde{\Gamma}_2$. The true values $\tilde{\Gamma}$ are given as dashed lines. The number of sample points is $N_s = 9$.

It is evident from fig. 4.11 that the mean values $\mu(\Gamma)$ of the parameter estimation results are only meaningful for small values of $\tilde{\sigma}_b$, since the magnitude of the standard deviation $\sigma(\Gamma)$ quickly eclipses that of the mean with growing noise level. The results at $\tilde{\Gamma} = 0$ form an exception to this observation: the standard deviation $\sigma(\Gamma)$ increases only slightly with $\tilde{\sigma}_b$ in this case. Generally, we find that, as we increase the true buoyancy flux ratio $\tilde{\Gamma}$, the standard deviation of the results increases more quickly with $\tilde{\sigma}_b$. This correlates with our observation from fig. 4.10, where we noted that the spread of the distributions of the results grows in $\Gamma_1 \cdot \Gamma_2$ with increasing $\tilde{\Gamma}$. Moreover, we found that the optimisation results accumulate at $\Gamma_1 = 0$ and $\Gamma_2 = 0$, as their distribution in the parameter space reaches these boundaries, i.e., they form the ‘boundary peaks’ discussed earlier. This likely limits the standard deviation of the optimisation results shown in fig. 4.11, where the limit is at greater values of Γ for greater values of the true buoyancy flux ratio $\tilde{\Gamma}$. Since the distance between the true buoyancy flux value $(\tilde{\Gamma}, \tilde{\Gamma})$ and the boundaries $\Gamma_1 = 0$ and $\Gamma_2 = 0$ is proportional to $\tilde{\Gamma}$, greater values of $\tilde{\Gamma}$ permit greater errors.

Unfortunately, it is difficult to draw on fig. 4.11 to find a simple relationship between the amplitude of the modelling error, $\tilde{\sigma}_b$, and the resulting accuracy of the parameter estimation. However, the fact that the sensitivity of $\sigma(\Gamma)$ with respect to $\tilde{\sigma}_b$ depends on the magnitude of the true buoyancy flux ratio $\tilde{\Gamma}$ indicates that we should consider a measure of the modelling error that is decoupled from the scale of the measured buoyancy field $\tilde{b}$, which is determined by $\tilde{\Gamma}$. In the context of measuring noisy signals, it is common to define a signal-to-noise ratio (SNR) to quantify the accuracy of the measurement. In order to stay consistent with our approach in this section, we instead define a noise-to-signal ratio

$$\text{NSR}_b = \frac{\tilde{\sigma}_b}{\Delta b^*(\tilde{\Gamma})}. \quad (4.42)$$

Here, we use the modelled difference Δb^* between the peaks of the buoyancy field’s PDF in place of

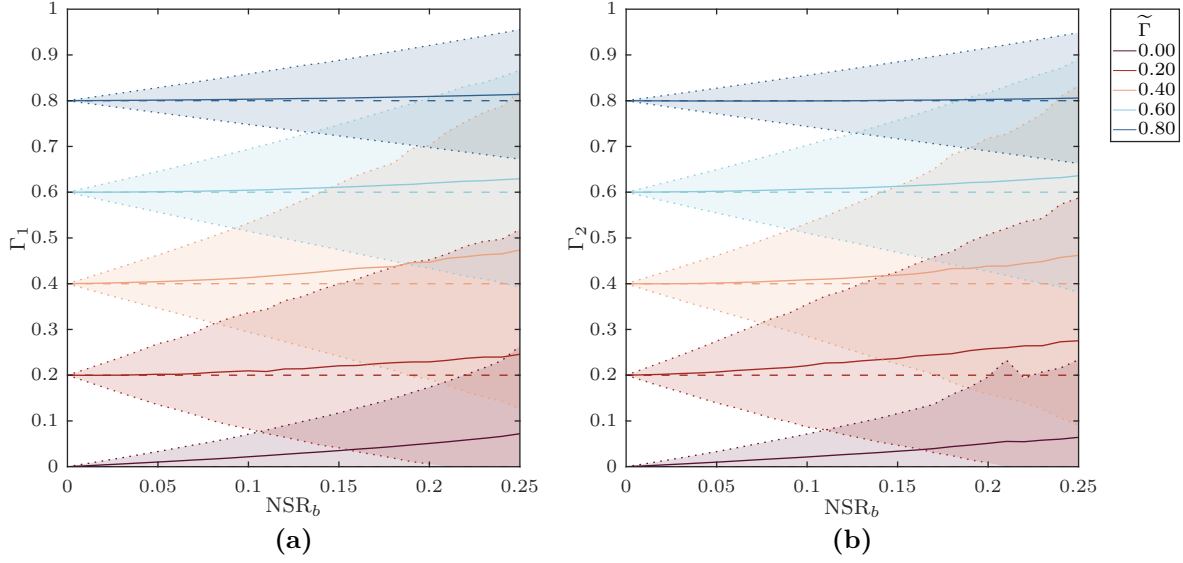


Figure 4.12: Parameter estimation results **(a)** Γ_1 and **(b)** Γ_2 , in terms of their ensemble mean (solid line) and standard deviation (shaded area), as a function of the noise signal ratio NSR_b (4.42) of the generated measured buoyancy for true buoyancy flux ratios $\tilde{\Gamma} \in \{0, 0.2, 0.4, 0.6, 0.8\}$, where $\tilde{\Gamma} = \tilde{\Gamma}_1 = \tilde{\Gamma}_2$. The true values $\tilde{\Gamma}$ are given as dashed lines. The number of sample points is $N_s = 9$.

the signal strength, since it characterises the buoyancy difference between the layers.

Fig. 4.12 shows the equivalent values to those in fig. 4.11 as a function of the noise-to-signal ratio, which corresponds to a rescaled measure of the modelling error. Evidently, the dependency between the rescaled noise level NSR and the standard deviation $\sigma(\Gamma)$ is simpler than the relationship presented in fig. 4.11: $\sigma(\Gamma)$ shows an approximately linear increase with the noise-to-signal ratio and the slope $d\sigma(\Gamma)/d\text{NSR}_b$ is of comparable magnitude in all considered cases of the true buoyancy flux ratio $\tilde{\Gamma}$. In fig. 4.11, the same absolute noise level $\tilde{\sigma}_b$ has a much greater impact on the parameter estimation results at high values of $\tilde{\Gamma}$ than on those at low $\tilde{\Gamma}$, since the noise is greater relative to the scale of the buoyancy field $\tilde{b}$ in the former case than in the latter. The rescaling of the Gaussian noise level $\tilde{\sigma}_b$ with Δb^* compensates this effect.

Necessarily, the noise-to-signal ratio considered in fig. 4.12 corresponds to different ranges of the absolute noise level $\tilde{\sigma}_b$ for each value of $\tilde{\Gamma}$; the respective ranges of $\tilde{\sigma}_b$ are given in tab. 4.3. Notably, the maximum NSR in fig. 4.12 corresponds to a Gaussian noise of only $\tilde{\sigma}_b = 0.13$ for $\tilde{\Gamma} = 0.80$. The decreasing range of $\tilde{\sigma}_b$ with increasing $\tilde{\Gamma}$ is also the cause of the decreasing slope $d\sigma(\Gamma)/d\text{NSR}_b$ that we observe for increasing $\tilde{\Gamma}$ at $\tilde{\Gamma} \geq 0.4$ in fig. 4.12. Since the modelled buoyancy difference Δb^* between the layers approaches zero as $\tilde{\Gamma}_1 \cdot \tilde{\Gamma}_2$ approaches 1, our definition of the noise-to-signal ratio is likely no longer a meaningful measure in the vicinity of $\tilde{\Gamma}_1 \cdot \tilde{\Gamma}_2 = 1$, which corresponds to $\tilde{\Gamma} = 1$ in the configurations considered here.

Table 4.3: Ranges of the absolute noise level $\tilde{\sigma}_b$ that correspond to the range of the noise-to-signal ratio $\text{NSR} \in [0, 0.25]$ displayed in fig. 4.12 for the true values of the buoyancy flux ratio $\tilde{\Gamma}$ shown there.

$\tilde{\Gamma}$	0	0.20	0.40	0.60	0.80
Range of $\tilde{\sigma}_b$	$\tilde{\sigma}_b \in [0, 1.69]$	$\tilde{\sigma}_b \in [0, 1.00]$	$\tilde{\sigma}_b \in [0, 0.58]$	$\tilde{\sigma}_b \in [0, 0.31]$	$\tilde{\sigma}_b \in [0, 0.13]$

To complete our picture of the impact of the modelling error amplitude on the results of the parameter estimation, we consider the results in a continuous range of true buoyancy flux values $\tilde{\Gamma}$ and noise-to-signal ratios. To this end, we define an equivalent $\sigma(\Gamma_1, \Gamma_2)$ to the standard deviation with respect to the true buoyancy flux ratio in the two-dimensional space (Γ_1, Γ_2) :

$$\sigma(\Gamma_1, \Gamma_2) = \sqrt{\frac{1}{N'_e} \sum_{i=1}^{N'_e} \left[(\Gamma_{1i} - \tilde{\Gamma})^2 + (\Gamma_{2i} - \tilde{\Gamma})^2 \right]}. \quad (4.43)$$

The above definition corresponds to the mean squared Euclidean distance between the parameter estimation result (Γ_1, Γ_2) and the true value $(\tilde{\Gamma}, \tilde{\Gamma})$.

Fig. 4.13 shows the contour plot of the standard deviation $\sigma(\Gamma_1, \Gamma_2)$ as a function of $\tilde{\Gamma}$ and NSR_b . Evidently, the same value of the noise-to-signal ratio produces very similar magnitudes of the standard deviation $\sigma(\Gamma_1, \Gamma_2)$ for a wide range of true buoyancy flux ratios $\tilde{\Gamma}$ and values of NSR_b . This makes the noise-to-signal ratio a suitable measure to determine the maximum level of inhomogeneity between the model and the measured data for a given acceptable error of the parameter estimation results. For example, according to our modelling of the inhomogeneity as Gaussian noise, we would need to aim for a noise-to-signal ratio of $\text{NSR}_b = 0.1$ to obtain at most a standard deviation of $\sigma(\Gamma_1, \Gamma_2) = 0.1$. This noise-to-signal ratio corresponds to absolute noise levels of e.g. $\tilde{\sigma}_b = 0.40$ for $\tilde{\Gamma} = 0.20$ and $\tilde{\sigma}_b = 0.12$ for $\tilde{\Gamma} = 0.60$. The relevant magnitude $\tilde{\sigma}_b$ of the maximal permissible Gaussian noise would then be determined by the range of true buoyancy flux ratios $\tilde{\Gamma}$ for which the parameter estimation is required to be accurate. Note, however, that fig. 4.13 only shows the relationship between the parameter estimation result and the signal-to-noise ratio for configurations with a true buoyancy flux ratio $\tilde{\Gamma}_1 = \tilde{\Gamma}_2 \equiv \tilde{\Gamma}$ and that we do not account for systematic errors of the model.

In the vicinity of $\tilde{\Gamma} = 0$ and 1, the relationship between the standard deviation of the parameter

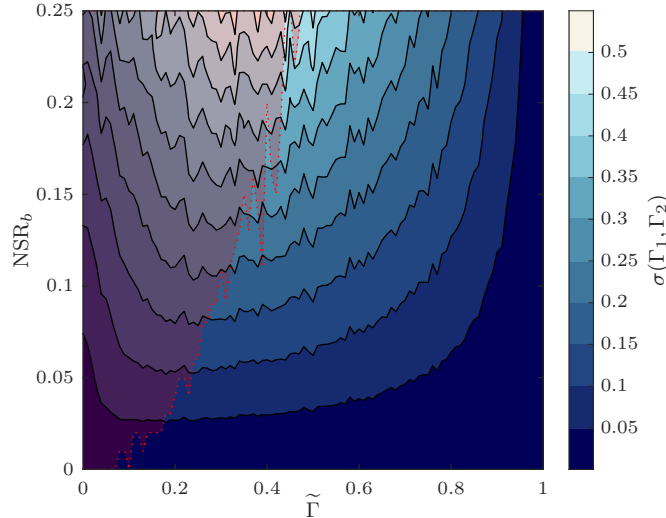


Figure 4.13: Contour plot of the mean squared Euclidean distance $\sigma(\Gamma_1, \Gamma_2)$ between the parameter estimation result (Γ_1, Γ_2) and the true value $(\tilde{\Gamma}, \tilde{\Gamma})$ (see (4.43)) as a function of $\tilde{\Gamma}$ and the noise signal ratio NSR_b of the buoyancy field. The red shaded area marks the points for which we find peaks at $\Gamma_1 = 0$ or $\Gamma_2 = 0$, based on a PDF of resolution 0.10 in Γ_1 and Γ_2 (cf. fig. 4.9). The number of sample points is $N_s = 9$.

estimation results $\sigma(\Gamma_1, \Gamma_2)$ and $\tilde{\Gamma}$ and NSR_b is not trivial. In both cases, the increase of the error $\sigma(\Gamma_1, \Gamma_2)$ with the noise level NSR_b is slower than at true buoyancy flux ratios $\tilde{\Gamma}$ more towards the centre of the range $\tilde{\Gamma} \in [0, 1]$. At values of $\tilde{\Gamma}$ close to zero, the growth of the standard deviation is limited because the true value $(\tilde{\Gamma}, \tilde{\Gamma})$ is close to the boundaries $\Gamma_1 = 0$ and $\Gamma_2 = 0$, and the character of the spread of the optimisation results in the parameter space causes results to accumulate at these boundaries (see fig. 4.9). In the PDFs of the parameter estimation results, the increased occurrence of results at $\Gamma_1 = 0$ or $\Gamma_2 = 0$ manifests as peaks at the corresponding boundaries, where the distance between the boundary peaks and the true buoyancy flux value $\tilde{\Gamma}$ approximately represents the largest possible error at the respective value of $\tilde{\Gamma}$. In fig. 4.13, we marked the cases for which we observed boundary peaks as a red shaded area, based on PDFs with a resolution of 0.10 in Γ_1 and Γ_2 . The correlation between the boundary of the red shaded area and the points in NSR_b and $\tilde{\Gamma}$ at which the standard deviation $\sigma(\Gamma_1, \Gamma_2)$ changes its behaviour indicates that the shallower slope $d\sigma(\Gamma_1, \Gamma_2)/d\text{NSR}_b$ in the vicinity of $\tilde{\Gamma} = 0$ is indeed caused by the process described above. Truly, this shallower slope does not only occur close to $\tilde{\Gamma} = 0$, but for increasingly larger values of $\tilde{\Gamma}$ with increasing noise level NSR_b .

While the shallow slope $d\sigma(\Gamma_1, \Gamma_2)/d\text{NSR}_b$ towards the boundary $\tilde{\Gamma} = 0$ is consistent with our observations of result distributions in the parameter space, the behaviour of $\sigma(\Gamma_1, \Gamma_2)$ in the vicinity of $\tilde{\Gamma} = 1$ is an artefact of the definition of the noise-to-signal ratio: the modelled buoyancy difference Δb^* between the layers approaches zero as $\tilde{\Gamma}$ approaches one, which causes NSR_b to approach infinity, as discussed earlier. Hence, our prediction of the relationship between the results of the parameter estimation and $\tilde{\Gamma}$ and NSR_b cannot be reliable close to $\tilde{\Gamma} = 1$.

4.5.3 Quantifying the difference between the DNS data and the model

Our attempt at a parameter estimation from DNS data gave results (Γ_1, Γ_2) that are widely distributed in the parameter space (fig. 4.6). The error of the parameter estimate, i.e., their deviation from the true buoyancy flux ratio $\tilde{\Gamma}$, can be described as composed of a systematic error and a ‘random’ error: the systematic error manifests as a shift of the results in $\Gamma_1 \cdot \Gamma_2$ from the true value $\tilde{\Gamma}$; the random error corresponds to a distribution of results along an isoline $\Gamma_1 \cdot \Gamma_2$ (cf. §4.5.1 and §4.5.2). We use the term ‘random error’ because of the distribution of results in the parameter space, which is approximately Gaussian in $(\Gamma_1)^2 - (\Gamma_2)^2$, the orthogonal of $\Gamma_1 \cdot \Gamma_2$. We do not assume that the source of the random error is inherently unpredictable, as would be the case for a truly random error.

The error in the parameter estimation is likely caused by discrepancies between the model and the DNS data, i.e., we assume that the systematic error in (Γ_1, Γ_2) arises from a systematic difference ε_{bS} between the model and the DNS buoyancy field; the random error occurs because the time-averaged DNS buoyancy field is more heterogeneous in each layer than the modelled buoyancy field, a difference which we term ε_{bR} . In the previous section, we modelled the difference ε_{bR} in homogeneity of the buoyancy field as Gaussian noise and indeed obtained results distributed similarly to those from the DNS data. For this modelled error ε_{bR} , we found that the accuracy of the parameter estimate is mainly dependent on the noise-signal-ratio of the error relative to the buoyancy difference between the layers of the stratification. Considering DNS data instead of a generated buoyancy field, can we confirm this relationship between the error of the modelled buoyancy field and the error of the estimated parameters? To answer this question, we have to quantify the respective errors.

Let us first consider the error of the modelled buoyancy field b^* , i.e., its deviation from the time-

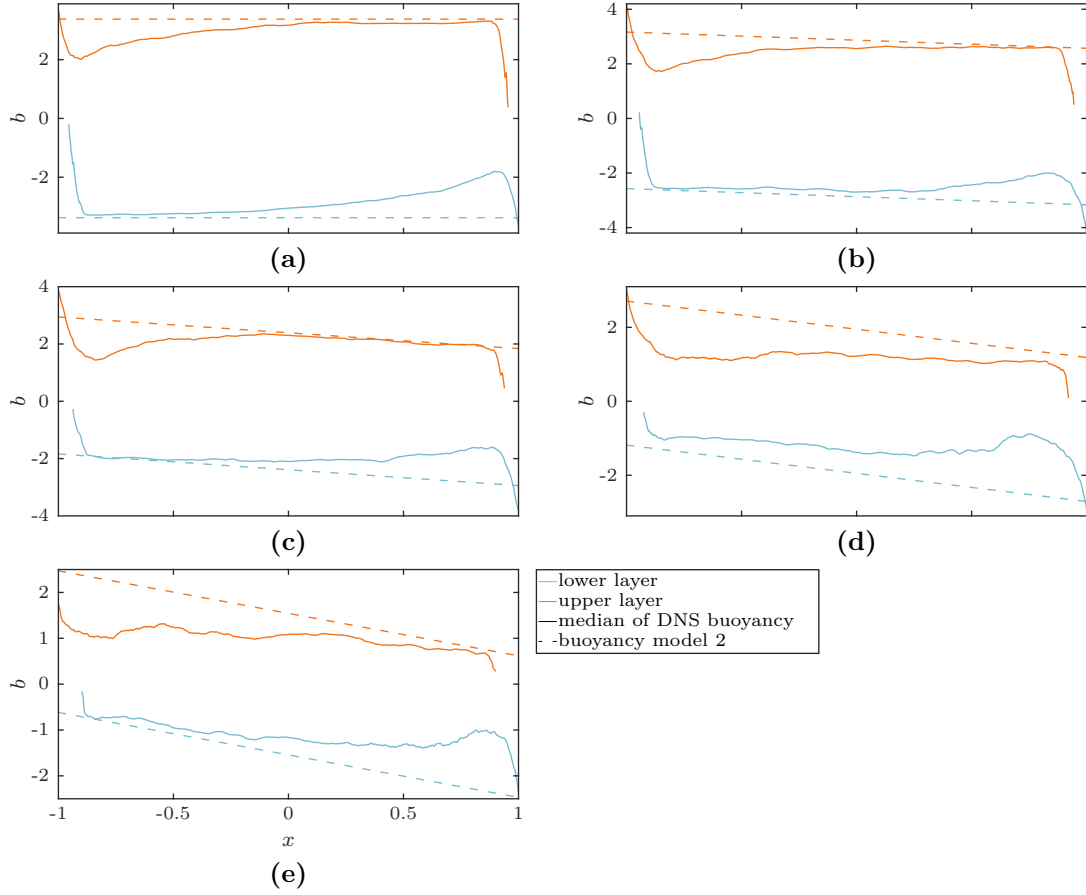


Figure 4.14: Comparing the modelled buoyancy (dashed lines) in layer 1 (blue) and layer 2 (red) with the time-averaged DNS buoyancy field (solid lines), where the latter is represented by the x -dependent median over the depth of each layer (see text). Displayed are the buoyancies at true buoyancy flux ratios (a) $\tilde{\Gamma} = 0$, (b) $\tilde{\Gamma} = 0.10$, (c) $\tilde{\Gamma} = 0.23$, (d) $\tilde{\Gamma} = 0.39$ and (e) $\tilde{\Gamma} = 0.60$. The median buoyancy per layer from DNS data is based on the layer definitions shown in fig. 4.1.

averaged DNS buoyancy field that was employed as measured buoyancy $\tilde{b}$ for the parameter estimation in §4.5.1. To investigate the systematic error ε_{bS} of model 2 with respect to the DNS data, we characterize the DNS buoyancy $\tilde{b}$ in each layer by its median. Specifically, we employ the definition of layer 1 and 2 displayed in fig. 4.1 and calculate the median of $\tilde{b}$ over the depth of the layer at each horizontal position x . The resulting medians of layer 1 and 2, $\text{med}_{a1}(\tilde{b})$ and $\text{med}_{a2}(\tilde{b})$, respectively, are displayed in fig. 4.14 as blue and red solid lines. The modelled buoyancy of each layer at the respective true buoyancy flux ratio $\tilde{\Gamma}$ is displayed as a dashed line. Note, that the median buoyancy of the layers is not defined at the position of the left- and right-hand plume for the lower and upper layer, respectively.

The difference between the modelled buoyancy and median DNS buoyancy displayed in fig. 4.14 is indicative of the systematic error ε_{bS} of model 2. Although there exists a reasonable agreement between the model and the DNS data for buoyancy flux ratios $\tilde{\Gamma} \leq 0.23$ (fig. 4.14a-c), the model generally overestimates the absolute value of the buoyancy in each layer, which corresponds to overestimating the local buoyancy difference $\delta b^* = b_{a2}^* - b_{a1}^*$ between the layers (cf. (4.4b)). This supports our assumption that the systematic error ε_{bS} in the buoyancy model causes the systematic error observed

in the parameter estimate (fig. 4.6), i.e., the shift of the results from the true buoyancy flux ratio $\tilde{\Gamma}$ towards values at $\Gamma_1 \cdot \Gamma_2 > \tilde{\Gamma}^2$. As the modelled buoyancy difference δb^* at $\tilde{\Gamma}$ exceeds the measured buoyancy difference $\delta \tilde{b}$, the buoyancy fluxes Γ_1 and Γ_2 are estimated at values greater than $\tilde{\Gamma}$ in order to reduce δb^* to the magnitude of $\delta \tilde{b}$ (see (4.4b)). Another indicator of the causal relationship between ε_{bS} and the systematic error of the estimated parameters is the significant increase of the deviation between modelled and DNS buoyancy as $\tilde{\Gamma}$ is raised from $\tilde{\Gamma} = 0.23$ to 0.39 (fig. 4.14c and 4.14d). This marked increase of ε_{bS} coincides with a notable shift of the estimated parameters away from the true value $\tilde{\Gamma}$, as can be seen from fig. 4.6c and 4.6d.

As a measure of the systematic error ε_{bS} of the model, we define a standard deviation $\tilde{\sigma}_{bS}$ between the modelled buoyancies of layer 1 and 2 and the median DNS buoyancy of the respective layer:

$$\tilde{\sigma}_{bS} = \sqrt{\frac{1}{2\Lambda} \int_{-\frac{\Lambda}{2}}^{\frac{\Lambda}{2}} \left[\left(b_{a1}^*(\tilde{\Gamma}) - \text{med}_{a1}(\tilde{b}) \right)^2 + \left(b_{a2}^*(\tilde{\Gamma}) - \text{med}_{a2}(\tilde{b}) \right)^2 \right] dx}. \quad (4.44)$$

In the above, we dropped the x -dependence of the modelled buoyancy and the median DNS buoyancy for better readability. Complementary to the above definition, we quantify the random error ε_{bR} of the model via a standard deviation $\tilde{\sigma}_{bR}$ between the time-averaged DNS buoyancy in each layer and the corresponding median

$$\tilde{\sigma}_{bR} = \sqrt{\frac{1}{\Lambda} \int_{-\frac{\Lambda}{2}}^{\frac{\Lambda}{2}} \int_{-\frac{\Lambda}{2}}^{\frac{\Lambda}{2}} \left[\left(m_{a1} \cdot \tilde{b} - \text{med}_{a1}(\tilde{b}) \right)^2 + \left(m_{a2} \cdot \tilde{b} - \text{med}_{a2}(\tilde{b}) \right)^2 \right] dx dz}, \quad (4.45)$$

where m_{a1} and m_{a2} are the mask functions of the layer definitions shown in fig. 4.1 (see (4.16)). As in (4.45), we dropped the x -dependency of the median and the (x, z) -dependency of the mask functions and the DNS buoyancy field.

The standard deviation $\tilde{\sigma}_{bR}$ represents the equivalent to the standard deviation $\tilde{\sigma}_b$ of the Gaussian noise in §4.5.2: both act as a measure of the random error between the modelled and the measured buoyancy. It might appear unintuitive that the measure $\tilde{\sigma}_{bR}$ of the random error of the buoyancy model is defined in (4.45) without reference to the modelled buoyancy. Indeed, a more rigorous approach might be to determine an ideal fit of the model to the DNS buoyancy field in each layer and employ this fitted modelled buoyancy in the definition of $\tilde{\sigma}_{bS}$ and $\tilde{\sigma}_{bR}$ instead of the DNS median. However, we chose the DNS median, because obtaining an ideal fit to the DNS data is non-trivial and because the median of the DNS buoyancy already behaves approximately in the manner of model 2, i.e., as a linear function in x over most of the interval $[-\frac{\Lambda}{2}, \frac{\Lambda}{2}]$. Non-linear behaviour of the median mainly occurs in the vicinity of the boundaries $x = \pm \frac{\Lambda}{2}$, where the layers as shown in fig. 4.1 border on a plume or include the jet-like continuation of the plume supplying the respective layer.

Fig. 4.15 shows the standard deviations $\tilde{\sigma}_{bS}$ and $\tilde{\sigma}_{bR}$ of the systematic and random error relative to the buoyancy difference $\Delta \tilde{b}$ between the peaks of the DNS buoyancy field's PDF in dependence of the true buoyancy flux ratio $\tilde{\Gamma}$. The resulting relative measure $\tilde{\sigma}_{bR}/\Delta \tilde{b}$ of the random error represents the equivalent to the noise-signal-ratio NSR_b of the Gaussian noise in §4.5.2.

Both the systematic and the random error of the modelled buoyancy, relative to the buoyancy difference $\Delta \tilde{b}$ between the layers, increase with the buoyancy flux ratio $\tilde{\Gamma}$ (fig. 4.15). Indeed, both errors show a similar behaviour over $\tilde{\Gamma}$, but for the marked increase of the systematic error between $\tilde{\Gamma} = 0.23$ and 0.39, which is absent in the random error. We discussed this abrupt increase of the

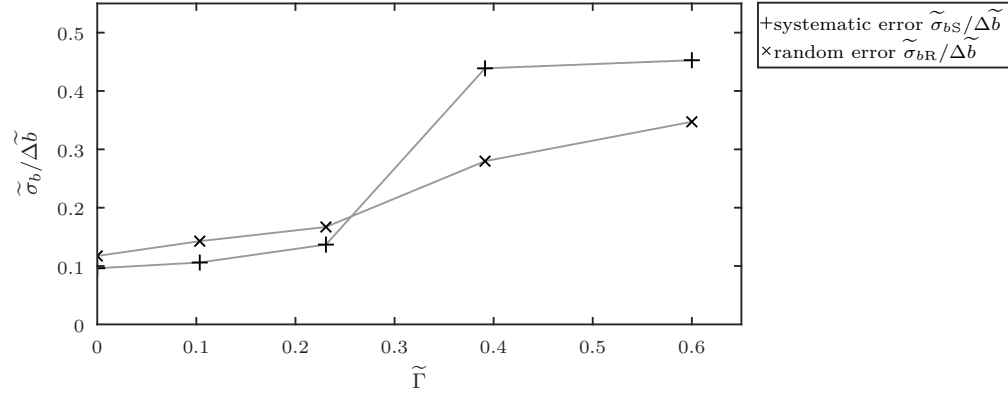


Figure 4.15: Systematic and random error of the modelled buoyancy field with respect to the DNS data in dependence of the true buoyancy flux ratio $\tilde{\Gamma} \in \{0, 0.10, 0.23, 0.39, 0.60\}$. The systematic and random error of the model are given in terms of the corresponding standard deviations, $\tilde{\sigma}_{bS}$ and $\tilde{\sigma}_{bR}$, respectively, relative to the buoyancy difference $\Delta\tilde{b}$ between the peaks of the DNS buoyancy field's PDF. The standard deviations are defined as given in (4.44) and (4.45).

systematic error above in context of fig. 4.14. For $\tilde{\Gamma} \leq 0.23$, $\tilde{\sigma}_{bS}$ and $\tilde{\sigma}_{bR}$ in fig. 4.15 are of similar magnitude. However, the systematic error in the corresponding estimated parameters (fig. 4.6a-c) is much less pronounced than the random error of the parameter estimate: the results (Γ_1, Γ_2) are shifted only marginally away from the true value $\tilde{\Gamma}$ in fig. 4.6a-c, but the spread of (Γ_1, Γ_2) around an isoline $\Gamma_1 \cdot \Gamma_2$ is significant. If the systematic and random error of the parameter estimation results are each caused by the systematic and random error of the buoyancy model, respectively, the random error of the model has a much greater impact on the parameter estimation than the systematic error of the model. The systematic error in the parameter estimate only becomes significant at $\tilde{\Gamma} \geq 0.39$ (fig. 4.6d-e), where the systematic error $\tilde{\sigma}_{bS}$ of the model notably exceeds the random error $\tilde{\sigma}_{bR}$, as shown in fig. 4.15.

With the standard deviations $\tilde{\sigma}_{bS}$ and $\tilde{\sigma}_{bR}$, we defined a measure of the systematic and random error of the buoyancy model 2. Let us now consider measures of the systematic and random error of the estimated parameters (Γ_1, Γ_2) from DNS data, in order to examine the relationship between errors of the buoyancy model and errors of the parameter estimation. It is possible to define standard deviations corresponding to the systematic and random error of (Γ_1, Γ_2) in a form equivalent to $\tilde{\sigma}_{bS}$ and $\tilde{\sigma}_{bR}$ in (4.44) and (4.45). In this case, the median is replaced by the parameter estimation result $(\Gamma_{1S}, \Gamma_{2S})$ that we expect if the buoyancy model differed from the DNS data solely by a systematic error, i.e., $(\Gamma_{1S}, \Gamma_{2S})$ should lie on the imagined isoline of $\Gamma_1 \cdot \Gamma_2$ around which the results are distributed. Following this approach, choosing $\Gamma_{1S} = \Gamma_{2S} = \sqrt{\text{med}(\Gamma_1 \cdot \Gamma_2)}$, we find that the resulting standard deviation associated with the random error gives near identical values to the general standard deviation $\sigma(\Gamma_1, \Gamma_2)$ of the estimated buoyancy fluxes with respect to the true value $\tilde{\Gamma}$ (see (4.43)). This agrees with our earlier observation that the error in the parameter estimation is dominated by the random error. Hence, we are mainly interested in the random error and refrain from quantifying the random and systematic error of the parameter estimate separately. Instead, we utilize the standard deviation $\sigma(\Gamma_1, \Gamma_2)$ of (4.43) as an approximate measure of the random error.

We are now able to consider the random error $\sigma(\Gamma_1, \Gamma_2)$ of the buoyancy fluxes estimated from DNS data in dependence of the random error $\tilde{\sigma}_{bR}$ of the buoyancy model and the true buoyancy flux ratio $\tilde{\Gamma}$. In §4.5.2, we examined the same relationship for a measured buoyancy whose difference to the

modelled buoyancy was modelled as Gaussian noise (fig. 4.13). However, in contrast to the approach in §4.5.2, we are now limited to a data set of five configurations, where both the true buoyancy flux ratio $\tilde{\Gamma}$ and the model error $\tilde{\sigma}_{bR}$ differ for each configuration. Thus, we cannot directly investigate the dependence of $\sigma(\Gamma_1, \Gamma_2)$ on $\tilde{\Gamma}$ or $\tilde{\sigma}_{bR}$, but rather compare the DNS results to those obtained with Gaussian noise. The errors $\sigma(\Gamma_1, \Gamma_2)$ of the estimated parameters for both types of measurement data are shown in fig. 4.16, displayed at the configurations $(\tilde{\Gamma}, \tilde{\sigma}_{bR})$ determined by the DNS data.

Fig. 4.16a shows the error $\sigma(\Gamma_1, \Gamma_2)$ of the parameter estimate plotted over the random error $\tilde{\sigma}_{bR}$ of the buoyancy model relative to the buoyancy difference $\Delta\tilde{b}$ between the layers; fig. 4.16b presents the same data in dependence of the true buoyancy flux ratio $\tilde{\Gamma}$. To relate the data points in both plots, the corresponding values of $\tilde{\Gamma}$ and $\tilde{\sigma}_{bR}/\Delta\tilde{b}$ are added at the top of fig. 4.16a and 4.16b, respectively. Recall, that the relative measure $\tilde{\sigma}_{bR}/\Delta\tilde{b}$ of the random error of the model is equivalent to the noise-signal ratio NSR_b of the Gaussian noise in §4.5.2.

From fig. 4.16, we find that the error $\sigma(\Gamma_1, \Gamma_2)$ corresponding to the DNS data considered in §4.5.1 (black ‘+’-markers) greatly exceeds the ‘modelled’ error values corresponding to the measured buoyancy generated with Gaussian noise in §4.5.2 (‘o’-markers). However, we did not expect these values to agree quantitatively: the concept of buoyancy values over the depth of a layer following a Gaussian distribution is a highly idealized one. Moreover, our definition of the random error $\tilde{\sigma}_{bR}$ between the modelled and the true buoyancy field is based on the buoyancy field of the entire domain without reference to the number N_s of sampling points. Hence, we expect the actual random error from a limited set of $N_s = 9$ buoyancy measurements to exceed $\tilde{\sigma}_{bR}$.

Qualitatively, the error $\sigma(\Gamma_1, \Gamma_2)$ from the DNS data behaves similarly to the error from the buoyancy data generated with Gaussian noise, although the former increases more rapidly with $\tilde{\Gamma}$ and/or $\tilde{\sigma}_{bR}/\Delta\tilde{b}$ than the latter. In particular, the increase of the error $\sigma(\Gamma_1, \Gamma_2)$ with $\tilde{\Gamma}$ and/or $\tilde{\sigma}_{bR}/\Delta\tilde{b}$ is com-

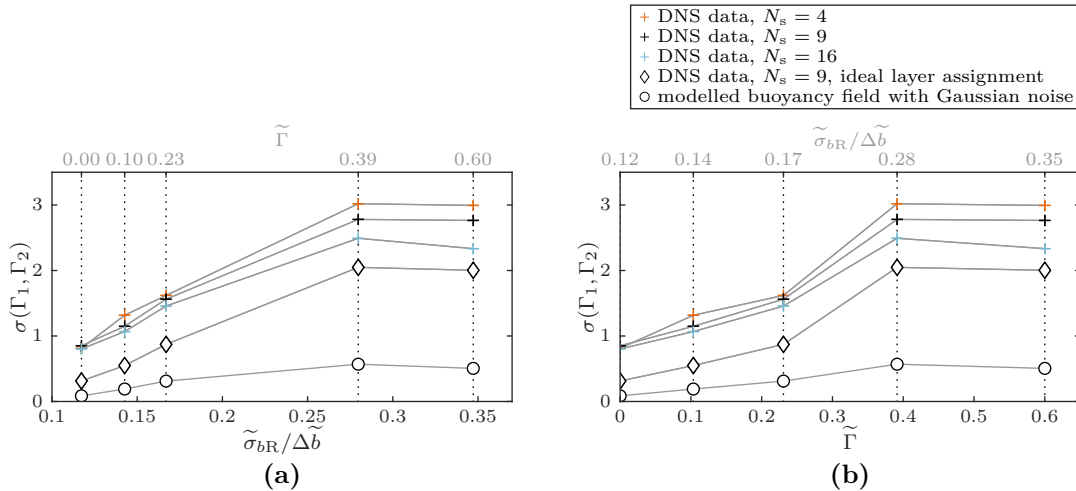


Figure 4.16: Relationship between the error $\sigma(\Gamma_1, \Gamma_2)$ of the estimated parameters, the random error $\tilde{\sigma}_{bR}$ of the buoyancy model and the true buoyancy flux ratio $\tilde{\Gamma}$: comparing results from the DNS data at different numbers N_s of sampling points (‘+’) and under ideal layer assignment (‘◇’) with the predictions made from Gaussian noise (‘o’) in §4.5.2. Both sub-figures display the same data, plotted over (a) the relative standard deviation $\tilde{\sigma}_{bR}/\Delta\tilde{b}$ of the random error of the buoyancy model and (b) the true value $\tilde{\Gamma}$ of the buoyancy flux ratio. To relate the data points of both plots, the respective values of $\tilde{\Gamma}$ or $\tilde{\sigma}_{bR}/\Delta\tilde{b}$ are added at the top of the graphs.

parable in both types of data sets ('+' and 'o'), if we consider $\tilde{\Gamma} \in \{0, 0.10, 0.23\}$ and $\tilde{\Gamma} \in \{0.39, 0.60\}$ separately. It is between $\tilde{\Gamma} = 0.23$ and 0.39 , where the behaviour of the error $\sigma(\Gamma_1, \Gamma_2)$ of both data sets differs most significantly, which coincides with a marked increase of the systematic error $\tilde{\sigma}_{bS}$ of the modelled buoyancy (fig. 4.14). Hence, the impact of $\tilde{\sigma}_{bS}$ on $\sigma(\Gamma_1, \Gamma_2)$ might be bigger than we assumed based on our attempt to isolate the random error in the parameter estimation result by employing $\text{med}(\Gamma_1 \cdot \Gamma_2)$. Alternatively, the distribution of estimated buoyancy fluxes around an isoline in $\Gamma_1 \cdot \Gamma_2$ might not solely arise from the random error $\tilde{\sigma}_{bR}$ in the modelled buoyancy but also be impacted by the systematic error $\tilde{\sigma}_{bS}$.

The notable increase of the error $\sigma(\Gamma_1, \Gamma_2)$ of the parameter estimate at $0.23 < \tilde{\Gamma} < 0.39$ in fig. 4.16b coincides with a change in the character of the stratification and flow (chapter 2). As the buoyancy flux ratio is increased from $\tilde{\Gamma} = 0.23$ to 0.39 , the secondary circulations of the mean flow disappear (fig. 2.7) and the two layers of the stratification become less distinct, as can be seen in the buoyancy field's PDF from the overlap of the two peaks at $\tilde{\Gamma} \geq 0.39$ (fig. 2.4). Thus, the estimation of the buoyancy flux ratios (Γ_1, Γ_2) performs better for stratifications consisting of layers of distinct buoyancy and is compromised when buoyancy values are not unique to the layers.

As we draw on a very limited data set of five configurations in fig. 4.16, we cannot make a definite statement about the behaviour of the error $\sigma(\Gamma_1, \Gamma_2)$ of the estimated parameters with respect to the random error $\tilde{\sigma}_{bR}$ of the modelled buoyancy field and the true buoyancy flux ratio $\tilde{\Gamma}$. However, we found similarities between the behaviour of $\sigma(\Gamma_1, \Gamma_2)$ from DNS data and buoyancy data generated with Gaussian noise ('+' and 'o' in fig. 4.16) as well as similarities between the corresponding distributions of estimated buoyancy fluxes in the parameter space (Γ_1, Γ_2) (cf. fig. 4.6, 4.9 and 4.10). This indicates that the random error of the parameter estimate is indeed caused by the random error $\tilde{\sigma}_{bR}$ of the modelled buoyancy, i.e., by a difference in homogeneity between the buoyancy field in each layer of the model and the DNS data, and that modelling this difference as Gaussian noise is sufficient to reproduce the effect on the parameter estimation qualitatively. Thus, it is indicated that the accuracy of the parameter estimation from the DNS data is indeed mainly dependent on the random error $\tilde{\sigma}_{bR}/\Delta\tilde{b}$ of the buoyancy model relative to the buoyancy difference between the layers, in a manner similar to that shown in fig. 4.13.

We do not assume that the error $\sigma(\Gamma_1, \Gamma_2)$ of the parameter estimate is solely caused by inaccuracies of the buoyancy model: the size N_s of the set of buoyancy measurements and the accuracy of the layer assignment also impact the parameter estimation. Indeed, we find that the results from a number of $N_s \in \{4, 9, 16\}$ sampling points, plotted as red, black and blue '+'-markers in fig. 4.16, respectively, decrease in $\sigma(\Gamma_1, \Gamma_2)$ with increasing N_s . This appears intuitive, since the buoyancy values of the clusters, which determine layer 1 or 2, more accurately resemble the buoyancy of the entire layers with increasing N_s (§4.3.4). In particular, we find that the number of sampling points has the greatest impact on the error $\sigma(\Gamma_1, \Gamma_2)$ of the estimated parameters at large values of the true buoyancy flux ratio $\tilde{\Gamma}$, where the buoyancy field is most heterogeneous relative to the buoyancy difference between the layers (see fig. 4.15) and a large sample size is more relevant to accurately represent the buoyancy of the layer. Although the sample size N_s impacts the accuracy of the parameter estimate, the difference in $\sigma(\Gamma_1, \Gamma_2)$ between different values of N_s is small compared to the absolute magnitude of the error. Hence, we consider the sample size as a point to be addressed last when aiming for accurate parameter estimation from simple models such as the one considered in this section.

In contrast, the correct layer assignment appears to play a significant role for an accurate parameter

estimation: the ‘ $\diamond$ ’-markers in fig. 4.16 show the error $\sigma(\Gamma_1, \Gamma_2)$ corresponding to a parameter estimate from a set of $N_s = 9$ buoyancy measurements that has been separated into layer 1 and 2 according to the layer definition shown in fig. 4.1, instead of via a clustering algorithm. The resulting error values $\sigma(\Gamma_1, \Gamma_2)$ are smaller than the errors we obtained for any of the parameter estimates from clustered samples at $N_s \in \{4, 9, 16\}$ (‘+’-markers in fig. 4.16). Particularly, the correct layer assignment significantly decreases the error at $\tilde{\Gamma} \leq 0.23$, where the sample size N_s has comparatively little impact. However, our comparison in §4.3.4 of the layers’ mean buoyancy obtained via clustering and under ideal layer assignment showed little difference between the corresponding PDFs (fig. 4.3). Hence, the great sensitivity of the parameter estimate with respect to the layer assignment might be caused by sample points that truly belong to the plumes but are assigned to one of the layers by the clustering. The ideal layer assignment, on which the results plotted as ‘ $\diamond$ ’-markers in fig. 4.16 are based, excludes sample points that belong to the plumes. Note, that the pronounced increase of $\sigma(\Gamma_1, \Gamma_2)$ at $0.23 < \tilde{\Gamma} < 0.39$ is similar for ideal layer assignment and layer assignment via clustering. Hence, the increase of $\sigma(\Gamma_1, \Gamma_2)$ that occurs as the buoyancy field becomes notably more heterogeneous is not an artefact of the layer assignment via clustering, or of our choice of clustering method or feature space.

Overall, we find that neither an increased number N_s of buoyancy measurements nor an ideal layer assignment give parameter estimation results from DNS data with a satisfactory accuracy; the smallest error $\sigma(\Gamma_1, \Gamma_2)$ from DNS data displayed in fig. 4.16 is of a magnitude $\sigma(\Gamma_1, \Gamma_2) \approx 0.3$. Hence, it might not be possible to achieve a reasonable parameter estimate from the buoyancy model 2 without a modification of the model or an adjustment of the cost functional that compensates the modelling error.

4.6 Conclusions

In this chapter, we considered the inverse problem of determining the buoyancy flux ratios Γ_1 and Γ_2 on the bottom and top boundary from sparse measurements of the DNS buoyancy field in the steady state. We based the parameter estimation on the general steady state model 2 (§2.8), since model 1 generally does not describe the buoyancy field as a bijective function of the buoyancy fluxes on the boundary. The resulting problem of minimizing a non-smooth cost functional, due to the non-smooth character of the modelled buoyancy field, was transformed into a smooth optimisation problem by splitting the problem into two parts. We first assign the sampling points at which buoyancy measurements are taken to the upper or lower layer of the stratified buoyancy field, using k -means clustering, and subsequently estimate the buoyancy flux ratios Γ_1 and Γ_2 by solving a least-squares problem via the method of steepest descent.

The results of the parameter estimation from DNS data are widely distributed in the parameter space, which suggests that the reconstruction of the buoyancy flux ratios Γ_1 and Γ_2 from samples of the buoyancy field suffers from several problems. The distribution of the estimated parameters in the parameter space is not Gaussian around the point of the true buoyancy fluxes, $(\Gamma_1, \Gamma_2) = (\tilde{\Gamma}, \tilde{\Gamma})$, but shows that the main issue of the parameter estimation is that it does not significantly favour symmetric configurations $\Gamma_1 = \Gamma_2$, which correspond to the true configurations, within a family of solutions that share a similar value $\Gamma_1 \cdot \Gamma_2$. Moreover, we observe a systematic error in the results, which generally overestimate the true buoyancy flux ratio $\tilde{\Gamma}$: $\Gamma_1 \cdot \Gamma_2 \gtrsim \tilde{\Gamma}^2$. At true buoyancy flux ratios $\tilde{\Gamma} > 0.23$, the spread in the product $\Gamma_1 \cdot \Gamma_2$ of the results and the systematic error increases noticeably in comparison

to $\tilde{\Gamma} \leq 0.23$.

The parameter estimation does not fail because the steepest descent method fails to minimize the cost functional, but due to the shape of the cost functional, whose minimum is not closely correlated with the true value of the buoyancy flux ratio. A comparison between parameter estimation from DNS data and noisy measurement data generated from model 2 suggests that the wide distribution of results in the parameter space occurs because the layers of the stratification are modelled as more homogenous than is the case for the DNS data. The resulting error in the estimated buoyancy flux ratios (Γ_1, Γ_2) , appears to be mainly dependent of the difference in homogeneity between model and DNS data relative to the buoyancy difference between the layers of the stratification. Thus, the parameter estimation is more sensitive to modelling errors at large values of the true buoyancy flux ratio $\tilde{\Gamma}$, where the buoyancy difference between the layers is small. Moreover, we find that the accuracy of the parameter estimate is correlated with the character of the buoyancy field's PDF. Specifically, we observed that stratifications with layers of distinct buoyancy result in notably smaller errors in the estimated buoyancy flux ratios compared to cases where buoyancy values are not unique to each layer. Hence, in attempts to discriminate localised and distributed sources from temperature measurements, stratifications of layers whose buoyancy values do not overlap may prove comparatively less challenging. Such stratifications could serve as a useful starting point for tackling more general source discrimination problems.

How could we improve estimates of the boundary buoyancy fluxes from samples of the buoyancy field in configurations of combined localised and distributed heating considered in this chapter? Simple (multi-) zone models with zones of homogeneous buoyancy and flow are commonly employed to solve inverse heat transport problems in building applications [7]. This suggests that, although modelling errors pose a problem in the parameter estimation, it may not be necessary to construct a more detailed model than the simple two-dimensional model utilised in this chapter. Indeed, there is a strong incentive for using simple models in parameter estimation problems since they require little computational effort and tend to be more reliable in their parameter estimate [54]. Instead of altering the model, it might be possible to successfully utilise model 2 for parameter estimation with an approach that compensates the modelling error, such as with a Bayesian framework [49, 103].

An inversion of model 2 would represent an approach for identifying different types of buoyancy flux sources in a steady state, which cannot be achieved if the buoyancy layers subjected to localised and distributed heating or cooling are modelled as uniform. This is particularly attractive, because we showed analytically that the exact position of the interface is not necessary to invert model 2, which would allow for a parameter estimation from a low number of sensors. The inversion of model 2 with respect to the buoyancy fluxes on the boundary is possible, because we can utilise the horizontal gradient of the buoyancy field in each layer. Note, that the horizontal buoyancy gradient is a result of distributed heating or cooling in combination with a flow over the corresponding source in the opposite direction to the gradient (§2.5.2). In settings of combined localised and distributed heating where a flow over the distributed source is not present, a horizontal buoyancy gradient might not exist or does not contain information about the distributed sources, such that localised and distributed sources would not be distinguishable in the steady state with an approach equivalent to the one presented here.

Inverse heat transport problems in buildings are typically formulated using a multi-zone model, where each zone is assumed to be well-mixed, such that parameter estimation may rely on as little as

one sensor per zone [78]. A parameter estimation from a stratified model requires at least one sensor per layer of the stratification and an additional sensor per layer if gradient information of the buoyancy field is to be used. In case of model 2 discussed in this chapter, this corresponds to a minimum of four sensors or sampling points, provided both layers of the stratification are sampled. Although an increase in the number of sampling points reduces the error of the parameter estimation, we found that this effect is most pronounced at high values of the buoyancy flux ratio $\tilde{\Gamma} > 0.23$, whereas, at smaller buoyancy flux ratios, the number of sampling points has comparatively little impact. Moreover, as noted above, parameter estimation results are less sensitive to discrepancies between model and measurement at low values of $\tilde{\Gamma}$ than at higher values $\tilde{\Gamma} > 0.23$. Thus, the cost in terms of sensors required and effort to solve the inverse problem would be lowest in scenarios where the buoyancy difference between the layers of the stratification is expected to be large, corresponding to a low value of the buoyancy flux ratio $\tilde{\Gamma}$. Conversely, in cases where the ratio of the distributed to the localised heating or cooling is large, i.e., where the effect of the distributed sources is less likely to be negligible, the inverse problem becomes more difficult and costly to solve.

Any inverse problem utilising a piecewise defined model of the buoyancy field, such as e.g. the emptying-filling box model, presents the challenge of minimising a non-smooth cost functional. Here, we assigned the sampling points to the upper or lower layer of the stratification via k -means clustering, resulting in a smooth cost functional that can be minimized with deterministic optimisation methods. However, the results of the parameter estimation in comparison with the results of the clustering imply that sample points that are located in a plume but are erroneously assigned to one of the layers significantly increase the error of the parameter estimation result. Such erroneous assignment was expected in our approach, since the clustering algorithm classifies all points as belonging to one of two clusters, which were interpreted as layer 1 or 2 according to their mean buoyancy. Note, however, that the probability for placing sampling points in the plumes might be smaller in similar configurations, depending on the aspect ratio of plumes in comparison with the bulk, and thus the issue of erroneously assigned sample points might be less pronounced. Regardless, the sensitivity of the parameter estimate with respect to samples of the plumes suggests that any approach of layer assignment should allow for the exclusion of outliers, whether the layer assignment is addressed separately, as in this thesis, or is included in the minimisation of a non-smooth cost functional, e.g. with a stochastic method.

In this chapter, we considered inverse problem for steady states of combined localised and distributed heating. Transient states contain additional information about the response of a system, which can be utilised in parameter estimation. Brouns et al. [23] for example realise a discrimination between two different additive heat sources by assuming characteristic dynamics for each. However, the estimation of time-dependent parameters from a transient state presents a more challenging problem than steady state parameter estimation, since it corresponds to the estimation of a time-dependent function in an infinite dimensional space of functions [83], and finding a suitable model of the transient state is non-trivial. The extension of model 1 for transient states introduced in chapter 3 might be too inaccurate a representation of the buoyancy field to be utilised in a parameter estimation. Apart from the differences between the model and the DNS data discussed in chapter 3, model 1 is based on the assumption that the transient buoyancy field consists of a stratification of two well-mixed layers at all times. Thus, it cannot reproduce spatially dependent processes such as the horizontal propagation of changes in the buoyancy and flow field, which characterize the transient state.

A generalisation of model 2 to transient states would allow for a spatially variable buoyancy field

and volume flux in the horizontal at the cost of solving non-linear partial differential equations at each iteration of the optimization routine. Moreover, the extension of the steady state model to transient states involves careful consideration to avoid discontinuities: under the assumption of quasi-steady plumes, abrupt changes of the localised buoyancy fluxes would result in spatial discontinuities of the modelled state variables in the horizontal. Hence, a transient model 2 might make the use of unsteady plume models necessary. Choosing the level of complexity of a model that balances sufficient representation and efficient computation is a general challenge of inverse problem settings and further work is required to determine a suitable choice of transient model for the configurations considered in this thesis.

In this chapter, we explored the potential of a simple model of stably stratified states in distinguishing between the causal localised and distributed sources from measurements of the buoyancy field. Such estimates of heat sources or sinks are of particular interest in building design and the control of indoor climates, typically oriented towards minimizing energy consumption, where the factors determining heat gains or losses may be difficult or expensive to measure directly. This task becomes more challenging if the considered system is subjected to multiple sources and the measured buoyancy field results from a superposition of the effect of all sources. In this case, different parameters that impact the thermal system may be identified by the character of the associated heat source or sink. Factors such as occupancy numbers and the operation of electrical appliances and lights, for example, could be associated with heating via localised sources, whereas time-variable solar gains due to the opening and shutting of blinds could be related to distributed sources. Parameter estimation based on a simple, and thus computationally affordable, model that captures the combine effect of distributed and localized sources on the buoyancy field may thus ultimately contribute to improve and sustain energy efficiency in buildings.

Chapter 5

Conclusions

In this thesis, we studied the effect of combinations of localised and distributed buoyancy sources on the boundary of a box on the buoyancy field and flow of the enclosed fluid. This configuration was considered both in a forward problem, determining the physical state from the causative boundary conditions, and in an inverse problem, attempting to estimate the boundary conditions from samples of the state. The case was chosen as an idealised example of the rich and challenging real-world problems that involve heterogeneous heating and cooling. In the following, we give a summary of the contributions of this work (§5.1), draw conclusions (§5.2) and give an outlook on further work (§5.3).

5.1 Contributions

Steady states (chapter 2)

Using direct numerical simulations, we investigated the steady states arising from a combination of localised and distributed sources on the top and bottom boundary of a closed domain under varying ratios Γ of the distributed to the localised source strength. In contrast to previous work on combined localised and distributed buoyancy sources [25, 47, 85, 116], the numerical approach allowed us to vary only the buoyancy flux ratio Γ while keeping the total buoyancy flux on each boundary constant, such that the impact of Γ could be studied without having to resort to a model. We find that the buoyancy flux ratio Γ is a key parameter in determining the response of the system. In the absence of distributed heating or cooling, localised sources result in two plumes of opposite orientation, which maintain a stable two-layer stratification. The two-layer stratification persists for finite distributed source strengths at $\Gamma < 1$, where the stabilising effect of the localised sources exceeds the destabilising effect of the distributed sources. The buoyancy difference between the layers decreases with increasing Γ , until the two-layer stratification is destroyed for $\Gamma > 1$.

Hunt, Holford and Linden [47] and Partridge and Linden [85] noted horizontal inhomogeneities of the buoyancy field for some configurations of combined localised and distributed sources in a ventilated enclosure, however, in these publications inhomogeneities were mainly of interest if they were so pronounced as to make a one-dimensional model of the buoyancy field inapplicable. To the best of our knowledge, this thesis is the first systematic investigation of horizontal structures arising in configurations of combined localised and distributed sources. For $\Gamma < 1$, we observed an increasing horizontal buoyancy gradient with increased distributed source strength and an increasingly tilted in-

interface between the two layers of the stratification. The tilt of the interface impacted the strength of the primary large-scale circulation and the mean flow structure. We were able to construct a simple two-dimensional model of the buoyancy field which accounts for the horizontal buoyancy gradient and is able to reproduce the buoyancy difference between the layers and the tilt of the interface with good accuracy, as well as approximating the volume flux of the primary large-scale circulation. A comparison of the two-dimensional model with a one-dimensional model in the tradition of previous publications on combined localised and distributed heating [25, 85, 116] showed that the horizontal buoyancy gradient can be neglected in predictions of the buoyancy difference between the layers at small values of the buoyancy flux ratio Γ but is crucial for the prediction of the volume flux.

Transient states (chapter 3)

We investigated transient states resulting from unsteady localised and distributed sources, where the initial and asymptotic final steady state is a stable two-layer stratification and the total buoyancy flux on each boundary is constant. A step-increase of the buoyancy flux ratio Γ corresponds to a simultaneous increase of the distributed source strength and a decrease of the localised source strength; for a step-decrease of Γ , the change of the respective source strengths is reversed. A stable stratification is maintained in the transient state, although the response of the system differs in character for a step increase and decrease of Γ . For a step-increase of Γ , convection from the distributed sources causes vertical mixing in each layer, such that the transient buoyancy field is similar to that of a steady state at every instant. In contrast, a step decrease of Γ to a configuration solely heated and cooled by localised sources initially results in a gravity current across the domain and the formation of additional layers above and below the original stratification, before a two-layer stratification is regained. We presume that the mixing in the layers due to convection from a distributed source strongly impacts the transition time to the final steady state, as we observed a significantly longer transition time for a decrease of Γ than for an increase of Γ .

Modelling the transient buoyancy field as a stratification of two homogeneous layers can give only a rough approximation of the observed state and shows a scaling of the transition time with Γ that contradicts observation. The accuracy of the model cannot be improved by considering the fluid discharged from the plumes following a buoyancy flux step change as additional layers, after the approach of Bower et al. [20] for modelling the stratification from unsteady localised sources in an enclosure. We observed that the horizontal propagation of buoyancy changes greatly impacts the dynamic of the transient system, causing a delayed response of the buoyancy field and non-monotonic behaviour in the strength of the large-scale circulation and the kinetic energy. Such dynamics cannot be reproduced by one-dimensional models, where the homogeneity of the layers corresponds to an instantaneous heat transfer.

Inverse heat transfer problem (chapter 4)

We attempted to estimate the buoyancy flux ratios Γ on the top and bottom boundary of the enclosure from samples of a stably stratified DNS buoyancy field in the steady state, utilising a two-dimensional model of the buoyancy field. Parameter estimation from any model of a stratification that involves a density jump at the interface between the layers corresponds to the minimisation of a non-smooth cost functional. In this thesis, the non-smooth aspect of the problem was separated from fitting the model to the DNS data by first assigning samples of the DNS buoyancy field to an upper or lower layer of

the stratification via clustering and subsequently minimising a smooth cost functional to estimate the buoyancy flux ratios on the boundaries. The inverse problem was simplified by reducing the parameter space to two dimensions, corresponding to the buoyancy flux ratios on the top and bottom boundary.

The estimation of buoyancy flux ratios on the boundaries from DNS data yielded results with a large standard deviation from the true values, due to differences in the homogeneity of the layers between the simple model and the DNS buoyancy field. The parameter estimation is more sensitive to differences between model and measurement for weak stratifications, i.e., from the set of DNS simulations considered in this thesis, for cases where the distributed sources notably impact the buoyancy field. The assignment of buoyancy samples to layers notably contributes to the error in the estimated buoyancy flux ratios, however, not because the clustering failed its objective, but because our approach did not allow outliers in the buoyancy samples to be excluded.

5.2 Discussion

How do combinations of localised and distributed sources affect the buoyancy and flow of a fluid? We showed that stable stratifications can arise from such a combination of sources, if the stabilising effect of the localised sources dominates over the destabilising effect of the distributed sources. However, in contrast to stratifications from purely localised sources, horizontal structures can arise in the flow and the buoyancy field that are crucial in characterising the physical state. It is important to recognize that the horizontal buoyancy gradient we observed in the configurations studied in this thesis, and consequently other characteristics such as the shape of the interface, arises from a horizontal flow over the distributed sources. The character of the flow over the distributed sources shapes the horizontal dependence of the buoyancy field in the bulk and the localised sources may be considered as amplifiers of the effect of the flow in the bulk, since the resulting plumes depend on the buoyancy of the ambient fluid. Hence, rather than implying a particular buoyancy structure for other configurations of combined localised and distributed sources, our work highlights the importance of including the flow in the bulk into considerations of the states arising from such heterogeneous thermal boundary conditions.

Horizontal dependencies are of different significance in the steady and transient states. In the steady state, a horizontal dependence of the buoyancy field may be neglected, if the strength of the distributed sources is small compared to the localised ones. In contrast, we observed spatial processes in the horizontal to be crucial for the time dependence of the transient state, since the change in the source strengths causes a change of buoyancy to propagate horizontally across the domain. If this spatial component is neglected, we cannot fully reproduce the time dependence even of quantities that are, in themselves, not spatially dependent. However, the effect of horizontal transport processes was most pronounced shortly after the change of the source strengths and may be negligible at later times, as the system approaches a steady state. Another difference between the steady and the transient states is the significance of the ratio Γ of the distributed to the localised source strength. For the steady states, Γ is a suitable parametrisation of the boundary conditions, which plays a key role in determining the resulting buoyancy field, e.g. being critical for the existence of a two-layer stratification. However, it is not clear from our observations whether Γ remains a meaningful parametrisation in the transient states. Indeed, localised and distributed sources drive different processes in the transient state, which we presume to be marked by different time-dependencies. Hence, we expect that in describing a transient state, distinguishing between localised and distributed source strengths may

be more appropriate than a conjunction of both in Γ . It should, however, be recognized that our investigation of transient states in this thesis is far from exhaustive: different behaviours may emerge for different amplitudes or rates of change of the unsteady source strengths and if the change of the localised and distributed sources is not synchronised. In particular, the generalised steady state model we developed suggests that the two-layer stratification may break down during the transient and re-establish in dependence of the rate of change of the sources.

If the stabilising effect of the localised sources dominates the destabilising effect of the distributed sources, the resulting buoyancy field can be modelled in the steady state as a simple two-layer stratification. At low distributed source strengths, the layers may be considered well-mixed, though generally, horizontal buoyancy gradients have to be accounted for, where the buoyancy gradient depends on the flow over the distributed sources. Such two-dimensional models can reproduce key characteristics of the buoyancy field with good accuracy, although we presume that they will not remain accurate close to $\Gamma = 1$, where localised and distributed sources are of equal strength and the two-layer stratification is predicted to break down. Modelling a transient state from combined localised and distributed sources is more challenging: a one-dimensional model, assuming homogeneous layers, does not give a good representation of the transient buoyancy field. Our work suggests that to improve this model, accounting for spatial dependence in the horizontal would be more promising than modelling the transient buoyancy field with a more sophisticated vertical stratification. However, to construct a two-dimensional model for the transient based on the corresponding steady state model presented in this thesis requires careful consideration to avoid discontinuities and would be more computationally demanding to solve than a one-dimensional model. Although the simple models presented in this thesis can reproduce central characteristics of the buoyancy field in the steady state, they cannot give an accurate representation of the entire spatially dependent buoyancy field. This limitation becomes crucial when utilising such models in an inverse problem setting.

How could we use our understanding of the effect of combined localised and distributed sources to determine heterogeneous thermal boundary conditions from measurements in the bulk? First, it is important to recognize that not all physical states that arise from combined localised and distributed sources of buoyancy allow for the sources to be distinguished using simplified models such as the ones employed in this thesis. A well-mixed buoyancy field, for example, may be caused by heterogeneous buoyancy sources whose effect is obscured by a sufficiently strong flow. However, we may be able to use measurements of the flow to identify cases that limit the conclusions that can be drawn in an inverse approach. Generally, we require flow and temperature information to discern localised and distributed sources. Moreover, if a stratification in distinct layers exists, measurements of the state in each layer are required, with several horizontally distributed sensors per layer to obtain information on the horizontal temperature gradient. As the structure of the temperature field is unknown, this corresponds to a large number of sensors. Sensor placement and the minimal number of sensors that is sufficient to analyse a state is a central problem when estimating source strength from a temperature field modelled as consisting of distinct layers. Moreover, rather than utilising a single model, as in this thesis, one would generally require a set of models, to cover cases with different numbers of layers or the break-down of a clear stratification.

Our work showed that to utilise simple stratification models in an inverse problem setting, special attention needs to be paid to compensating the difference between model and measurement, for example via a Bayesian approach. It is, however, not clear whether an accurate parameter estimate can thus

be obtained from simple stratification models. In particular, the increased sensitivity of the estimated parameters with respect to modelling errors for cases where both localised and distributed sources have a significant impact, may, unfortunately, limit the applicability of simple models of combined localised and distributed sources in cases where accounting for both source types would be most appropriate. If simple stratification models can be used in parameter estimation, the associated cost would generally exceed that of modelling spaces as well-mixed, due to a large number of sensors, the analysis required to compensate modelling errors and the increased computational effort to minimize a non-smooth cost functional. Hence, careful consideration needs to be given of the cost versus the benefit of estimating heterogeneous thermal boundary conditions in each application.

The work presented in this thesis on a simple configuration of combined localised and distributed sources of buoyancy flux may be considered as a starting point in the investigation of more general non-uniformly heated or cooled domains or, on a higher level, fluids subjected to heterogeneous forcing. Predicting the effect of non-uniform forcing on the flow and temperature field can be employed to solve the inverse problem of estimating source characteristics from flow and/or temperature measurements - in particular to determine what information can be inferred from such measurements. Reconstructing inhomogeneous sources from measurements is relevant in various contexts, such as for the thermal design and control of buildings, though its applications can extend to oceanic or atmospheric systems.

The work of this thesis aligns best with applications in built environments, as our models are similarly simplistic to (multi-)zone models commonly used for parameter estimation in buildings. Typically, parameter estimation applications for buildings aim to reduce energy consumption, while maintaining thermal comfort. In this context, parameters of interest significantly impact energy consumption but are difficult, expensive or inaccurate to measure. Such factors include occupancy presence and human building interactions, like the closing and opening of windows and blinds and usage of electrical appliances, the (movable) internal mass, such as furniture or commercial goods, and air infiltration rates of windows and doors, where the latter may also depend on climatic conditions. Including such parameter estimates in a thermal model of a building enables various applications, such as the development of predictive climate control strategies, that may incorporate predictions of occupancy, weather forecasts, solar gains and/or electrical grid loads to achieve a comfortable indoor climate energy efficiently [69]. Other applications include monitoring the performance or diagnosing faults in heating, ventilation and air conditioning systems [120] or predicting the energy savings that can be achieved by retrofitting existing buildings to inform decision making in this respect [122]. Incorporating the modelling of inhomogeneous sources into such applications may allow for more refined and extensive parameter reconstruction and thus improve existing approaches or open avenues for new applications.

5.3 Further work

The space of heterogeneous thermal boundary conditions and the associated physical states can be understood as bounded by two extremal cases: a configuration of purely localised buoyancy sources, corresponding to a stable stratification in distinct layers, and a configuration of homogeneously distributed sources, resulting in a well-mixed state similar to Rayleigh-Bénard convection. In this thesis, we focused on configurations of combined localised and distributed sources that are dominated by the localised sources and hence show a two-layer stratification. However, when the distributed source strength exceeds the localised source strength and the two-layer stratification is destroyed, the resulting

buoyancy field is not well-mixed but retains a heterogeneous structure. Further work could be directed towards exploring the flow regimes and buoyancy structures that arise in configurations of combined localised and distributed sources as the extremal case of purely distributed sources is approached, thus completing the picture of the effect of combined localised and distributed sources.

In choosing the configurations investigated in this thesis, we prioritized the simplicity of the system over practical applicability, in order to expose the connection between the distribution of the buoyancy flux on the boundaries and the resulting state. A natural extension of this work would be to consider heterogeneous boundary conditions in practical settings: conceptually, by considering asymmetric settings and allowing for ventilation and, experimentally, by investigating combined localised and distributed sources in a real-world building application. Regarding the latter point, it would be of particular interest to observe the effect of complex domain geometries on features of the buoyancy field such as its horizontal gradient, which we showed to contain crucial information on the nature of the thermal boundary conditions. This would have fundamental implications on the capability of employing the horizontal spatial dependence of a measured buoyancy field to discern different types of buoyancy sources in an inverse problem setting.

To estimate localised and distributed source strengths from measurements in the bulk, it would be desirable to extend the inverse problem from steady to transient states. Measurements in practical applications would be unlikely to correspond to steady states and a system's dynamic contains additional information to what can be inferred from its steady state. In particular, we expect that spatial inhomogeneities in the boundary conditions would translate to some temporal inhomogeneity of the state. Since we were not able to identify characteristics of the time-dependence that relate to the localised or distributed source strength in this thesis, more groundwork on the transients from inhomogeneous boundary conditions is required, such as considering the transients arising from independent changes of the localised and distributed sources and constructing a model that can reproduce the time-dependent behaviour. It would be especially interesting if horizontal spatial information could be utilised, such as implied by the steady state model, as this would offer a new approach to identify sources with simple models. Brouns et al. [23] successfully solved a source separation problem for heat sources in building applications by approaching the problem purely from the aspect of time-dependence. Combining such an approach with source information gained from spatial dependencies might offer a robust method for determining different sources of different character.

Appendix A

Planar plumes

We consider wall-bounded planar plumes in a quiescent environment from a source of buoyancy flux F_ℓ . At an elevation ζ sufficiently far above the plume source to consider the source as one-dimensional, the plume's buoyancy flux $\tilde{F}$ relative to the ambient of the plume, the volume flux Q and momentum flux M can be modelled as

$$\frac{d\tilde{F}}{d\zeta} = -Q \frac{db_a}{d\zeta}, \quad \frac{dQ}{d\zeta} = \alpha \frac{M}{Q}, \quad \frac{dM}{d\zeta} = \frac{\tilde{F}Q}{M}, \quad (\text{A.1a})$$

$$\tilde{F}(0) = F_\ell, \quad Q(0) = 0, \quad M(0) = 0. \quad (\text{A.1b})$$

with

$$\tilde{F}(\zeta) = \int_{\mathcal{I}} \overline{w\tilde{b}}(x, \zeta) dx, \quad Q(\zeta) = \int_{\mathcal{I}} \overline{w}(x, \zeta) dx, \quad M(\zeta) = \int_{\mathcal{I}} \overline{w^2}(x, \zeta) dx. \quad (\text{A.2})$$

Here, α is the entrainment coefficient such that $\frac{dQ}{d\zeta} = \alpha \frac{M}{Q}$ and $\tilde{b} \equiv b - b_a$ is the relative buoyancy of the plume to its ambient of buoyancy b_a . The domain $\mathcal{I}$ is the interval that corresponds to the horizontal extent of the plume. In an unstratified environment, $db_a/d\zeta = 0$, (A.1) can be solved to give

$$\tilde{F} = F_\ell, \quad Q(\zeta) = \alpha^{\frac{2}{3}} F_\ell^{\frac{1}{3}} \zeta, \quad M(\zeta) = \alpha^{\frac{1}{3}} F_\ell^{\frac{2}{3}} \zeta. \quad (\text{A.3})$$

The model (A.1), and its special case (A.3), is equivalent to the model of a wall-bounded axisymmetric plume by Ezhova, Cenedese and Brandt [34], where we neglect wall-shear stress due to the free-slip condition imposed on the side walls of our simulated domain. The expressions (A.1) and (A.3) correspond to those describing an unconfined plume of half the source strength F_ℓ and half the width (cf. e.g. Bremer and Hunt [21]). The effect of the side walls and of the confinement on the plume will be addressed later in this section.

In the following, we consider the vertical flow arising from purely localised heating ($\Gamma = 0$) with respect to plume scaling relations. All simulation data correspond to the left-hand plume. We define the integral quantities in (A.2) by taking the integration interval $\mathcal{I}$ to be one half of the domain, $\mathcal{I}_1 = [-\frac{\Lambda}{2}, 0]$ (blue curves in fig. A.1). This approach relies on the assumption that the vertical velocity outside the plume is negligible. The resulting volume flux (blue curve in fig. A.1a) indicates that this assumption is not suitable. Close to $x = 0$, the secondary circulations induce a non-negligible

vertical velocity component in the mean flow of both layers (cf. fig. 2.7a), which leads to a volume flux profile in the lower layer ($z < 0$) that is not consistent with plume scaling (A.3).

A more suitable integration interval is $\mathcal{I}_2 = [-\frac{\Lambda}{2}, x_\psi]$, where the point (x_ψ, z_ψ) marks the centre of the left-hand secondary circulation, manifest as a local extremum of the stream function. The interval $\mathcal{I}_2$ can be understood as the smallest integration interval of constant width which contains the plume and the adjoining jet. Using $\mathcal{I}_2$, we obtain a volume flux which scales according to (A.3) up to $z \approx 0$, where the plume penetrates the interface between the layers (fig. A.1a, red curve).

In fig. A.1b, the displayed buoyancy flux is calculated as

$$\tilde{F} = \int_{\mathcal{I}} \bar{w} (\bar{b} - \bar{b}_a) + \overline{w'b'} dx, \quad (\text{A.4})$$

with the ambient buoyancies $\bar{b}_{a1}$ and $\bar{b}_{a2}$, for the intervals $\mathcal{I}_1$ and $\mathcal{I}_2$, respectively, being defined as

$$\bar{b}_{a1} \equiv 2 \Lambda^{-1} \int_{\mathcal{I}_1} \bar{b} dx, \quad \bar{b}_{a2} \equiv |x_\psi|^{-1} \left[\int_{\mathcal{I}_1} \bar{b} dx - \int_{\mathcal{I}_2} \bar{b} dx \right]. \quad (\text{A.5})$$

The relative buoyancy flux differs only slightly between the two integration intervals (fig. A.1b). In agreement with (A.3), the relative buoyancy flux in the lower layer is approximately constant at the buoyancy flux value $F_\ell = 1$ of the localised source. At the bottom boundary, $\tilde{F}(-\frac{1}{2}) = 0$ is unequal to the strength F_ℓ of the localised source, since $\tilde{F}$ as defined in (A.4) does not include a diffusive buoyancy flux. As the plume penetrates the interface between the layers ($z \approx 0$), $\tilde{F}$ decreases abruptly, but does not reduce to zero. In contrast, the mean flow contribution to $\tilde{F}$ goes to zero in the upper layer ($z > 0$). Thus, the flow in the upper layer corresponds to a jet in the sense of integrals of mean quantities $\bar{b}$ and $\bar{w}$ [29], but carries a residual buoyancy flux, since $\overline{w'b'}$ is unequal zero in the upper layer.

To evaluate the models of section §2.6, we require the value of the plume entrainment coefficient. Two independent estimates of the entrainment coefficient can be deduced from observations, using the plume equations (A.3) [29]. Inverting the expression for the volume flux in (A.3) at the interface $z = 0$,

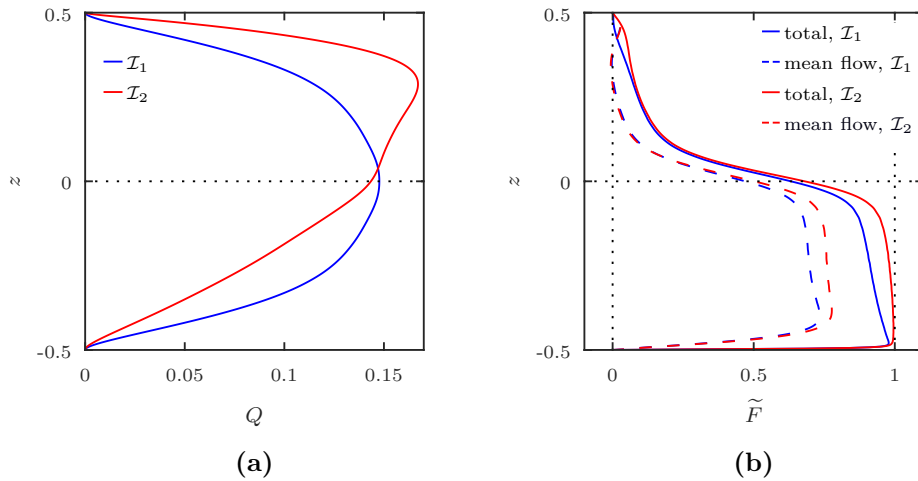


Figure A.1: Scaling of the plumes' (a) volume flux Q and (b) relative buoyancy flux $\tilde{F}$ at $\Gamma = 0$. Both the total buoyancy flux $\tilde{F}$ of the plume and its contribution from the mean flow are shown. $\tilde{F}$ and Q are calculated from (A.2) and (A.4), respectively, for two integration intervals, $\mathcal{I}_1$ and $\mathcal{I}_2$ (see text).

i.e. $\zeta = \frac{1}{2}$, we define an entrainment coefficient:

$$\alpha_Q \equiv F_\ell^{-\frac{1}{2}} \left(\frac{1}{2} \right)^{-\frac{3}{2}} Q(\frac{1}{2})^{\frac{3}{2}} = 2^{\frac{3}{2}} F_\ell^{-\frac{1}{2}} \left(\int_{-\frac{\Delta}{2}}^0 \bar{w}(x, \frac{1}{2}) dx \right)^{\frac{3}{2}}. \quad (\text{A.6})$$

We use $\mathcal{I}_1$ for simplicity, as the difference to the result from $\mathcal{I}_2$ is small at $z = 0$ (fig. A.1a).

Assuming plumes of width r_m with top-hat profiles of velocity w_m and a relative buoyancy $\tilde{b}_m$, we obtain from (A.3)

$$r_m(\zeta) = \alpha \zeta, \quad w_m(\zeta) = \alpha^{-\frac{1}{3}} F_\ell^{\frac{1}{3}} = \text{const}, \quad \tilde{b}_m(\zeta) = \alpha^{-\frac{2}{3}} F_\ell^{\frac{2}{3}} \zeta^{-1}, \quad (\text{A.7})$$

where we neglect turbulent contributions to the relative buoyancy flux. Inverting the expression for $\tilde{b}_m$ at $\zeta = \frac{1}{2}$, we define a second approximation of the entrainment coefficient:

$$\alpha_b \equiv F_\ell \left(\frac{1}{2} \right)^{-\frac{3}{2}} \tilde{b}_m(\frac{1}{2})^{-\frac{3}{2}} = F_\ell \left(\frac{1}{2} \right)^{-\frac{3}{2}} \Delta b^{-\frac{3}{2}}. \quad (\text{A.8})$$

The buoyancy of a layer corresponds to the buoyancy of its supplying plume where it penetrates the interface. Therefore, the relative buoyancy of the plume at the interface is $\tilde{b}_m(\frac{1}{2}) = \bar{b}_a - (-\bar{b}_a) = \Delta b$, where Δb is the distance between the peaks of the buoyancy field's PDF.

The entrainment coefficients can be estimated from the DNS data via (A.6) and (A.8) as

$$\alpha_Q \approx 0.161, \quad \alpha_b \approx 0.169. \quad (\text{A.9})$$

The good agreement between the two entrainment coefficients α_Q and α_b confirms that the vertical flows from the line sources at $\Gamma = 0$ can be modelled as planar plumes from sources at $z = \pm \frac{1}{2}$. The agreement between both values also attests to a sufficiently small width λ of the localised sources for them to act as virtual line sources. The buoyancy-based entrainment coefficient α_b is slightly larger than α_Q , possibly due to the neglected term of turbulent buoyancy transport in (A.7). Accordingly, the value of α_Q is used as the entrainment coefficient in this work.

While the macroscopic characteristics of a wall-bounded plume can be modelled similarly to those of a plume in an unconstrained environment (A.3), a turbulent flow along a wall differs from a freely evolving one. The entrainment of wall-bounded plumes is significantly reduced compared to free plumes, with an entrainment coefficient slightly larger than half of that of a free plume [84]. The adjoining wall prevents the large-scale wavering motion present in free plumes [84], thus reducing mixing, and has been proposed to suppress cross-stream turbulent fluxes [98].

The entrainment coefficient $\alpha \approx 0.161$ we obtain is closer in magnitude to values of α typical for free planar plumes than to those of wall-bounded plumes (cf. tab. A.1). This might partly be due to the wall shear stress, which is non-zero in all experimental realisations of wall-bounded plumes (Tab. A.1), but disappears in our configurations because of free-slip boundaries. Parker et al. [84] expect an increased entrainment with reduced wall shear stress. A second factor that potentially increases plume entrainment is our specific configuration of two confined plumes connected by a large-scale circulation with background turbulence. In a related set-up of confined axisymmetric plumes, Craske and Davies Wykes [29] observed entrainment coefficients of slightly less than twice the value typical for unconfined

Table A.1: Literature values for the entrainment coefficient of planar plumes from experiments. Given are the values of the entrainment coefficient α' as defined in the respective publication and of the corresponding α consistent with the definition used in the present work, i.e. $\frac{dQ}{d\zeta} = 2\alpha \frac{M}{Q}$ for free plumes and $\frac{dQ}{d\zeta} = \alpha \frac{M}{Q}$ for wall-bounded plumes.

			α'	α
free plumes	Lee and Emmons (1961)	$\alpha = \sqrt{2} \alpha'$	0.16	0.23
	Kotsovinos (1975)	$\alpha = \sqrt{2} \alpha'$	0.11	0.16
	Ramaprian and Chandrasekhara (1989)	$\alpha = \alpha' / \sqrt{2}$	0.23	0.16
	Yuana and Cox (1996)	$\alpha = \sqrt{2} \alpha'$	0.13	0.18
	Parker et al. (2020)	$\alpha = \alpha'$	0.14	0.14
wall- bounded plumes	Grella and Faeth (1975)	$\alpha = \sqrt{2} \alpha'$	0.067	0.095
	Lai and Faeth (1987)	$\alpha = \sqrt{2} \alpha'$	0.071	0.100
	Sangras, Dai and Faeth (2000)	$\alpha = \sqrt{2} \alpha'$	0.068	0.096
	Parker et al. (2020)	$\alpha = \alpha'$	0.08	0.08

axisymmetric plumes, noting that background turbulence disrupts the near-source necking of lazy plumes.

The equations (A.3) model a plume in an unstratified environment. In the following, we derive an analytical solution of (A.1) for a wall-bounded planar plume above a density step in its ambient, equivalent to the approach of Cooper and Linden [28] for an axisymmetric plume, where the ambient buoyancy field b_a above the density step and the ambient buoyancy field b_a^* below it are unstratified (see fig. A.2). The plume above the density step at elevation ζ_{ds} can be considered as a plume from an area source at finite volume and momentum flux, Q_{ds} and M_{ds} , respectively, as sketched in fig. A.2. Modelling the plume with the differential equations (A.1a), the latter can be combined to give

$$\frac{dM}{dQ} = \frac{\tilde{F} Q^2}{\alpha M^2}, \quad (\text{A.10})$$

where the relative buoyancy flux above the density step is constant, $\tilde{F} = \tilde{F}_{ds}$, since $db_a/d\zeta = 0$. Consequently, the volume and momentum flux at an arbitrary elevation ζ are connected by the relationship

$$M(\zeta)^3 = \frac{\tilde{F}_{ds}}{\alpha} [Q(\zeta)^3 + \Omega^3], \quad (\text{A.11})$$

where Ω is defined by the behaviour of the plume at its area source at elevation ζ_{ds} :

$$\Omega \equiv \left(\frac{\alpha}{\tilde{F}_{ds}} M_{ds}^3 - Q_{ds}^3 \right)^{\frac{1}{3}}. \quad (\text{A.12})$$

Inserting (A.11) into the second equation of (A.1a) results in an implicit expression for the volume

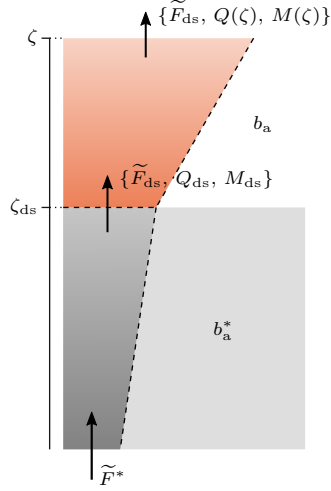


Figure A.2: Modelling a plume with a density step in its ambient: the highlighted section marks the plume above the density step at ζ_{ds} , which is modelled as a plume from an area source at finite volume and momentum flux, Q_{ds} and M_{ds} , respectively. The ambient buoyancy above and below the step change, b_a and b_a^* , respectively, and the relative buoyancy flux of the plume above and below the density step, $\tilde{F}$ and $\tilde{F}^*$, respectively, are constant in the vertical.

flux $Q(\zeta)$ above the density step:

$$\zeta - \zeta_{\text{ds}} = \frac{\Omega}{\alpha^{\frac{2}{3}} \tilde{F}_{\text{ds}}^{\frac{1}{3}}} \int_{\frac{Q_{\text{ds}}}{\Omega}}^{\frac{Q(\zeta)}{\Omega}} [1 + q^{-3}]^{-\frac{1}{3}} dq. \quad (\text{A.13})$$

Below the density step, the ambient buoyancy b_a^* and thus the relative buoyancy flux $\tilde{F}^*$ of the plume are constant in the vertical. Thus, the buoyancy flux of the plume above and below the density step are connected by

$$\tilde{F}_{\text{ds}} - \tilde{F}^* = -Q_{\text{ds}} (b_a - b_a^*). \quad (\text{A.14})$$

Appendix B

Interface between the layers of the stable stratification

The two layers of the stable stratification ($\Gamma < 1$) are separated by an interface at zero buoyancy. This isosurface is generally tilted and shows a local maximum or minimum in z close to where the plumes penetrate the interface. Fig. B.1 shows an example of the buoyancy field, with the isosurface's extrema marked as points B and C. We define the interface between the two layers as the isosurface of zero buoyancy between its local extrema, i.e. $\overline{BC}$. We continue the curve of the interface from B and C by horizontal segments to the left and right, respectively, which intersect the vertical boundaries at points A and D. Buoyancy exchanged between the two layers of the stratification is either transported across the interface, $\overline{BC}$, or via the plumes, i.e. across $\overline{AB}$ and $\overline{CD}$. The entire curve over the points A, B, C and D will be denoted as s .

The buoyancy flux across an arbitrary surface S can be calculated as

$$F_S = \frac{1}{\Lambda_y} \int_S \sum_i f_i n_i dS, \quad (\text{B.1})$$

where $f_i = u_i b - \text{Pe}^{-1} \partial_i b$ is the local buoyancy flux in the spatial direction specified by i and n_i

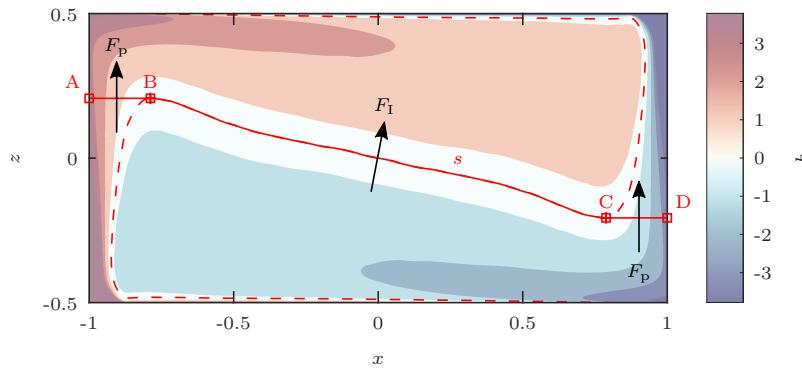


Figure B.1: Schematic for the definition of a separating surface between the two layers of the stratification, using the mean buoyancy field. The red dashed line marks the isosurface at zero buoyancy. The solid red line corresponds to the separating curve s (see text).

are the components of the unit vector perpendicular to the surface. Thus, the mean buoyancy flux between the two layers, calculated across the separating curve s , is

$$F_s = \int_{-\frac{\Lambda}{2}}^{\frac{\Lambda}{2}} \left[-\frac{dz_s}{dx} \cdot \bar{f}_x(x, z_s(x)) + \bar{f}_z(x, z_s(x)) \right] dx \equiv \int_{-\frac{\Lambda}{2}}^{\frac{\Lambda}{2}} f_s(x) dx, \quad (\text{B.2})$$

with f_s defined as the corresponding mean local buoyancy flux. Here, $z_s(x)$ is the elevation of the separating curve s . The buoyancy flux F_s is well-defined, since z_s is differentiable at the junction of the segments $\overline{AB}$, $\overline{BC}$ and $\overline{CD}$.

Separating the buoyancy flux F_s into the buoyancy transport of the two plumes and the buoyancy transport across the interface, $F_s = 2 F_p + F_I$, we define

$$F_p = \frac{1}{2} \int_{-\frac{\Lambda}{2}}^{x_A} f_s(x) dx + \frac{1}{2} \int_{x_B}^{\frac{\Lambda}{2}} f_s(x) dx, \quad F_I = F_s - 2 F_p. \quad (\text{B.3})$$

Equivalently, the volume flux of the plumes is determined from the simulation data as

$$Q_p = \frac{1}{2} \int_{-\frac{\Lambda}{2}}^{x_A} \bar{w}(x) dx + \frac{1}{2} \int_{x_B}^{\frac{\Lambda}{2}} \bar{w}(x) dx. \quad (\text{B.4})$$

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