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Evaporation-driven turbulent convection in water pools heated from below

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Abstract

In this thesis, we study turbulent thermal convection driven by free-surface evaporation in water pools. The studied physical phenomenon is closely related to the flow that occurs in the early stages of a spent-fuel pool (SFP) loss-of-cooling accident such as that which occurred at Fukushima 2011, which acts as one of the motivations for this research. Over a series of studies, we investigate numerically the turbulent flow structures water-side of this thermal convection set-up, at each stage incorporating more physics and hence gradually building up in difficulty. This strategy allows us to assess the relative importance of the various modelling choices.

We start by introducing the important interdependent physical phenomena associated with the first stages of the SFP loss-of-cooling-accident, that of free-surface evaporation and turbulent thermal convection. We consider only the upper volume of the pool, and make geometric simplifications, so that the heat source is considered as a uniformly heated bottom wall. Doing so allows comparisons against similar thermal convection configurations from the literature such as turbulent Rayleigh-Bénard Convection (RBC) and evaporative cooling. In this introductory chapter, we describe how our configuration is distinguished from these two well known alternatives. Furthermore, we summarise the most pertinent experimental research in the domain of free-surface evaporation into a quiescent air-side environment.

In chapter 2, we provide the governing equations for the problem in hand; the low-Mach-number expansion of the compressible Navier-Stokes-Fourier equations. We then discuss how these equations are discretised spatially and temporally before detailing the numerical algorithms used to solve the equations. Throughout the thesis, we have used the open-source Computational Fluid Dynamics (CFD) package OpenFOAM® v1806. We develop a low-Mach-number flow solver, by updating the relevant Navier-Stokes algorithm, for both single and two phase applications, the latter being included in the Appendix. In this chapter, we also provide details on the turbulence modelling adopted in the thesis. Here, we employ the integrated models with OpenFOAM®, with small adaptations leading to improvements when applied to the flow in question.

In chapter 3, we investigate a novel configuration, similar to turbulent RBC set-up but with a free-slip upper boundary condition as a first approximation of a free surface. We enforce fixed temperature, Dirichlet, boundary conditions above and below, corresponding to a temperature drop across the domain of 20 K. As such, this chapter concentrates on the role of the free-slip and non-Oberbeck-Boussinesq effects on the mean flow properties and turbulent statistics. The former is shown, for the first time, to play a role on heat transfer in the domain and on the homogeneity of the thermal

boundary layer heights. We also provide a turbulent-kinetic-energy (TKE) budget, which suggests that even though the deviations from the Oberbeck–Boussinesq conditions are small, the effect of such deviations is significant on determining the important terms in the budget.

In chapter 4, we carry out our first estimation of the full problem and build on the previous chapter by significantly improving the thermal boundary condition above. Here, we prescribe a representative evaporative heat flux leaving the domain, mathematically this implies a non-zero Neumann boundary condition for the temperature. We provide a detailed explanation on the calculation of this gradient based on realistic evaporation rates from experiments. This boundary condition is prescribed uniformly above, however, the result is a spatially variable temperature at the upper boundary; this set-up is thus closer to the physical problem. The originality of the results is in the time-averaged properties of the flow, which are shown to be influenced by the presence of the free surface. Specifically, the large-scale circulation (LSC), which gives an indication of the mean flow structures, is effected, leading to inhomogeneous recirculation zones for the cubic container investigated. In this chapter, we also find novel Rayleigh number (Ra) scaling of the global Nusselt number (Nu) for the current thermal convection configuration. Here, we find a remarkably similar exponent to that found in turbulent RBC, but with an increased prefactor accounting for the shear-free boundary.

In chapter 5, we again build on previous work by implementing a novel dynamic thermal boundary condition based on evaporative and convective heat loss at the free surface. We then investigate, for the first time, the role of the aspect ratio in slender cuboidal domains. We continue to consider only the water-side domain in the system of governing equations. However, we fix ambient conditions and model the heat loss locally, that is based on a local (cell-dependent) film temperature. As a result, we have a spatially variable Neumann thermal boundary condition for the temperature above, representative of the total heat losses at an evaporating free surface. This leads to non-uniform upper boundary temperatures and, without modelling both the gas- and water-side domains, is as close as possible to modelling the full physical problem. We then decrease the aspect ratio of the domain and assess the impact on the LSC state. The LSC switches from a stable single-roll, to a dual-roll state, which changes the temperature and velocity fields at the free surface. However, we find no discernible impact on the evaporation rate at the free surface.

Finally, in chapter 6, we draw conclusions and make recommendations for future work.

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Contents

1	Introduction	1
1.1	Motivation	2
1.2	Thermal convection	4
1.3	Natural convection-driven evaporation	10
1.4	Outline and objectives of the thesis	12
2	Governing equations and numerical algorithms	15
2.1	Introduction	15
2.2	Governing equations	16
2.3	Numerical algorithms	18
2.3.1	Discretisation	18
2.3.2	Pressure-velocity coupling	20
2.3.3	Turbulence modelling	23
2.3.4	Parellelisation	27
2.4	Summary	27
3	Thermal convection with a free-slip upper boundary	29
3.1	Introduction	29
3.2	Numerical set-up	31
3.3	Resolution requirements	33
3.3.1	Direct numerical simulation resolution requirements	33
3.3.2	Large-eddy simulation resolution requirements	36
3.4	Numerical results	38
3.4.1	Analysis of moderate-Rayleigh-number flow	38
3.4.2	Analysis of higher-Rayleigh-number flows	51
3.5	Conclusions	55
4	Evaporation-driven thermal convection in water pools	57
4.1	Introduction	57
4.2	Numerical set-up	60
4.3	Estimation of evaporation rates	61

4.4	Boundary conditions	66
4.5	Resolution requirements	68
4.6	Numerical results	70
4.6.1	Mean flow properties	71
4.6.2	Flow statistics	78
4.7	Conclusions	84
5	Thermal convection driven by dynamic free-surface evaporation	87
5.1	Introduction	87
5.2	Numerical set-up	89
5.2.1	Sub-grid scale modelling	90
5.3	Evaporation model	91
5.4	Boundary conditions	94
5.5	Resolution criteria	97
5.6	Numerical results	99
5.6.1	Validation of the modelling approach	99
5.6.2	Study of the effect of the aspect ratio	106
5.7	Conclusions	115
6	Conclusions and future perspectives	117
6.1	Concluding remarks	117
6.2	Future perspectives	120
A	A two-phase approach for simulating an evaporating free surface	123

List of Figures

1.1	Important physical phenomena in the pre-uncovery phase of the SFP loss-of-cooling accident	3
1.2	Plot showing approximate evaporative mass flux at a free surface based on bulk equilibrium temperatures	5
1.3	A comparison of thermal convection configurations and their temperature profiles	5
1.4	Mean velocity vectors in the LSC plane of a cubic domain	8
3.1	Vertical and horizontal grid resolution for the DNS at $Ra = 10^7$	36
3.2	Vertical and horizontal grid resolution for the LES at $Ra = 10^8$	38
3.3	Plots of the time- and area-averaged components of Nu_y at $Ra = 10^7$.	40
3.4	Time-averaged streamlines of DNS at $Ra = 10^7$ coloured by dimensionless mean vertical velocity, $\langle \hat{v} \rangle_t$	41
3.5	Colour plot of $\hat{\theta}_{\text{rms}}$ with superimposed velocity vectors of the DNS at $Ra = 10^7$	41
3.6	Colour plot of the instantaneous normalised temperature $\hat{\theta}$ of the DNS at $Ra = 10^7$	42
3.7	Colour plot of the instantaneous normalised temperature $\hat{\theta}$ with superimposed velocity vectors of the DNS at $Ra = 10^7$	42
3.8	Velocity rms plots of $Ra = 10^7$ at mid-width, $\hat{x} = 0.5$	43
3.9	Mean normalised temperature, $\langle \hat{\theta} \rangle$, plots of $Ra = 10^7$ at mid-width, $\hat{x} = 0.5$	44
3.10	Normalised temperature rms, $\hat{\theta}_{\text{rms}}$, plots of $Ra = 10^7$ at mid-width, $\hat{x} = 0.5$	45
3.11	Turbulent heat flux, $\langle \hat{\theta}'\hat{v}' \rangle$, plots of $Ra = 10^7$ at mid-width, $\hat{x} = 0.5$. .	46
3.12	Horizontal TKE budget of DNS at $Ra = 10^7$ at mid-height, $\hat{y} = 0.5$. . .	49
3.13	Horizontal TKE budget of DNS at $Ra = 10^7$ at mid-height, $\hat{y} = 0.5$. Zoom on the right-hand-side wall of figure 3.12.	50
3.14	Vertical TKE budget of DNS at $Ra = 10^7$ at $\hat{x} = 0.5$	50
3.15	Vertical TKE budget of DNS at $Ra = 10^7$ at $\hat{x} = 0.5$	51
3.16	LES plots of the time- and area-averaged Nu_y at increasing Ra	52
3.17	LES plots of velocity rms at increasing Ra at mid-width, $\hat{x} = 0.5$	53

3.18	LES plots of mean normalised temperature, $\langle \hat{\theta} \rangle$, at increasing Ra at mid-width, $\hat{x} = 0.5$	53
3.19	LES plots of the rms of normalised temperature fluctuations, $\hat{\theta}_{\text{rms}}$, at increasing Ra at mid-width, $\hat{x} = 0.5$	54
3.20	LES plots of turbulent heat flux, $\langle \hat{\theta}'\hat{v}' \rangle$, at increasing Ra at mid-width, $\hat{x} = 0.5$	55
4.1	Instantaneous isosurfaces of the temperature field at different Ra	68
4.2	Time-averaged normalised temperature, $\langle \hat{\theta} \rangle$, at the interface and lower wall for $Ra = 9.0 \times 10^7$	71
4.3	Diagonal planes showing $\hat{\theta}_{\text{rms}}$ fields at $Ra = 5.0 \times 10^7$	73
4.4	Time-averaged streamlines coloured by the mean vertical velocity, $\langle \hat{v} \rangle$, at $Ra = 5.0 \times 10^7$	74
4.5	Plot of the mean dimensionless vertical velocity, $\langle \hat{v} \rangle$, along the diagonal line containing the LSC	75
4.6	Ra -scaling plots	76
4.7	Plots of the time- and area-averaged components of Nu_y	78
4.8	Plots of the rms of velocity fluctuations across the vertical direction . .	79
4.9	Plots of the mean normalised temperature, $\langle \hat{\theta} \rangle_{xz}$, across the vertical direction	81
4.10	Plots of the rms of the normalised temperature fluctuations, $\hat{\theta}_{\text{rms}}$, across the vertical direction	81
4.11	Plots of the normalised temperature skewness, $\hat{S}_{\theta}$, across the vertical direction	83
5.1	A flowchart of the free-surface evaporation algorithm.	95
5.2	Plots of the time- and area-averaged components of Nu_y at $Ra = 1.2 \times 10^7$	101
5.3	Plots of the rms of velocity fluctuations at $Ra = 1.2 \times 10^7$	102
5.4	Plots of the temperature at $Ra = 1.2 \times 10^7$	102
5.5	Plots of third-order statistics at $Ra = 1.2 \times 10^7$	104
5.6	Comparisons between LES predictions and experimental measurements of the evaporative mass flux, $\dot{m}''$, and interface temperature, T_{int}	105
5.7	Time-averaged streamlines in the aspect ratio $\Gamma = 1$ domain at $Ra = 1.2 \times 10^8$	106
5.8	Time-averaged velocity vectors scaled by magnitude with superimposed large-scale structures in the cubic ($\Gamma = 1$) domain	107
5.9	Time-averaged streamlines in the domain of aspect ratio $\Gamma = 1/2$ at $Ra = 1.1 \times 10^9$	107
5.10	Time-averaged velocity vectors scaled by magnitude with superimposed large-scale structures for aspect ratio $\Gamma = 1/2$	108

5.11	Time-averaged flow structure in the domain of aspect ratio $\Gamma = 1/4$ at $Ra = 8.8 \times 10^9$	109
5.12	Time-averaged normalised interface temperatures, $\langle \hat{\theta} \rangle$ with superimposed mean velocity vectors scaled by magnitude	111
5.13	Plots of the time- and area-averaged components of Nu_y as Ra is increased (Γ is decreased)	112
5.14	Plots of the rms of velocity fluctuations as Ra is increased (Γ is decreased)	113
5.15	Temperature plots as Ra is increased (Γ is decreased)	114

List of Tables

3.1	Polynomial coefficients for water thermodynamic properties over the temperature range 323.15–343.15 K	31
3.2	Reference values for nondimensionalisation purposes for simulations of chapter 3	32
3.3	DNS grid resolution criteria of chapter 3	34
3.4	LES grid resolution criteria of chapter 3	37
3.5	Boundary layer heights at $Ra = 10^7$	44
3.6	Time-averaged results for chapter 3	55
4.1	Example polynomial coefficients for water thermodynamic properties at $Ra = 5 \times 10^7$	61
4.2	Gaseous mixture properties far from the interface	62
4.3	Gaseous mixture properties at the interface	63
4.4	Gas-side dimensionless parameters	64
4.5	Fluxes at the interface	65
4.6	Thermal boundary conditions for the simulations of chapter 4	67
4.7	Reference values for nondimensionalisation purposes for simulations of chapter 4	67
4.8	Resolution criteria for the DNS of chapter 4	69
4.9	Time-averaged results for chapter 4	72
4.10	Vertical limits of the recirculation zones	74
5.1	Example polynomial coefficients for variable water thermodynamic properties for the $Ra = 1.3 \times 10^8$ case	90
5.2	Thermal boundary conditions for the simulations of the cubic ($\Gamma = 1$) domain	96
5.3	Nondimensionalisation reference values for the cubic ($\Gamma = 1$) domain	96
5.4	Nondimensionalisation reference values for the study of the aspect ratio	97
5.5	Resolution criteria for the simulations of chapter 5	100
5.6	Time-averaged results for cubic ($\Gamma = 1$) domain	103
5.7	Thermal boundary conditions for the study of the aspect ratio	110
5.8	Time-averaged results for the study of the aspect ratio	113

Nomenclature

(.) The hat superfix denotes dimensionless quantities.

All quantities are in S.I units unless specifically stated otherwise.

Acronyms

CFD Computational Fluid Dynamics

DNS Direct Numerical Simulation

LES Large-Eddy Simulation

LSC Large Scale Circulation

MPI Message Passing Interface

NSF Navier–Stokes–Fourier

PISO Pressure-Implicit with Splitting of Operators

RBC Rayleigh-Bénard Convection

rms Root Mean Square

SFP Spent-Fuel Pool

TKE Turbulent Kinetic Energy

Constants

$\mathbf{g} = (0, -9.814, 0)$ Gravitational acceleration vector

$a = 0.482$ Empirical constant for calculation of boundary layer points

$E = 0.982$ Empirical constant for calculation of boundary layer height

Dimensionless numbers

$\Gamma = \frac{W}{H} =$ Aspect ratio

$Le = \frac{Sc}{Pr} =$ Lewis number

Nu Nusselt number (ratio of convective to conductive heat transfer)

$Pr = \frac{\nu}{\kappa} =$ Prandtl number

$Ra = \frac{|g|\beta\Delta TH^3}{\nu\kappa} =$ Rayleigh number

$Re = \frac{v_{rms}H}{\nu} =$ Reynolds number

$Ri = \frac{1}{|\bar{\mathbf{S}}|^2} \frac{|g|}{\rho_{ref}} \cdot \nabla \bar{\rho} =$ (Gradient) Richardson number

$Sc = \frac{\nu}{D} =$ Schmidt number

$Sh = \frac{W}{\delta_c} =$ Sherwood number

Subscripts

∞ A distance far from the interface

θ Thermal

c Critical

f Face

g Gas

l Index of neighbouring cells

l Liquid

P Index of an arbitrary cell-centre

r Reduced

r_i Recirculation zones, with $i = 1-4$

add Added to interface from water-side

c Concentration

conv Convective

ctr Centre

eff Effective

evap Evaporative

f	Film
G	Global (volume averaged)
int, Γ	Interface
l	Lower
lhs	Left hand side
max	Maximum
min	Minimum
ref	Reference
rhs	Right hand side
rms	Root-mean-square
t	Turbulent
tot	Total
u	Upper
v	Vapour
w	Water-side

Variables

β	Thermal expansion coefficient
$\boldsymbol{\tau}$	Deviatoric part of the viscous stress tensor
$\boldsymbol{\tau}^r$	Subgrid-scale stress tensor
$\boldsymbol{q}^r$	Subgrid-scale heat flux
$\boldsymbol{S}$	Rate-of-strain tensor
$\boldsymbol{u}$	Velocity vector
ΔT	Temperature difference between the lower wall and upper boundary
Δ	Cell size
δ	Boundary layer height

$\delta(\boldsymbol{x} - \boldsymbol{x}_\Gamma)$	Dirac delta function
$\dot{m}''$	Mass flux
$\dot{q}''$	Heat flux
ϵ_k	TKE dissipation
η	Kolmogorov scale
η_B	Batchelor scale
η_C	Corrsin scale
η_l	Taylor microscale
$\hat{\theta}$	Normalised temperature
$\hat{S}_\theta$	Temperature skewness
κ	Thermal diffusivity
λ	Thermal conductivity
$\mathcal{H}(\boldsymbol{u})$	Transport part of the semi-discretized momentum equation
μ	Dynamic viscosity
ν	Kinematic viscosity
Φ_k	TKE mean pressure work
ϕ_k	TKE fluctuating pressure work
Π_k	TKE correlation between pressure and dilatation of fluctuating velocity
ρ	Density
P_k	TKE production
$\mathbf{I}$	Identity matrix
$\mathbf{S}_f$	Face area vector
ζ	Bulk viscosity
A	Matrix coefficient in semi-discretized momentum equation
B_m	Mass transfer driving force

C_k	TKE convection
c_p	Specific heat capacity
D	Mass diffusivity
D_k	TKE diffusion
F	Mass flux through a face
f	Indicator function field
H	Height of the domain
h	Heat transfer coefficient
h_{lv}	Latent heat of vapourisation
k	Turbulent kinetic energy
L	Length of the domain
L_{mn}	Relation for subgrid-scale stresses at Δ and 2Δ
M	Molar mass
M_{mn}	Relation for resolved rate of strain tensors at Δ and 2Δ
N_u	Number of points inside hydrodynamic boundary layer
N_{DNS}	Total Number of cells in DNS
N_{LES}	Total Number of cells in LES
N_θ	Number of points inside thermal boundary layer
N_i	Number of cells in i -direction, where $i = x, y, z$
p	Pressure
p'	Modified pressure
p_0	Thermodynamic pressure
p_1	2nd-order term of the low-Mach-number expansion of the pressure
p_v	Bulk viscous pressure
s	Interface area

T	Temperature
t	Time
T_k	TKE transport
t_{avg}	Averaging time
t_{ff}	Free-fall time
u, v, w	Velocity components
U_{ff}	Free-fall velocity
V	Cell volume
W	Width of the domain
x, y, z	Spatial coordinates
Y	Mass fraction
RH	Relative humidity

Chapter 1

Introduction

This thesis is an in-depth numerical study of turbulent thermal convection driven by free-surface evaporation in water pools. Thermal convection itself is defined as fluid motion generated not by external mechanical work, but by a thermal energy, or heat, source. It is an ever-present phenomenon in both nature and in industrial flows and has been a key area of research for centuries. In the literature, which is comprehensive, thermal convection is interchangeably referred to as free, or natural, convection. Hereafter, the same terminology is adopted in the thesis.

Early examples of literature, in the domains of atmospheric [1, 2] and oceanic [3, 4] flows, observed and studied experimentally thermal convection cellular structures. With respect to industrial applications, it was the domain of metallurgy [5, 6] that drove research, as here, an understanding of natural convection effects on melting and freezing is critical. Knowledge of thermal convection is crucial also in geophysical [7] and astrophysical [8] convection where the flows experience large temperature, density and transport property variations. It is then no exaggeration, to say that thermal convection is one of the most widely observed types of flow in the universe [9].

The specific form of thermal convection induced by an evaporating free surface, is often referred to simply as evaporative convection, or evaporative cooling, and is normally studied in fluid layers. The difference between studying a water layer and a water pool is significant. As we will cover in more detail later, the water-side turbulence is greatly influenced by the representative length, the height, of the studied domain. A further difference between evaporative convection and the type of thermal convection studied herein, is in the form of the primary heat source. For example, in the study of evaporation from the surface layers of lakes and oceans, the heat source is external to the water-side domain, in the form of solar energy from above. The motivation for our work is quite different: the thermal convection occurring in the Spent-Fuel Pools (SFP) of nuclear facilities under accidental conditions.

1.1 Motivation

At-reactor spent-fuel pools are located in the buildings adjacent to (light-water) reactors, this enables easy fuel transfer and storage. The primary role of an at-reactor SFP is to safely store spent (used) fuel removed from the reactor. The stored fuel assemblies, fresh from the reactor, release decay heat as a result of the radioactive decay of unstable fission products (radioisotopes). Some of these fission products have long half-lives which require the spent-fuel to be stored on site for years. As such, the fuel assemblies are stored in fuel racks located at the bottom of the pool, and are covered by a large volume of coolant and the SFP itself is housed within a fuel building.

SFP dimensions are such that the $\sim 4\text{m}$ long fuel assemblies can be stacked vertically within fuel racks and still be covered by enough water ($\sim 7\text{m}$) to act as a biological shield and prevent harmful radiation release. This makes the pool approximately 11m deep. Assuming a rectangular SFP, a typical length and width of 12m and 8m respectively results in more than 1000 m^3 of coolant inventory. We consider the coolant as pure water throughout the thesis, although reactor designs differ in this respect. Under normal conditions, the nominal maximum SFP operating temperature is $\sim 323.15\text{ K}$ and the decay heat is evacuated via a system of pumps and external heat exchangers. Further, any evaporation at the free surface is compensated for by make-up water injection.

On the other hand, in the event of a “station blackout”, defined as the complete loss of electric power on a nuclear facility, the systems for heat removal fail and, in a worst-case scenario, there is no make-up water injection. Forced convection in the pool also stops, and as a result the fuel assemblies heat up. The physical phenomena associated with this loss-of-cooling-accident scenario motivates this work.

To understand the main physical phenomena involved in the early-stages of an SFP loss-of-cooling-accident, it suffices to (falsely) assume that shortly after a station blackout we obtain an entirely quiescent SFP. A pocket of water in contact with the fuel assembly cladding will be heated and rise through the fuel racks and up to the surface due to an added buoyancy force. Assuming it does not diffuse all of its heat on the way up, such a pocket will arrive at the free surface, evaporate into the air, and in doing so, cool-down a neighbouring pocket of water at the surface. This cooler pocket in turn sinks back down towards the fuel assemblies and a natural convection loop is created. We therefore have a flow governed by the inter-dependent flow phenomena of free-surface evaporation and *turbulent* natural convection. The flow is always in a turbulent state, due to the depth of the pool. Figure 1.1 displays these phenomena in schematic form.

We concentrate solely on the phenomena of free-surface evaporation and turbulent natural convection highlighted in figure 1.1. The aim is then to better understand

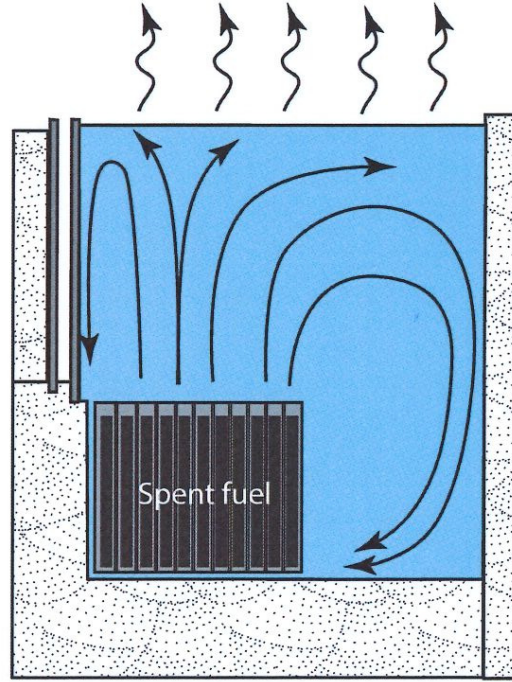


Figure 1.1: Important physical phenomena in the pre-uncovery phase of the SFP loss-of-cooling accident. The figure shows the water-side natural convection loop, driven by free surface evaporation above and the internal heat source (fuel assemblies) below. This figure is reproduced with permission from the National Academy of Sciences, Courtesy of the National Academies Press, Washington, D.C. [10].

the physics whilst ensuring that experimental (or numerical) data is available in the literature for comparison and validation purposes. Further, owing to the fact that we use numerical software to attack the problem, we are limited by computational resources and geometric simplifications of the problem in hand are therefore necessary.

In view of the above restraint, only the upper volume of the pool is modelled, that is the region above the fuel assemblies. We further consider the fuel assemblies as a uniformly heated horizontal bottom (lower) wall; this is a significant simplification of the overall problem. However, this decision allows the important aforementioned physical phenomena to be studied and leaves more complicated approaches, such as assuming the fuel assemblies as a porous media, to future work. Even with these geometric simplifications, the dimensions of the SFP are such that it is not feasible to model the full upper volume of the pool. Consequently, we estimate the upper volume as a (much smaller) cuboidal domain and increase the height of the domain to ensure a turbulent flow; the natural state of an SFP.

The evaporation that occurs at the free surface has important consequences on the coolant inventory. The spent-fuel will heat-up the SFP towards an equilibrium bulk temperature whose value is determined by how efficiently heat is removed from the system. The decay heat from the assemblies is evacuated by conductive ($< 5\%$ to

pool walls), radiative ($< 3\%$ to surroundings) and convective plus evaporative ($\sim 90\%$ from free surface) heat losses. As a result, the pool water evaporates away at the air/water interface, the extent to how gradually this process occurs is, of course, of great importance and interest to nuclear safety. Hereafter, we use the terms (air/water) *interface* and *free surface* interchangeably.

In the pre-uncovery phase of the accident, that is, prior to the fuel racks being exposed to steam and/or air, boiling point is not breached in the SFP. The equilibrium bulk pool temperature is such that there is no nucleation, and heat is predominantly evacuated at the free surface via evaporation. This assumption is based on observations of Fukushima 2011, where even the SFP containing the highest decay heat did not reach boiling point in the early-stages of the accident. The time required for the pool level to descend to the top of the fuel assemblies, that is the time until uncovery, depends on the initial SFP volume and temperature, storage pattern of fuel assemblies in the pool, and how recently after reactor shutdown the fuel assemblies have been stored. In figure 1.2 we show approximate values of the equilibrium bulk pool temperatures and decay heat for two different SFP cases at Fukushima 2011 (adapted from Wang *et al.* [11]). The grey line represents an approximative evaporative mass flux at the free surface; these different mass fluxes correspond to 19 and 79 tonnes/day inventory loss for the equilibrium bulk temperatures of 343.15 K and 361.15 K respectively [10]. With only moderate changes in temperature having a significant impact on inventory loss, it is clear that the accurate modelling of free-surface evaporation is critical for SFP loss-of-cooling accident safety studies.

For clarity purposes, in this thesis, our motivation is entirely from the pre-uncovery phase of the accident. Even within this limitation, in our studies we do not account for the possibility of flashing and other boiling phenomena which could occur in specific scenarios. The important and complex phenomena that occur in the post-uncovery phase, that is, post the exposure of the fuel assemblies to steam and/or air, are not covered. As such, this thesis is not a comprehensive study of the entirety of physical phenomena that occur in an SFP loss-of-cooling-accident. Instead, this thesis is a study of the thermal convection induced by free-surface evaporation; we now cover these two topics and discuss the scientific motivations of the thesis in more detail.

1.2 Thermal convection

In order to fix ideas, consider an open container filled with water and an initially quiescent velocity field water-side. Evaporation at the free surface would induce convective motion below. Thermal plumes would then descend through the domain before interacting with a lower adiabatic bottom wall. This configuration is the evaporative convection mentioned earlier; schematically it is represented by figure 1.3a. Conversely,

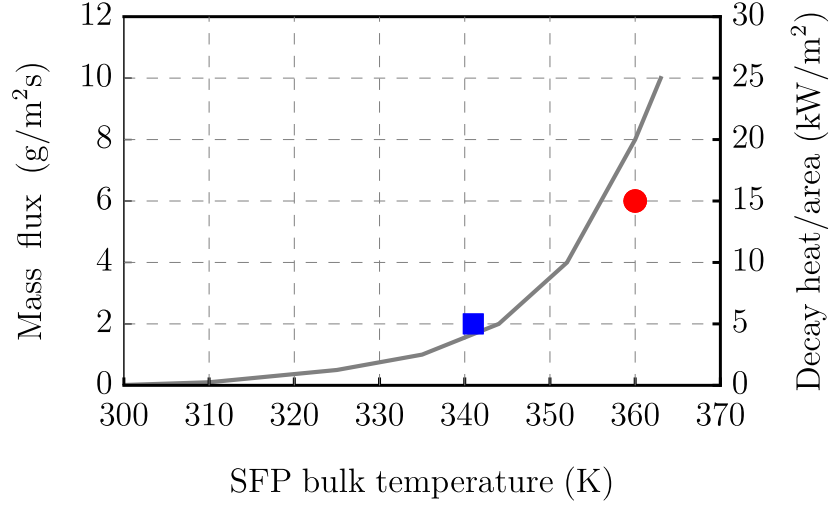


Figure 1.2: Plot showing approximate evaporative mass flux at a free surface based on bulk equilibrium temperatures. The plot markers approximately correspond to measured values of SFP bulk temperatures for the decay heat power per surface area of SFP2 and SFP4 at Fukushima, 2011. The legend is as follows: approximate mass flux (—), approximate SFP2 decay heat per unit area (■), approximate SFP4 decay heat per unit area (●). This figure is adapted from [11] and [12] as a useful guide to approximate quantities and should not serve as a data source.

if heat is added from below and simultaneously evacuated above then a flow is induced similar to the most well-known of all thermal convection configurations, that of turbulent Rayleigh-Bénard Convection (RBC); see figure 1.3b. The problem studied in this thesis, which is shown schematically in figure 1.3c, can be understood as a combination of these two well-known thermal convection configurations.

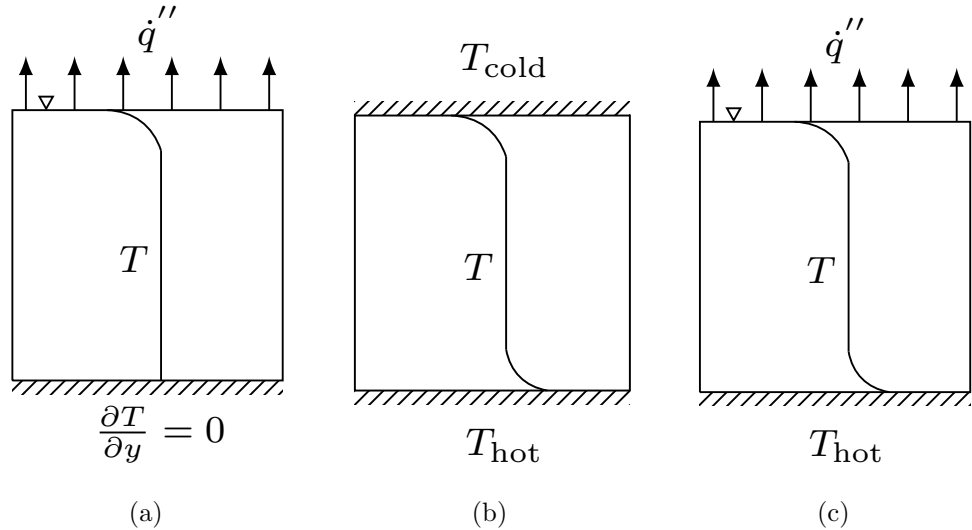


Figure 1.3: A comparison of thermal convection configurations and their temperature profiles: (a) evaporative convection, (b) turbulent RBC, and (c) current configuration. In this figure, $\dot{q}''$ represents the heat flux away from a free surface.

Clearly, figure 1.3c is only a schematic representation of the thermal convection configuration we intend to study. However, a keen eye will find this figure to make bold assumptions about the thermal convection it purports to represent. For instance, the presence of symmetric thermal boundary layers and a uniform bulk temperature gradient. We will attack these points in more detail later in the thesis. Furthermore, we add that free-surface evaporation is always spatially non-uniform and this is not evident in figure 1.3c. This flow feature is just one example distinguishing our set-up from turbulent RBC whose upper wall is a (spatially and temporally constant) Dirichlet thermal boundary condition. As we advance through this thesis, we will continue to compare the investigated configuration to the closely related turbulent RBC. For this reason, it is worth summarizing the state-of-the-art in this area before moving on.

With respect to RBC, Bénard's initial experiments were carried out with an upper boundary open to atmosphere [13], hence surface tension at the interface played a pivotal role. Bénard in fact investigated, for the first time, what has come to be known as the Bénard-Marangoni instability. RBC is most commonly studied, however, as a fluid uniformly heated from below and cooled from above with solid upper and lower boundaries. Rayleigh's theoretical contribution to the subject came immediately after Bénard's and was the first to study the instability that arises uniquely from the temperature nonuniformity in fluid layers [9]. The resulting dimensionless Rayleigh number that governs a flow of this type was named after him and it is this latter subject that is most commonly referred to today as RBC.

The flow and thermal dynamics in RBC are determined by the geometry of the system, the temperature difference across it and the resulting variation in fluid properties. The two dimensionless parameters that then govern the flow are the aforementioned Rayleigh number,

$$Ra = \frac{|\mathbf{g}|\beta\Delta T H^3}{\nu\kappa}, \quad (1.1)$$

and Prandtl number, $Pr = \nu/\kappa$. In these expressions, $|\mathbf{g}|$ is the magnitude of gravitational acceleration, β the thermal expansion coefficient, H the height of the domain, ν the kinematic viscosity, ΔT the temperature difference between lower and upper walls and κ is the thermal diffusivity. The system response to a given Ra and Pr is measured in terms of the dimensionless heat flux and turbulence; respectively the Nusselt (Nu) and Reynolds (Re) numbers [14]. We provide formal definitions of these quantities later on.

Early interest in RBC was related to pattern formation and nonlinear dynamics at low Ra . Under low Ra conditions a cellular structure forms whereby the horizontal length-scale is comparable to the height of the domain [15]. As Ra is increased, this cellular structure breaks-down and is replaced by chaotic plumes. The recent literature, since the 80s, has mostly focused on turbulent RBC. This new regime is entered when

$Ra > 10^6$. Here, plumes are transported in one direction near the lower wall and in the opposite direction near the upper boundary by a large-scale flow, more recently known as a large-scale circulation (LSC).

It is uniquely turbulent RBC that we refer to in this thesis for the obvious reason that an SFP is always in a turbulent state. For reference, Rayleigh numbers up to 10^{14} are expected in SFPs. Simulating this level of turbulence is beyond the computational resources available today. However, throughout the thesis, we refer only to simulations of $Ra > 10^7$. Furthermore, the term true Rayleigh-Bénard convection is reserved for fluid layers which extend infinitely in the horizontal directions [16] (i.e. horizontal periodicity), but the term is often used in the literature, and indeed throughout this thesis, to refer to contained geometries.

Reviews of turbulent RBC include those of Siggia [17] and Ahlers *et al.* [14]. The former, from 1994, was likely the first attempt to represent thermal convection as a branch of turbulence. Therein, the theoretical framework was provided for the exact predictions of Nu based on the Oberbeck-Boussinesq approximation of the Navier-Stokes-Fourier (NSF) equations [18]. Here, the NSF equations are the mass, momentum and energy balance laws of the fluid written in differential form, and the Oberbeck-Boussinesq approximation assumes that variations in density and transport properties are sufficiently small that they are taken into account only in the gravitational term of the momentum equation which drives the flow. This approximation is thus only valid for small temperature variations.

Siggia [17] also summarised the contemporary experimental findings at high Ra , made possible due to the cryogenic helium experiments [19]. Further, they distinguished the regimes of turbulence in thermal convection, where although depending slightly on aspect ratio, *hard* turbulence was suggested to exist above $Ra > 2 \times 10^7$. Finally, and of particular interest to this thesis, the large-scale circulation, was also discussed in detail. Siggia [17] noted how Krishnamurti and Howard [15] discovered the buoyancy-generated coherent flow structure in the soft turbulence regime of turbulent RBC, that is $Ra \approx 2 \times 10^6$. The LSC, or mean wind, sweeps across the upper and lower boundaries stabilizing the thermal boundary layers, and simultaneously creates a hydrodynamic boundary layer with its shear [20]. The shape of the container, and particularly its aspect ratio, has been shown to be a further control parameter which plays a particularly important role in determining the structure of the LSC (see for example [16]). We will frequently return to this subject during the thesis, but demonstrate an example LSC plane in figure 1.4. Here the LSC is a diagonal plane, which occupies the entire height of the cubic domain. The specific example shown in figure 1.4 represents an LSC in its single-roll state.

On the other hand, the review of Ahlers *et al.* [14], released in the 2009, predominantly focused on the Nu , Re and boundary layer height dependence on Ra ; they also

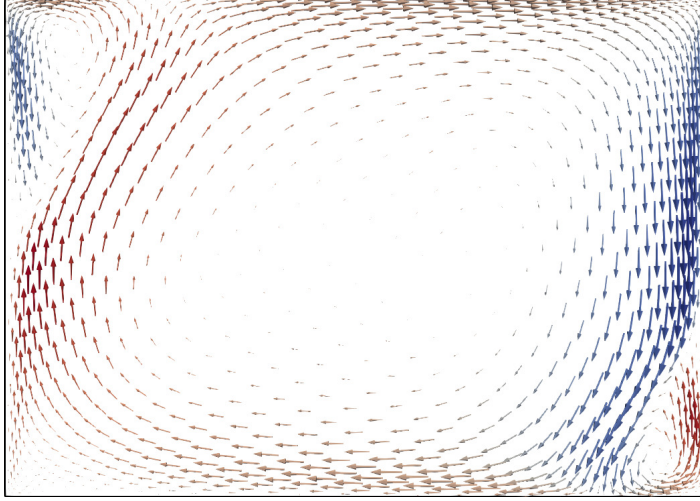


Figure 1.4: Mean velocity vectors in the LSC plane of a cubic domain at $Ra = 10^7$ from an example simulation from this thesis. The magnitude of the vectors is demonstrated by the arrow length and the colour represents vertical velocity (blue negative, red positive). The LSC shown in the figure is the diagonal plane of a cube, hence the horizontal dimension is larger than the vertical.

covered the role of non-Oberbeck–Boussinesq effects on these quantities. The significant advancements made in computational resources since the publication of Siggia [17], meant that much of the research reviewed in Ahlers *et al.* [14] was computational. For the most part, these simulations were carried out with numerical software that utilised the Oberbeck–Boussinesq approximation of the NSF equations. We will cover this in more detail in the next chapter, but we do not implement this approximation in the simulations that make up this thesis.

Much of the scaling in turbulent RBC summarised in Ahlers *et al.* [14] was carried out by Grossmann and Lohse [21]. Wherein, flow regimes are defined in a Ra – Pr parameter space depending on the relative thicknesses of the hydrodynamic and thermal boundary layers and on the dominant contribution (either bulk or background) to the turbulent kinetic energy and fluctuating temperature variance dissipation rates [22]. Ahlers *et al.* [14] also reviewed the contemporary research into LSC reorientations. By this time, experiments had shown the LSC to be nonstationary, i.e. the LSC does not stay in one plane for the entirety of its existence, it reorientates itself, that is changes axes, via cessations or rotations (see for example Cioni *et al.* [23]).

One of the principle scientific objectives of this thesis is to distinguish the investigated thermal configuration from that of turbulent RBC. In other words, we try to answer the question: what is the effect of a free surface in thermal convection? To do so, we make comparisons against the aforementioned turbulent RBC literature.

As already mentioned, evaporative cooling is the second thermal convection configuration from which our set-up borrows attributes. This is the study of the liquid-side flow induced by an evaporating interface [24] with no other heat source participating

in driving the flow. Early observations of an evaporating water layer, noted that cool water accumulates along lines on the free surface before plunging downwards in vertical sheets, taking surrounding fluid with it and creating an uneven surface layer [25]. The role of an upper thermal boundary layer as a source for thermal plumes has qualitative similarities to turbulent RBC where plumes break away from a cooled upper wall, falling rapidly into the interior [26]. However, in evaporative cooling the plunging sheets are broken-up and dissipated by diffusion before interacting with a lower boundary. There is a clear deviation from turbulent RBC here where the container bottom wall is heated and from which thermal plumes are also released from a second thermal boundary layer; see figure 1.3.

More recently, Flack *et al.* [27] measured velocities and subsequent turbulence quantities beneath an evaporating water surface. In that study, measurements were made for a shear-free, clean surface, i.e. without surfactants, where it was found that the turbulent kinetic energy peaked at the free surface. Bukhari and Siddiqui [28] also observed the turbulent structure beneath an air/water interface and noted that these vortices increase in number and magnitude as a result of an increasing heat flux.

Specifically, and in relation to turbulent RBC, evaporation-driven thermal convection shares the attribute of plume formation at both boundaries, hence also the presence of a LSC. Likewise, from evaporative cooling, the current set-up shares the attribute of the maximum root mean square (rms) of velocity and temperature fluctuations occurring at the free surface. Throughout the thesis, the free surface in our thermal convection configuration, is approximated by a shear free upper boundary. This represents a novel set-up, and it is of interest to study the heat transfer effectiveness in the current configuration as a result of its shear-free upper boundary. This is achieved later by developing a $Ra-Nu$ power-law, and making comparisons with the more classical turbulent RBC equivalent.

The configuration shown in figure 1.3c *has* been investigated experimentally in the past, however, the aims were to better understand the gas-side flow and, importantly, to measure evaporation rates [29, 30]. In this latter reference, Bower and Saylor [30] considered whether water-side natural convection can affect evaporation rates. A result with considerable importance to the modelling of free-surface mass loss rates from SFP-LOCAs, which are up to 11m deep. Therein, it was argued that two different tanks of different depths, and hence Ra , could lead to different water-side turbulence intensities, and in turn, different mass fluxes at the free surface. Indeed, according to the experiments in [30], progressively deeper tanks lead to an increased free surface temperature and hence evaporative mass flux. This experimental study, however, was inconclusive, and it was hypothesised that the results could be due to an experimental artifact. One of the scientific motivations for this thesis is then to try and answer the open question of whether water-side turbulence plays a role on free-surface evaporation

rates.

As discussed above, this thesis concentrates on the water side mixing and, with the exception of the Appendix, we never attempt to simulate the gas-side phenomena. It is important, however, to understand the type of free-surface evaporation that is taking place at the free surface of a heated water pool.

1.3 Natural convection-driven evaporation

The process of evaporation from a free surface is simply the liquid changing to its vapour state. From the kinetic theory viewpoint, evaporation occurs when more molecules leave the interface from the water-side than enter from the gas-side. The liquid molecules are dynamic and some have enough energy to escape via the interface to enter the gaseous phase. The rate at which molecules escape is a function of the kinetic energy of the liquid molecules, that is of the temperature of the water. Likewise, immediately above the liquid, there are gaseous molecules which continuously strike the interface, some with enough energy to enter the liquid phase.

Evaporation from a free surface stops when the number of liquid molecules leaving the interface equals the number of gaseous molecules entering. The liquid is then said to be in equilibrium with its own vapour. The vapour pressure is then defined as the pressure exerted by the water vapour on the liquid water for a specific temperature; it is an indication of the liquid's evaporation rate and is reduced by the presence of the other gases that make up air [31].

For evaporation from the free surface to continue, the water vapour molecules must be further removed; this occurs first via diffusion then convection. The molecules must first pass through a concentration boundary layer. Once this has been achieved, the molecules are then transported further away by convection. The state of the surrounding gas, i.e. whether we have free or forced convection, plays here an important role. We add that this scenario differs from Stefan's quasi-static diffusion problem of evaporation which is relevant only for long and narrow tubes where convection plays no role [32, 33].

The above process is analogous to heat transfer from a heated horizontal surface to cooler surrounding air. In this latter situation, heat is conducted, or diffused, first through the thermal boundary layer before being transported more completely by convection. The overall heat losses from a heated plate are often assumed to be proportional to the difference between the temperature of the solid, and the ambient gas-side temperature, with the heat transfer coefficient, h , as the proportionality coefficient. Of course, such a heat transfer coefficient is found experimentally and has a specific validity range, based on Ra . The same is true for natural convection mass transfer from an evaporating free surface. Instead of forming a Ra – Nu relation, we have a

Ra – Sh relation, where Sh is the Sherwood number; a measure of the dimensionless mass flux and previously known as the mass Nusselt number. We again provide a formal definition of Sh later on in the text. To the authors knowledge, the first to make such an analogy between heat and mass transfer was Hickox [31] and Boelter *et al.* [29] from the University of California, Berkeley. The relevant dimensionless number in the scaling is Ra due to the gas-side velocity being generated from free convection.

Gas-side free convection also happens to be the natural state in the fuel building of an SFP in a Station-Black-Out. Here, the back-up electricity supply is unavailable for an extended period of time and, consequently, any eventual ventilation fails inside the fuel building. Unfortunately, the body of research on natural convection-driven evaporation is very limited, especially at high surface temperatures. This is important as an SFP can see both low or high surface temperatures during an accident and hence will experience both low and high free-surface evaporation regimes; figure 1.2 displays this well.

The work of Boelter *et al.* [29] studied “free evaporation into air of water from a free horizontal quiet surface” and dates from 1946. This is indeed close to the scenario that we assume to exist in an SFP. However, evaporation rates were measured from tanks into a quieting chamber, which ensured that the air-flow above the free surface was restricted. They looked at evaporation from a cylindrical tank of 0.3 m diameter of distilled water at interface temperatures ranging from 290.15 K to 361.15 K; above this ceiling boiling was observed, that is bubbles were seen to nucleate, on the heated lower tank wall. The air-side conditions, that is the relative humidity and temperature, were also measured, with the former playing a limited role in determining the evaporation rates. They plotted the water vapour concentration difference (from the surface to a distance far away) against the evaporation rates and were the first to find Ra – Sh scaling for this type of flow.

A full sixty years later, Bower and Saylor [30] reviewed the literature for evaporative free-surface natural convection from liquid pools and found only two references, that of Boelter *et al.* [29] and Sparrow *et al.* [34]. This latter paper looked only at the case where the water was cooler than the air above, and is thus not pertinent here. Further, it was noted that the work of Boelter *et al.* [29] over-restricted the airflow in their use of a quieting chamber and this had an important influence on the evaporation rates. Consequently, Bower and Saylor [30] set about extending the relevant literature by presenting their own experimental work. The work of Bower and Saylor [30] can be considered the first true study of evaporation from a water body where the air-flow is not restricted, yet is still under natural convection conditions; this is the situation of the SFP. The results of their work are later incorporated into the evaporation model that we develop in this thesis.

Following Fukushima 2011, there were other works that, although focusing specif-

ically on the SFP accident, did also develop their own models for free surface evaporation. Of particular note here are Wang *et al.* [11] and Quinn Brewster [35]. Later experimental work [36] showed that the former over-predicts and the latter under-predicts the actual mass flux from a free surface. The evaporation model that we develop has similarities with both Wang *et al.* [11] and Quinn Brewster [35] and we validate the final model against the experimental work of Martin and Migot [36].

1.4 Outline and objectives of the thesis

In summary, we investigate an evaporation-driven turbulent thermal configuration similar to the well-known configurations of turbulent RBC and evaporative convection. One of our motivations is to better understand the physical phenomena occurring during the pre-uncovery phase of an SFP loss-of-cooling accident. The scientific motivations are then as follows:

1. Study and evaluate the impact of the free surface on thermal convection
2. Study the role of non-Oberbeck–Boussinesq effects in the flows of interest
3. Develop, implement and validate a model for evaporation at a free surface
4. Determine the role of water-side turbulence on free-surface evaporation rates

To date, the above scientific questions have only been partially addressed. Answering these open questions will both contribute to the thermal convection literature and help the nuclear industry understand better evaporative mass losses during the early stages of a SFP-LOCA. More concretely, the rest of the thesis is structured as follows:

In chapter 2, we provide the governing equations for the problem in hand, that is the low-Mach-number expansion of the NSF equations. We also discuss how these equations are discretised spatially and temporally and then detail our implementation of the resulting numerical algorithm. In this chapter, we also provide details on the turbulence modelling adopted in the thesis.

In chapter 3, we carry out a numerical study where we fix a temperature drop across a cuboid domain without taking into account evaporation. The set-up is a modified turbulent RBC set-up with a free slip upper boundary condition as a first approximation of a free surface. The originality of this chapter is in the study of the role of the free-slip and non-Oberbeck–Boussinesq effects on the mean flow properties and turbulent statistics. A final novel aspect is in the turbulent-kinetic-energy (TKE) budget that we perform.

In chapter 4, we build on the previous chapter by significantly improving the thermal boundary condition above. Here, we prescribe a representative evaporative heat flux

leaving the domain in the form of a non-zero Neumann boundary condition for the temperature. We provide a detailed explanation on the calculation of the temperature gradient based on representative evaporation rates from experiments before carrying out a series of direct-numerical simulations. The originality here is in the assessment of the statistical properties of the flow, the Ra – Nu scaling and analysis of the LSC structure for this novel configuration.

In chapter 5, we again build on the previous work by implementing a novel dynamic thermal boundary condition based on evaporative and convective heat loss at the free surface. We consider only the water-side domain in the system of governing equations. However, we fix ambient conditions and model the heat loss locally, that is based on a local, cell-dependent, film temperature. On the upper boundary we therefore have a variable non-zero Neumann boundary condition for the temperature representative of natural convection-driven heat losses. Without modelling both the gas- and water-side domains, this configuration is as close to the full physical problem as possible. The original aspects of this chapter are the assessment of the role of aspect ratio on the LSC structure and the investigation of water-side turbulence effects on evaporation rates above. We also extend the parameter space of the Ra – Nu scaling in the previous chapter by carrying out simulations at high Ra .

Finally, in chapter 6 we draw conclusions and discuss future research avenues.

Chapter 2

Governing equations and numerical algorithms

2.1 Introduction

In thermal convection, it is uniquely variations in the temperature field that drive the flow. Evidently then, if simulations are to be used to study the problem in hand, it is important to take into account the accompanying variations in fluid properties. As we touched upon in the Introduction, Direct Numerical Simulations (DNS) can be expensive and certain approximations, such as that of Oberbeck–Boussinesq, can simplify the governing equations and hence enable the use of quicker and more efficient numerical algorithms.

The role of DNS in understanding the physics of turbulent thermal convection is well-known; numerical experiments enable data acquisition to an extent that is not possible in a laboratory. However, in the specific case of turbulent RBC, there is the further advantage of simulating an *ideal* numerical experiment. This means the possibility of exact temperature boundary conditions, the absence of conductive heat losses through sidewalls, which are purely adiabatic in simulations, and the unconditional validity of the Oberbeck–Boussinesq approximation, which is invoked in the majority of finite-volume simulations in the turbulent RBC literature [14].

Our approach in this thesis is to adopt a flexible numerical method that is applicable in both single and multi-phase flows. As discussed in the Introduction, the high-mass transfer regime is indicative of high interface temperatures. Consequently, under such conditions, large temperature variations exist between the interface and the ambient gas-side conditions. As a result, density variations are also expected, and it is imperative to adopt a numerical method that takes this into account.

One method that accounts for such transport property variations, is to develop software which solves the low-Mach-number approximation of the compressible NSF

governing equations. Such an approximation requires that the Mach number of the flow is low. For example, it can be shown that in flows with small density variations, that is $\Delta\rho \ll \rho$, the Mach number is low [37]. More generally, when the density variations regardless of their amplitude, are induced by thermal as opposed to mechanical means, then the flow evolves at low-Mach numbers and is said to be incompressible.

The low-Mach number equations are derived by expanding all the flow variables in a power series by a perturbation parameter based on the Mach number. In the resulting equations, the pressure is decomposed into thermodynamic and dynamic contributions. The former appears uniquely in the energy equation, whereas the only pressure appearing in the gradient term of the momentum equation is the dynamic contribution. Further, the contribution to the energy equation from viscous work terms in incompressible, and low-Mach number, flows is negligible. For these reasons, the momentum and energy equations are decoupled. This approach has a significant advantage over solving the full set of NSF equations as the compressible terms have been removed and with it, the significant restrictions on the maximum time-step. If required, more detailed explanations of the low-Mach number expansion of the NSF equations are available in the literature [37, 38].

Although the use of the low-Mach number approximation of the NSF equations could be considered excessive for the water-side flow where density variations are small, the variations in other transport properties are significant and this approach remains valid for both liquid and gases.

In what follows we present the important numerical features of our scientific software. We provide only an outline of the finite-volume method in the open-source software OpenFOAM[®] and how it can be used to simulate low-Mach number flows. More details of the OpenFOAM[®] code are available at [39]. The rest of the chapter is structured as follows: we first provide the governing equations before elaborating on the numerical algorithms. Within, the algorithm section we also discuss how the governing equations are discretised in space and in time as well as providing the additional equations for the modelling of turbulence.

2.2 Governing equations

In this thesis, we consider only the flow beneath an evaporating surface and as such the working fluid is liquid water, which is treated as Newtonian. The exception to this rule is the Appendix, where we present a two-phase approach for simulating an evaporating free surface. We investigate flows without invoking the Oberbeck–Boussinesq approximation and therefore variations of the density and transport properties with temperature are taken into account. For this reason, the system of governing equations is the low-Mach number approximation of the compressible NSF equations [38, 40],

which in dimensional form reads,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (2.1)$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \nabla \cdot \boldsymbol{\tau} - \nabla p + \rho \mathbf{g}, \quad (2.2)$$

$$\frac{\partial (\rho c_p T)}{\partial t} + \nabla \cdot (\rho c_p \mathbf{u} T) = \nabla \cdot (\lambda \nabla T) + \frac{dp_0(t)}{dt}, \quad (2.3)$$

with $\mathbf{u} = (u, v, w)$ as the velocity vector.

In (2.2), p stands for the sum of the 2nd-order term of the low-Mach-number expansion of the pressure, p_1 , and the bulk viscous pressure, p_v , that is $p = p_1 + p_v$. Here, $p_v = \zeta (\nabla \cdot \mathbf{u})$, with ζ as the bulk viscosity [41, 42]. Also, $\boldsymbol{\tau}$ stands for the deviatoric part of the viscous stress tensor, defined as,

$$\boldsymbol{\tau} = \mu \left(2\mathbf{S} - \frac{2}{3}(\nabla \cdot \mathbf{u})\mathbf{I} \right), \quad (2.4)$$

where $\mathbf{I}$ is the identity matrix, μ the dynamic viscosity and the rate-of-strain tensor $\mathbf{S}$ is given by,

$$\mathbf{S} = \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T). \quad (2.5)$$

In (2.3), c_p is the specific heat and λ the thermal conductivity. The $p_0(t)$ term is the 1st-order component of the asymptotic expansion of pressure at the zero-Mach limit, interpreted as the thermodynamic pressure. According to the low-Mach number expansion, it is spatially uniform, that is $\nabla p_0 = 0$. For open domains, p_0 is constant and equal to the ambient pressure, whereas for closed domains, p_0 varies with time and is evaluated from the equation of state of the working medium.

In order to close the system of governing equations, an isobaric “equation of state” for the water density is required. More specifically, a ρ - T relation is introduced. This relation is a fourth-order polynomial fit, which for a generic quantity ϕ reads,

$$\phi = c_4 T^4 + c_3 T^3 + c_2 T^2 + c_1 T + c_0. \quad (2.6)$$

The tabulated data is taken for water density at one atmosphere and over a case-dependent temperature range of interest [43]. The other fluid thermodynamic properties, λ and μ are also calculated from a quartic polynomial fit of the form (2.6) with data originating from the same reference. Example sets of coefficients for the fits of ρ/p_0 , λ and μ are provided in chapters 3–5.

Throughout the thesis, the simulations with the largest ΔT involve large variations of the dynamic viscosity and the thermal conductivity across the domain. In other words, even though the density variations are small, the induced variations in the transport properties of water are non-negligible. On the other hand, c_p varies very

little over the temperature ranges investigated herein. It is thus taken as a constant, case-dependent, value in all simulations. We note also that with the aforementioned variations in fluid properties, Pr varies across the domain in all simulations.

2.3 Numerical algorithms

Throughout this thesis we have used the open-source CFD code OpenFOAM® v1806 to develop numerical software. The intention has been to develop a code that can incorporate more physics in future research, if and when required. The primary focus of the PhD is on marginal improvements to the pre-existing OpenFOAM® solvers and applying them to the novel physical phenomena described in the Introduction. What follows is, for the most part, adapted from Jasak [44] and Ferziger and Perić [45], which should act as points of reference for a more detailed explanation.

2.3.1 Discretisation

In the finite-volume method, which OpenFOAM® is based on, the term discretisation refers to both the discretisation of the computational domain and to the discretisation of the partial differential conservation equations into their algebraic form.

Discretisation of the computational domain provides the mesh on which the algebraic version of the governing equations, that is (2.1)–(2.3), will be solved. In other words, it is the process of deciding the spatial positions where we seek a solution. For unsteady problems, such as the turbulent thermal convection investigated in this thesis, we must also integrate the equations in time. To achieve the desired second-order accuracy, we must discretise the differential equations into their algebraic form with (at least) second-order accuracy both spatially and temporally.

As OpenFOAM® uses a collocated grid arrangement, all variables are computed and stored in the centroid of the control volume (cell-centres). We use non-uniform hexahedral grids throughout so that a generic cell of volume, V_P , has the point P located at its cell-centre. All cell faces are flat and shared with neighbouring cells (or boundaries). In this way, the cell faces are either internal or at a boundary. The face area vector, $\mathbf{S}_f$, is then defined as normal to the face, with its magnitude equal to its area. Herein, we use the subscript f to relate to any quantity at the cell face.

The accuracy of the discretisation process depends on the variation of the conserved quantity in time and space. In order to demonstrate the adopted discretisation schemes we first provide the energy equation in integral form for an arbitrary control volume, where Gauss theorem has been used to convert the volume integrals into

surface integrals as follows,

$$\int_{V_P} \frac{\partial}{\partial t} (\rho c_p T) dV + \oint_{\partial V_P} (\rho \mathbf{u} c_p T) \cdot d\mathbf{S}_f = \oint_{\partial V_P} (\lambda \nabla T) \cdot d\mathbf{S}_f + \int_{V_P} \frac{dp_0(t)}{dt} dV. \quad (2.7)$$

The first term on the left-hand side (lhs) of (2.7) is the unsteady term. For the time-marching part of the numerical solution of (2.1)–(2.3) we employ the second-order accurate, implicit, backward differencing scheme for all terms, taking into account the current and the two previous time steps,

$$\int_{V_P} \frac{\partial}{\partial t} (\rho c_p T) dV = \frac{c_p \rho^n}{\Delta t} \left(\frac{3}{2} T^{n+1} - 2T^n + \frac{1}{2} T^{n-1} \right) V_P. \quad (2.8)$$

In the above equation, T is then the average temperature in V_P . For second-order schemes such as the central differencing used here, this coincides with the centroid value. Further, the superscripts “ $n+1$ ”, “ n ” and “ $n-1$ ” correspond to the current, previous and “second previous” time-steps. Here, the time-step is defined as the time taken to go from time-step n to $n+1$, and is calculated dynamically in relation to a Courant number of 0.25. Finally, in (2.8) the density is analysed at time-step n as there are only very small changes between time-steps; in this manner the algorithm is greatly simplified without loss of accuracy. As noted earlier in this chapter, c_p , is constant at all time-steps.

The second term on the lhs of (2.7) is the convective term. Discretising into algebraic form gives,

$$\oint_{\partial V_P} (\rho \mathbf{u} c_p T) \cdot d\mathbf{S}_f \approx \sum_f (\rho \mathbf{u} c_p T)_f^{n+1} \cdot \mathbf{S}_f \approx \sum_f (c_p T)_f^{n+1} (\rho \mathbf{u})_f^n \cdot \mathbf{S}_f, \quad (2.9)$$

where the second approximation in (2.9) is a result of using the mass flux through the face at the known time-step n , defined as $(\rho \mathbf{u})_f^n \cdot \mathbf{S}_f$, in accordance with the conservative formulation of the governing equations. This approximation is consistent with the use of ρ^n in (2.8) and allows for a simplification of the algorithm. Regarding the spatial discretisation, the convective flux term requires face-interpolated values which are found from the second-order accurate (linear) central difference scheme. As such, the face values are interpolated from the cell-centre values either side.

Similarly, the first term on the right-hand side (rhs) of (2.7) is the diffusive term, which we discretise as follows,

$$\oint_{\partial V_P} (\lambda \nabla T) \cdot d\mathbf{S}_f \approx \sum_f (\lambda \nabla T)_f^{n+1} \cdot \mathbf{S}_f = \sum_f \lambda_f^n (\nabla T)_f^{n+1} \cdot \mathbf{S}_f, \quad (2.10)$$

where we again evaluate λ_f at time-step “ n ” to simplify the algorithm. This is permit-

ted as the change between consecutive time-steps is small. In order to evaluate (2.10), the temperature surface normal gradient, $(\nabla T)_f \cdot \mathbf{S}_f$, must be evaluated. This gradient is calculated at the cell face by subtracting the value at the cell-centre on one side of the face from the cell-centre value at the other side and dividing by the distance. That is, $(\nabla T)_f \cdot \mathbf{S}_f \approx (T_l - T_p) |\mathbf{S}_f|/|\mathbf{d}|$, where T_l is the cell-centre temperature in a neighbouring cell. This results in a second-order accurate scheme if the vector connecting the cell-centres is orthogonal to the face, which is the case throughout this thesis.

Finally, the second term on the rhs of (2.7) is the pressure term. As p_0 is uniform in space, it is approximated as follows,

$$\int_{V_P} \frac{dp_0(t)}{dt} dV \approx \frac{p_0^n - p_0^{n-1}}{\Delta t} V_P. \quad (2.11)$$

Combining (2.8)–(2.11) and dividing through by volume gives the semi-discretised form the energy equation as,

$$\begin{aligned} \frac{c_p \rho^n}{\Delta t} \left(\frac{3}{2} T^{n+1} - 2T^n + \frac{1}{2} T^{n-1} \right) + \frac{1}{V_P} \sum_f (c_p T)_f^{n+1} (\rho \mathbf{u})_f^n \cdot \mathbf{S}_f \\ = \frac{1}{V_P} \sum_f \lambda_f^n (\nabla T)_f^{n+1} \cdot \mathbf{S}_f + \frac{p_0^n - p_0^{n-1}}{\Delta t} V_P. \end{aligned} \quad (2.12)$$

We add that the pressure term on the rhs of (2.12) is zero for the liquid flows investigated herein. This is so because it is assumed that the thermodynamic pressure of the liquid is temperature independent and therefore constant. Finally, we note that as terms from time-step $n+1$ appear on both the lhs and rhs of (2.12), the above temperature equation must be solved implicitly.

2.3.2 Pressure–velocity coupling

For the pressure–velocity coupling a PISO (Pressure Implicit with Splitting of Operators) projection method is used, similar to the methods for incompressible flows [46, 47]. The divergence of the momentum equation is taken and the continuity equation is used as a constraint to formulate the variable-coefficient Poisson equation to be solved for p . In this low-Mach-number PISO algorithm, the temporal derivative of the density, $\frac{\partial \rho}{\partial t}$, emerges on the left-hand side of the Poisson equation which would be zero for the incompressible case. An outline of the PISO algorithm, adapted from Jasak [44], is now provided.

The PISO projection method involves an implicit predictor and multiple explicit corrector steps. Before we elaborate on how the pressure equation is determined we note that, for robustness purposes, the buoyancy term in the momentum equation is included inside a modified pressure variable as, $p' = p - \rho(\mathbf{g} \cdot \mathbf{h})$, the momentum

equation then reads,

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \nabla \cdot \boldsymbol{\tau} - \nabla p' + \mathbf{g} \cdot \mathbf{h} \nabla \rho, \quad (2.13)$$

A semi-discretised version of (2.13), where we leave the source terms in differential form is formulated as,

$$A_P \mathbf{u}_P + \sum_l A_l \mathbf{u}_l + \frac{(\rho_P \mathbf{u}_P)^n}{\Delta t} = -\nabla p' - \mathbf{g} \cdot \mathbf{h} \nabla \rho, \quad (2.14)$$

where P is again the index of an arbitrary cell-centre, the index l denotes neighbouring points that appear in the discretised momentum equation, so that A_P and A_l are the matrix coefficients corresponding to the arbitrary cell-centre and its neighbours, respectively. From the above we can get a relation for the velocity at point P as follows,

$$\mathbf{u}_P = \frac{1}{A_P} \mathcal{H}(\mathbf{u}) - \frac{1}{A_P} \nabla p' - \frac{1}{A_P} \mathbf{g} \cdot \mathbf{h} \nabla \rho, \quad (2.15)$$

where $\mathcal{H}(\mathbf{u})$ is defined as,

$$\mathcal{H}(\mathbf{u}) = - \sum_l A_l \mathbf{u}_l - \frac{(\rho_P \mathbf{u}_P)^n}{\Delta t}. \quad (2.16)$$

The first term on the rhs of (2.16) represents the current estimate of the neighbouring values and the second term on the rhs is the transient term from the previous time-step (or outer iteration). Multiplying (2.15) by ρ_P , the cell-centre density, then gives the term inside the divergence operator of the continuity (2.1) as follows,

$$\rho_P \mathbf{u}_P = \frac{\rho_P}{A_P} \mathcal{H}(\mathbf{u}) - \frac{\rho_P}{A_P} \nabla p' - \frac{\rho_P}{A_P} \mathbf{g} \cdot \mathbf{h} \nabla \rho. \quad (2.17)$$

One feature of collocated grids is the possibility of pressure odd-even decoupling when using central difference schemes. In such a situation, spurious pressure profiles can arise. To avoid this, OpenFOAM[®] uses a flux interpolation technique on the collocated grid [38, 48–50]. To this end, the terms in the above equation are linearly interpolated to their face values,

$$(\rho \mathbf{u})_f = \left(\frac{\rho}{A_P} \mathcal{H}(\mathbf{u}) \right)_f - \left(\frac{\rho}{A_P} \right)_f (\nabla p')_f - \left(\frac{\rho}{A_P} \right)_f (\mathbf{g} \cdot \mathbf{h})_f (\nabla \rho)_f, \quad (2.18)$$

and we write the discretised form of the continuity equation (2.1) as,

$$\nabla \cdot (\rho \mathbf{u}) = \sum_f (\rho \mathbf{u})_f \cdot \mathbf{S}_f = - \left(\frac{\partial \rho}{\partial t} \right)_P. \quad (2.19)$$

Then, combining (2.18) and (2.19) gives the pressure Poisson equation as follows,

$$\nabla \cdot \left(\frac{\rho}{A_P} \nabla p' \right) = \sum_f \left(\frac{\rho}{A_P} \mathcal{H}(\mathbf{u}) \right)_f \cdot \mathbf{S}_f - \sum_f \left(\frac{\rho}{A_P} \right)_f (\mathbf{g} \cdot \mathbf{h})_f (\nabla \rho)_f \cdot \mathbf{S}_f + \left(\frac{\partial \rho}{\partial t} \right)_P. \quad (2.20)$$

The Laplacian on the lhs of (2.20) is solved at the cell-faces using a second-order central-difference scheme.

Finally, we obtain a relation for the face flux by taking the dot product of (2.18) with the face area vector, $\mathbf{S}_f$,

$$(\rho \mathbf{u})_f \cdot \mathbf{S}_f = \left(\frac{\rho}{A_P} \mathcal{H}(\mathbf{u}) \right)_f \cdot \mathbf{S}_f - \left(\frac{\rho}{A_P} \right)_f (\mathbf{g} \cdot \mathbf{h})_f (\nabla \rho)_f \cdot \mathbf{S}_f - \left(\frac{\rho}{A_P} \right)_f (\nabla p')_f \cdot \mathbf{S}_f. \quad (2.21)$$

The aim of the PISO projection method is to use a segregated approach to solve the discretised NSF system of equations just described. Starting with ρ^n , T^n , $\mathbf{u}^n$ and p'^n , the algorithm to advance one step in time is as follows:

1. Solve for $\mathbf{u}^*$ from (2.14) using p'^n (momentum predictor step)
2. Solve for T^{n+1} from (2.12) (implicit temperature solution step)
3. Find ρ^{n+1} from (2.6) using T^{n+1}
4. Formulate $\mathcal{H}(\mathbf{u})^*$ from (2.16)
5. Solve for p'^* from (2.20) (implicit pressure solution step)
6. Solve for $\mathbf{u}^{**}$ from (2.14) using p'^* (explicit velocity correction step)
7. Repeat steps 4–6
8. Using $\mathbf{u}^{n+1}$ and p'^{n+1} find new conservative flux, $(\rho \mathbf{u})_f^{n+1} \cdot \mathbf{S}_f$, from (2.21)
9. If final time not reached, advance to next time-step

Step 7 deserves further explanation. As the velocity correction in step 6 takes into account only the updated pressure, it is necessary to complete three *outer* iterations (steps 4–6 above), wherein convergence is achieved within a tolerance of 10^{-9} . This ensures that the $\mathcal{H}(\mathbf{u})$ term is updated and, according to [46], ensures second-order accuracy with our chosen time integration scheme. In order to validate the numerical algorithm described in this section, we successfully reproduced the results of a classical turbulent RBC from the literature [51].

2.3.3 Turbulence modelling

The high potential of direct numerical simulations as a tool for studying turbulence is well-known. A desire for data from simulations where all eddies are resolved and the time history of the velocity field is available has driven turbulence research since the 1970s. All of this has been driven by an advancement in computational power, and at the same time, the relatively slow progress in computing power is holding back DNS as a useful tool in modelling industrial turbulent flows [52].

The Large-Eddy-Simulation (LES) approach offers a computationally cheaper alternative to fully resolved DNS. According to it, only the large, energy containing eddies are resolved and the effects of the unresolved scales on the flow are modelled. At the heart of LES is thus the requirement for a subgrid-scale modelling. The large scale field is captured as much as one can afford, whilst trying to model the effect of the small scales on the large scales.

The main argument behind LES is that, in the quest to understand turbulent flows, we are often predominately interested in the larger scales. The additional oomph required in resolving the intermediate to small scales, i.e. the backbone of DNS, is often not of primary importance. As a result, solutions on far coarser meshes can be sought and the time-scales for simulating flows can be reduced.

Among the first to propose the idea was Leonard [53], who filtered the governing equations, (2.1)–(2.3), in the aim of removing the smallest scales. For any flow quantity ϕ , such a low-pass filtering operation reads

$$\overline{\phi(\mathbf{x})} = \int_{-\infty}^{\infty} \phi(\mathbf{x} - \mathbf{x}') G(\mathbf{x}') d\mathbf{x}', \quad (2.22)$$

where the box filter function $G(\mathbf{x}')$ is defined as follows,

$$G(\mathbf{x}') = \begin{cases} \frac{1}{L}, & \text{for } |\mathbf{x}'| < \frac{L}{2}, \\ 0, & \text{otherwise,} \end{cases} \quad (2.23)$$

with L as the filter width. Then, $\overline{\phi(\mathbf{x})}$ can be considered a local average of ϕ in the (x, y, z) vicinity of $\mathbf{x}$. The advantage of the above *box* filter is that, the grid can play the implicit role of filtering out the smaller scales; that is the filter width is found from the local grid as $L = \Delta = (\Delta x \Delta y \Delta z)^{1/3}$. Here, the cube-root of the local cell is the simplest method for choosing for local filter width, and is the method used throughout this thesis.

The quantity $\overline{\phi(\mathbf{x})}$ is then filtered, i.e. smoothed, and all fluctuations associated with eddies smaller than the local grid size are removed. The standard procedure is to choose a filter width that lies in the inertial sub-range so that the majority ($\approx 80\%$)

of the energy containing eddies are resolved [52].

In order to avoid subgrid-scale terms in the continuity equation, Favre [54] introduced a mass-weighted filter for variable density flows. Using such a strategy, Favre-filtering a generic quantity ϕ reads,

$$\tilde{\phi} = \frac{\overline{\rho\phi}}{\bar{\rho}}, \quad (2.24)$$

and Favre-filtering (2.1)–(2.3) gives the following system of governing equations,

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{\mathbf{u}}) = 0, \quad (2.25)$$

$$\frac{\partial (\bar{\rho} \tilde{\mathbf{u}})}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{\mathbf{u}} \tilde{\mathbf{u}}) = -\nabla \bar{p} + \nabla \cdot \mu \left(2\tilde{\mathbf{S}} - \frac{2}{3}(\nabla \cdot \tilde{\mathbf{u}})\mathbf{I} \right) - \nabla \cdot \boldsymbol{\tau}^r + \bar{\rho} \mathbf{g}, \quad (2.26)$$

$$\frac{\partial \bar{\rho} c_p \tilde{T}}{\partial t} + \nabla \cdot (\bar{\rho} c_p \tilde{\mathbf{u}} \tilde{T}) = \frac{dp_0(t)}{dt} + \nabla \cdot (\lambda \nabla \tilde{T}) + \nabla \cdot \mathbf{q}^r, \quad (2.27)$$

where on the right-hand side of (2.26), $\tilde{\mathbf{S}}$ is now the filtered strain-rate tensor defined as,

$$\tilde{\mathbf{S}} = \frac{1}{2} (\nabla \tilde{\mathbf{u}} + (\nabla \tilde{\mathbf{u}})^\top). \quad (2.28)$$

Further, in the filtered governing equations, $\boldsymbol{\tau}^r$ and $\mathbf{q}^r$ stand for the subgrid-scale stress tensor and heat flux, respectively defined as,

$$\boldsymbol{\tau}^r = \bar{\rho}(\tilde{\mathbf{u}}\tilde{\mathbf{u}} - \widetilde{\mathbf{u}\mathbf{u}}) \quad (2.29)$$

and

$$\mathbf{q}^r = \bar{\rho}(\tilde{\mathbf{u}}\tilde{T} - \widetilde{\mathbf{u}T}). \quad (2.30)$$

Many LES studies of thermal convection [55–58] have used the eddy-viscosity model of Smagorinsky [59]. Wherein, the influence of the filtered-out eddies are approximated as a viscous contribution on the resolved fields. With respect to the subgrid-scale stress tensor this leads to,

$$\boldsymbol{\tau}^r - \frac{1}{3}\text{Tr}(\boldsymbol{\tau}^r) = \mu_t \left(2\tilde{\mathbf{S}} - \frac{2}{3}(\nabla \cdot \tilde{\mathbf{u}})\mathbf{I} \right), \quad (2.31)$$

where μ_t is the turbulent viscosity. The residual kinetic energy term in (2.31), $\frac{1}{3}\text{Tr}(\boldsymbol{\tau}^r)$, is incorporated into the pressure term $\bar{p}$ of (2.26), so that $\bar{p} = \bar{p}_1 + \bar{p}_v + \frac{1}{3}\text{Tr}(\boldsymbol{\tau}^r)$. In other words, we group together all the aforementioned surface force terms, which enter the governing equations via their gradient only. On the other hand, for the subgrid-scale

heat flux, the assumption of a turbulent diffusive contribution leads to,

$$\mathbf{q}^r = \lambda_t \nabla \tilde{T}, \quad (2.32)$$

with λ_t as the turbulent conductivity, which is found using the Reynolds analogy, $\lambda_t = \mu_t c_p / Pr_t$, and where Pr_t is a constant turbulent Prandtl number to be defined later.

Due to the low-Mach number approximation, no subgrid-scale terms associated with compressibility arise upon Favre-filtering (2.1)–(2.3). All that remains then is to choose a strategy for taking into account the eddies at scales smaller than Δ , where it is necessary only to extend the widely-used incompressible subgrid-scale models to take into account the variable density [60].

The closure of (2.26) only requires therefore an expression for μ_t , where Smagorinsky proposed the following relation,

$$\mu_t = \bar{\rho} C_s^2 \Delta^2 |\tilde{\mathbf{S}}|, \quad (2.33)$$

In (2.33), C_s is the model constant and $|\tilde{\mathbf{S}}|$ is defined as the square root of twice the double inner product of the filtered strain-rate tensor, that is $|\tilde{\mathbf{S}}| = (2\tilde{\mathbf{S}} : \tilde{\mathbf{S}})^{1/2}$. The idea behind computing the rate-of-the-strain tensor in (2.33) from the filtered velocity field is based on a physical argument. It is argued that μ_t should be determined by the unresolved eddies containing the most energy; that is the eddies of size comparable to cut-off length Δ [52].

Around the same time as Smagorinsky, Lilly [61] extended (2.33) using dimensional analysis, to account for the turbulence owing to buoyancy caused by the temperature gradients of the large-scale flow. The inclusion of a buoyancy production term gives the following relation for the turbulent viscosity,

$$\mu_t = \bar{\rho} C_s^2 \Delta^2 |\tilde{\mathbf{S}}| \left(1 - \frac{Ri}{Pr_t}\right)^{0.5}, \quad (2.34)$$

with the Richardson number, Ri , given by

$$Ri = \frac{1}{|\tilde{\mathbf{S}}|^2} \frac{|\mathbf{g}|}{\rho_{\text{ref}}} \cdot \nabla \bar{\rho}. \quad (2.35)$$

We note that (2.34) reduces to the Smagorinsky model for isothermal flows. Further, (2.35) is an approximation of the gradient Richardson number, Ri , which is valid for low-Mach number flows. The gradient Richardson number is equivalent to the square of the buoyancy frequency, presented herein is the form familiar to the oceanography community [62], with ρ_{ref} as a reference density.

In our study, we employ the Lagrangian dynamic model [63] adapted for variable density flows [64]. As such, the resolved scales are used to compute C_s locally and at each time-step. This model employs the procedure of Germano [65], to calculate C_s dynamically from,

$$C_s^2 = \frac{\langle L_{mn}M_{mn} \rangle}{\langle M_{pq}M_{pq} \rangle}. \quad (2.36)$$

where L_{mn} and M_{mn} respectively relate to the subgrid-scale stresses and resolved rate of strain tensors at two different filter widths, Δ and 2Δ . We add that the numerator and denominator appearing in (2.36) are referred to as $\mathcal{F}_{LM} = \langle L_{mn}M_{mn} \rangle$ and $\mathcal{F}_{MM} = \langle M_{mn}M_{mn} \rangle$, respectively. Further, the $\langle \cdot \rangle$ represents an averaging procedure. In Germano [65], the averaging procedure in (2.36) is carried out over directions of statistical homogeneity and leads to highly variable eddy-viscosity fields containing a significant fraction of negative values. To avoid this, Meneveau *et al.* [63] propose to carry out the sampling over flow pathlines. This is essential for the contained thermal convection investigated in this thesis.

The averaging procedure therefore requires the solution of two further transport equations, which when adapted for variable density and written in conservative form gives,

$$\frac{\partial}{\partial t}(\rho\mathcal{F}_{LM}) + \nabla \cdot (\rho\mathbf{u}\mathcal{F}_{LM}) = \frac{1}{\mathcal{T}}(L_{ij}M_{ij} - \mathcal{F}_{LM}), \quad (2.37)$$

and

$$\frac{\partial}{\partial t}(\rho\mathcal{F}_{MM}) + \nabla \cdot (\rho\mathbf{u}\mathcal{F}_{MM}) = \frac{1}{\mathcal{T}}(M_{ij}M_{ij} - \mathcal{F}_{MM}), \quad (2.38)$$

with $\mathcal{T}$ as a relaxation time-scale, which we take as the recommended value proposed in [65]. Further details about the above procedure are available in the same reference.

All terms are discretised as in section 2.3.1, except for the temporal derivative of (2.38) which uses the first-order accurate Euler backward scheme. Meneveau *et al.* [63] state that although the solution of two further transport equations increases the computational cost, high numerical accuracy in solving (2.37) and (2.38) is unnecessary. The idea behind using the Lagrangian dynamic subgrid-scale model is thus to remove negative viscosity and to enable the correct behaviour of C_s at near-wall locations. Indeed, although some clipping is required in our simulations it is always limited to a few percent.

In chapter 3 we dynamically calculate μ_t using the Smagorinsky relation for C_s from (2.33) and take Pr_t as constant and equal to 0.9 as recommended for liquid water [41]. Later, in chapter 5 we still dynamically calculate μ_t but use Lilly's updated model for C_s from (2.34) and take Pr_t , also present in (2.34), as constant and equal to 0.4 as recommended in Eidson [55]. The latter approach therefore builds upon and improves the results from the earlier chapter. It is noted that some references have calculated Pr_t dynamically [57, 66], but it is debatable if this extra effort is worthwhile.

2.3.4 Parallelisation

To conclude this chapter, we note that OpenFOAM[®] offers the option of running parallel simulations on distributed processors, using the openMPI implementation of message passing interface (MPI). All simulations in this thesis were completed on decomposed domains, whereby the computational domain and fields are divided-up and allocated to separate processors and the solver is run in parallel. A geometric decomposition is used, whereby the domain is split into pieces so that each processor handles approximately the same number of cells. Such a method allows for increased mesh refinement and speeds up simulations significantly.

2.4 Summary

In this chapter, we have introduced the governing equations for the problem in hand: the low-Mach number expansion of the NSF equations. Further, we have introduced the discretisation methods used in the finite-volume method adopted by OpenFOAM[®]. We then outlined an updated PISO algorithm for the low-Mach number flows in question, which allows for the solution of the governing equations. Moreover, we have also provided the modeling strategy used throughout this thesis for taking into account turbulence, that is the LES subgrid-scale models. These have been expanded upon and the Lagrangian dynamic procedure has been introduced. Finally, we discussed the method of parallelisation adopted, which enables longer simulations on more refined meshes.

Chapter 3

Thermal convection with a free-slip upper boundary

3.1 Introduction

In this chapter, we report on direct numerical and large-eddy simulations of turbulent thermal convection without invoking the Oberbeck–Boussinesq approximation. The working medium is liquid water and we employ a modified turbulent RBC set-up with a free-slip upper boundary condition. The domain is a cavity heated from below with a free surface above. Such a set-up is a coarse approximation of the problem of an evaporating free surface. We ignore completely the mechanisms and details of evaporation and apply fixed temperatures at both boundaries. This should be considered as an over-simplified model, but it allows for role of the free surface in thermal convection to be examined.

Turbulent RBC is most commonly studied numerically by invoking the Oberbeck–Boussinesq approximation for a fluid uniformly heated from below and cooled from above with solid upper and lower boundaries [16, 68–71]. This type of flow will be henceforth referred to as *classical turbulent RBC*. As discussed in the Introduction, the flow and thermal dynamics are then determined by the geometry of the cavity, the temperature difference across it and the resulting variation in fluid properties. The two dimensionless parameters Pr and Ra then govern the flow, with the system response measured in terms of the Nu and Re , where the velocity for the latter is representative of the large-scale circulation.

Although it is noted that Bénard’s initial experiments were carried out with an upper boundary open to atmosphere [13], the vast majority of numerical and experimental work has concentrated on the container bounded by upper and lower walls (see [14, 17, 72] and references therein). As a first attempt to understand the effects of the

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free surface on turbulent RBC, we carry out a DNS at $Ra = 10^7$ and a series of LES up to $Ra = 10^9$ where the free surface is approximated as a free-slip upper boundary. We further allow for variations of the density and other fluid properties by using a low-Mach number solver. To the authors' knowledge, this type of flow has not been investigated before.

A literature review suggests the most similar study to the flow examined herein is Zikanov *et al.* [57], in which the authors studied numerically the turbulent convection occurring in warm shallow ocean during adverse weather events. A heat flux was implemented at the free-slip upper surface to represent evaporation and the lower boundary was a rigid wall. The main differences between [57] and our study are the increased ΔT , the unstably stratified initial condition and the energy conservation introduced here by the fixed temperatures at the upper and lower boundaries (which also implies fixed ΔT).

The Oberbeck–Boussinesq approximation assumes that density variations have no effect on the fluid properties or on the flow field other than the buoyancy force. Accordingly, the density is assumed to be constant in all terms of the governing equations except in the gravitation term. This simplifies greatly the system of equations to be solved but remains valid for only small variations in temperature [73, 74]. The experimental pursuit of higher Rayleigh numbers has inevitably resulted in increasing ΔT , larger density variations and, with it, deviations away from the validity of the Oberbeck–Boussinesq approximation. This deviation is known as the non-Oberbeck–Boussinesq effect of the working fluid. Ahlers *et al.* [75] showed that, although variable viscosity and thermal diffusivity affect boundary layer heights and temperature profiles in turbulent RBC, both Nu and Re , based on large-scale circulation velocity, are insensitive to such non-Oberbeck–Boussinesq effects, even with a $\Delta T = 40$ K.

In this thesis, we take into account variable fluid properties to ensure that other qualitative flow features are not lost. Moreover, the effect of variable fluid properties on the different components of Nu , which includes the vertical turbulent heat flux, merits further attention. Finally, allowing for density variation allows for a more comprehensive analysis of the TKE budget.

The rest of the chapter is structured as follows: the numerical set-up is described further in section 3.2. Next, in section 3.3, we provide justifications for the DNS and LES grid resolutions. The numerical results are presented in section 3.4, where the global structure of the moderate Rayleigh number flow is first analysed, comparisons with the LES are made and a TKE budget is provided. We then present the results of the LES at higher Rayleigh numbers and assess the impact of the non-Oberbeck–Boussinesq and free-slip conditions on the first- and second-order flow statistics. Finally, conclusions are drawn in section 3.5.

3.2 Numerical set-up

The working fluid is liquid water, treated as Newtonian, at a mean temperature of 333.15 K corresponding to $Pr = 3$. Further, a ΔT of 20 K is applied between the lower wall and upper free-slip boundary. These temperatures correspond well to those seen in a loss-of-cooling accident in a spent-fuel pool during the heat-up stage of the accident, however, the ΔT itself is too high to represent evaporation. As mentioned in the Introduction to this chapter, the thermal boundary conditions enable analysis of both the free slip and non-Oberbeck–Boussinesq effects.

The significant changes in fluid properties over the thermodynamic range of interest must be taken into account as, with water as the working fluid, the ΔT used could render the use of the Oberbeck–Boussinesq approximation questionable [73, 74]. For this reason, the system of governing equations for the DNS is the low-Mach number approximation of the compressible NSF equations [38, 40], which are provided in dimensional form as (2.1)–(2.3). On the other hand, for the LES carried out in this chapter, the system of equations is (2.25)–(2.27). For the numerical solution of both sets of equations, we follow section 2.3.1 and for the pressure–velocity coupling we use the PISO projection method outlined in section 2.3.2.

In order to close the system of governing equations, we use the isobaric ‘equation of state’ given earlier as (2.6). This corresponds to the tabulated data in [43] for water density at one atmosphere and over the temperature range of interest for this chapter, which corresponds to 323.15–343.15 K. The coefficients of the polynomial fit are provided in table 3.1. According to (2.6), the liquid density varies by 1% over the range of interest. All other fluid properties are also calculated from a quartic polynomial of the form (2.6) with corresponding coefficients given in table 3.1.

	c_4	c_3	c_2	c_1	c_0
ρ/p_0	-2.87×10^{-12}	3.92×10^{-9}	-2.04×10^{-6}	4.7×10^{-4}	-0.031
μ	1.10×10^{-11}	-1.57×10^{-8}	8.43×10^{-6}	-2.0×10^{-3}	0.185
λ	3.6×10^{-11}	-3.4×10^{-8}	2.2×10^{-6}	5.4×10^{-3}	-0.59

Table 3.1: Polynomial coefficients for variable water thermodynamic properties over the temperature range 323.15–343.15 K [43]. We note that the c_p is set constant at 4183 J/kg/K.

The dynamic viscosity, μ , and the thermal conductivity, λ , vary, respectively, by 35% and 3 % over the temperature range of interest. In other words, even though the

density variations are small, the induced variations in the transport properties of water are significant. On the other hand, the specific heat, c_p , varies by only 0.2% over the domain and is thus taken as constant in the simulations. Moreover, we note that as a result of the aforementioned variations of the fluid properties, Pr varies by 40% across the domain.

The reference values of the fluid properties at $T_{\text{ref}} = 333.15$ K are $\rho_{\text{ref}} = 983.2$ kg m⁻³, $c_{p,\text{ref}} = 4183$ J kg⁻¹ K⁻¹, $\lambda_{\text{ref}} = 0.65$ W m⁻¹ K⁻¹, and $\alpha_{\text{ref}} = 1.6 \times 10^{-7}$ m² s⁻¹. These are later used for nondimensionalisation purposes along with the other Ra -dependent variables provided in table 3.2. Wherein, $U_{\text{ff}} = (|\mathbf{g}|H\beta\Delta T)^{1/2}$ is the free-fall velocity, later used to calculate the free-fall time from $t_{\text{ff}} = H/U_{\text{ff}}$.

Ra	H (m)	U_{ff} (m/s)
10^7	0.019	0.045
10^8	0.041	0.066
10^9	0.090	0.096

Table 3.2: Reference values for nondimensionalisation purposes. In this table, H is the height of the domain and U_{ff} is the free-fall velocity. As the thermal boundary conditions are constant between the simulations the reference values are provided in the text.

Dimensionless variables are denoted with a hat symbol ($\hat{\cdot}$), and we denote the normalised temperature as $\hat{\theta} = (T - T_{\text{ref}})/\Delta T$. The domain is a (1 : 1 : 6) cuboid with the unity aspect ratio corresponding to the first horizontal (x) and vertical (y) directions. The second longitudinal (z) direction is periodic with a length of $\hat{L} = 6\hat{H}$. The lower wall is located at $\hat{y} = 0$, the upper boundary at $\hat{y} = 1$ and, likewise, the side walls at $\hat{x} = 0$ and $\hat{x} = 1$, respectively.

The side walls are assumed to be adiabatic; as such, the condition $\partial\hat{\theta}/\partial\hat{x} = 0$ is prescribed at them. The lower (hot) and upper (cold) walls are isothermal and kept at $\hat{\theta} = 0.5$ and $\hat{\theta} = -0.5$ respectively. No-slip velocity boundary conditions are enforced at the side and lower walls, whereas the free-slip condition is prescribed at the upper-boundary, i.e. $\partial\hat{u}/\partial\hat{y} = \partial\hat{w}/\partial\hat{y} = 0$ and $\hat{v} = 0$ at $\hat{y} = 1$. As a result of the aforementioned boundary conditions there are three hydrodynamic boundary layers, one at each the vertical side walls and one at the lower wall. On the other hand, there are only two thermal boundary layers, one each at the lower wall and upper boundary.

With regard to initial conditions for the DNS, we employ a linear temperature profile across the vertical and a quiescent velocity field to which we apply small random perturbations. This initially unstable stratification results in the formation of convective patterns which then break down into turbulent motion until a statistically

stationary state is reached.

We run simulations for 100 free-fall times before assuming a statistically stationary state has been reached. This is sufficient time to wash out all transient effects [71]. Subsequently, averages are taken over a further 200 free-fall times, which is a longer averaging period than that used in [76] for the DNS of turbulent RBC at the same Ra and in a geometrically similar domain. The criterion for determining whether sufficient statistical data have been taken is elaborated on in section 3.4. Regarding the initial conditions for the LES at $Ra = 10^7$ and $Ra = 10^8$, the temperature and velocity fields are initialised from the DNS solution. Likewise, the flow fields for the LES at $Ra = 10^9$ are initialised from the LES solution of $Ra = 10^8$; this process reduces the time required for a statistically stationary solution to be found.

3.3 Resolution requirements

We start with the justification for the DNS resolution at $Ra = 10^7$, before moving onto the LES resolution at $Ra = 10^7$, $Ra = 10^8$ and $Ra = 10^9$.

3.3.1 Direct numerical simulation resolution requirements

The accuracy of a DNS is ensured only when the smallest length scales of the flow are everywhere resolved. The first criterion is therefore to ensure adequate resolution of the hydrodynamic and thermal boundary layers in the vertical direction. A universal criterion based on the laminar Prandtl–Blasius boundary layer theory has been developed by Shishkina *et al.* [77].

The *a priori* estimate of the dimensionless thermal boundary layer heights is found from the relation $\hat{\delta}_\theta = \frac{1}{2Nu}$. On the other hand, the *a priori* estimate of the dimensionless hydrodynamic boundary layer height, $\hat{\delta}_u$, is given by

$$\hat{\delta}_u = \frac{1}{2}E^{-1}Nu^{-1}Pr^{\frac{1}{3}}, \quad (3.1)$$

where the empirical constant $E = 0.982$. Then, according to Shishkina *et al.* [77], the minimum resolution requirements for $\hat{\delta}_u$ and $\hat{\delta}_\theta$, denoted by N_u and N_θ respectively, are

$$N_u = \sqrt{2a}E^{\frac{1}{2}}Nu^{\frac{1}{2}}Pr^{\frac{1}{3}}, \quad (3.2)$$

$$N_\theta = \sqrt{2a}E^{\frac{3}{2}}Nu^{\frac{1}{2}}, \quad (3.3)$$

where the empirical constant $a = 0.482$. For the flow under study, the values of N_u and N_θ are rounded to the next integer, so that we have $N_u = 5$ and $N_\theta = 4$. We also

provide these values in table 3.3, where they are shown to be minimum requirements for the number of points inside the boundary layers. In fact, as can be seen by the difference in values of those in parentheses and those outside, we intentionally over-resolve by more than a factor of two.

Ra	N_θ	N_u	N_x	N_y	N_z
10^7	10 (4)	13 (5)	110	110	360

Table 3.3: DNS grid resolution criteria. In this table, N_θ and N_u are the number of cells in the thermal and hydrodynamic boundary layers, respectively, and N_x , N_y and N_z are the number of cells x , y and z directions. In the second and third columns, the numbers in parentheses correspond to the minimum resolution requirements according to [77].

Further, in turbulent RBC the dissipation of turbulent kinetic energy peaks in the near-wall regions. It is therefore important to ensure that the grid is adequately refined in these regions too. Accordingly, we choose to refine equally in vertical (y) and horizontal (x) directions using a hyperbolic-tangent expansion from a minimum cell size at the boundaries to a maximum in the centre.

The second resolution criterion is to ensure that the bulk of the domain is adequately resolved. A satisfactory refinement can be predicted *a priori* by using the method of Stevens *et al.* [71], itself based originally on Grötzbach [78]. To this end, we recall that the Kolmogorov scale η is defined as $\eta = (\nu^3/\epsilon)^{\frac{1}{4}}$, with ϵ as the kinetic-energy dissipation. Moreover, for fluids at $Pr > 1$, it is the temperature microscale and not the Kolmogorov equivalent that is limiting. Interestingly however, the temperature microscale itself is Pr -dependent. That is, for fluids at $Pr \leq 1$, the relevant temperature microscale is the Corrsin scale, $\eta_C = \eta/Pr^{\frac{3}{4}} = (\kappa^3/\epsilon)^{\frac{1}{4}}$. Whereas, for $Pr > 1$ the Batchelor scale, $\eta_B = \eta/Pr^{\frac{1}{2}} = (\kappa^3 Pr/\epsilon)^{\frac{1}{4}}$, should be used [79]. As a side-note, $\eta_C = \eta_B$ for the case of $Pr = 1$ [80]. The above analysis suggests that the relevant temperature microscale for fluids at $Pr > 1$ should always be η_B ; however Grötzbach [78], Stevens *et al.* [71] and many other authors in the turbulent RBC literature use η_C .

Now, we let Δ be the maximum length of a given computational cell in the inhomogeneous direction, that is $\Delta = \max(\Delta x, \Delta y)$. The maximum wave-number seen by the grid, $k_{\max} = \pi/\Delta$, must then be greater than the reciprocal of the Kolmogorov and temperature microscales [71, 78]. The combination of the above relations leads to the following constraints,

$$\Delta \leq \pi\eta = \pi(\nu^3/\epsilon)^{\frac{1}{4}}, \quad (3.4)$$

and either

$$\Delta \leq \pi \eta_C = \pi (\kappa^3 / \epsilon)^{\frac{1}{4}}, \quad (3.5)$$

or

$$\Delta \leq \pi \eta_B = \pi (\kappa^3 Pr / \epsilon)^{\frac{1}{4}}. \quad (3.6)$$

For fluids at $Pr > 1$, the condition (3.5) oft-used by the turbulent RBC community is more stringent. For this reason, it is constraint (3.5) that is used from hereon based on η_C , with this latter quantity now referred to as the temperature microscale, η_θ .

Deardroff and Willis [81] argued that the turbulent kinetic energy dissipation profile in turbulent RBC is flat in the bulk of the flow. This led Grötzbach [78] to assume this dissipation to be constant and equal to the buoyant production. The ‘hydrodynamic resolution requirement’ based on the smallest Kolmogorov scale is then given by,

$$\Delta \leq \pi \eta \approx \pi H \left(\frac{Pr^2}{Ra Nu} \right)^{\frac{1}{4}}, \quad (3.7)$$

with H as the height of the domain. Next, using the Corrsin scale relation, $\eta_\theta = \eta / Pr^{\frac{3}{4}}$, (3.7) is transformed into the ‘thermal resolution requirement’ as follows,

$$\Delta \leq \pi \eta_\theta \approx \pi H \left(\frac{1}{Ra Pr Nu} \right)^{\frac{1}{4}}, \quad (3.8)$$

Technically, (3.7) and (3.8) are valid only for homogeneous isotropic turbulence but they are considered here as reasonable *a priori* predictions for adequate resolution in the bulk of the domain.

We note that (3.7) and (3.8) require an estimation of Nu in advance. To the authors knowledge, there are no correlations in the literature for the system studied here, hence the refinement procedure can be seen as an iterative process. Previous studies showed that a first estimate for Nu can be obtained via a classical Ra – Nu correlation from the literature, for example $Nu = 0.124 Ra^{0.309}$ [82], which is then updated *a posteriori* in (3.8) and the bulk resolution recalculated.

We provide the total number of cells for the DNS in table 3.3. Further, the DNS refinement in the vertical (and horizontal) direction at $Ra = 10^7$ is shown in figure 3.1 along with estimates of the hydrodynamic and thermal resolution requirements, respectively (3.7) and (3.8). The cells are clustered near the walls to capture the sharp gradients in temperature and velocity.

The above resolution requirements result in $\Delta y_{\max} = \Delta x_{\max}$ in the centre of the cavity. For the DNS, the uniform longitudinal grid resolution is determined from the maximum cell height (and width) found in the centre, that is $\Delta z = \Delta y_{\max} = \Delta x_{\max}$, used to calculate N_z from $L / \Delta z$.

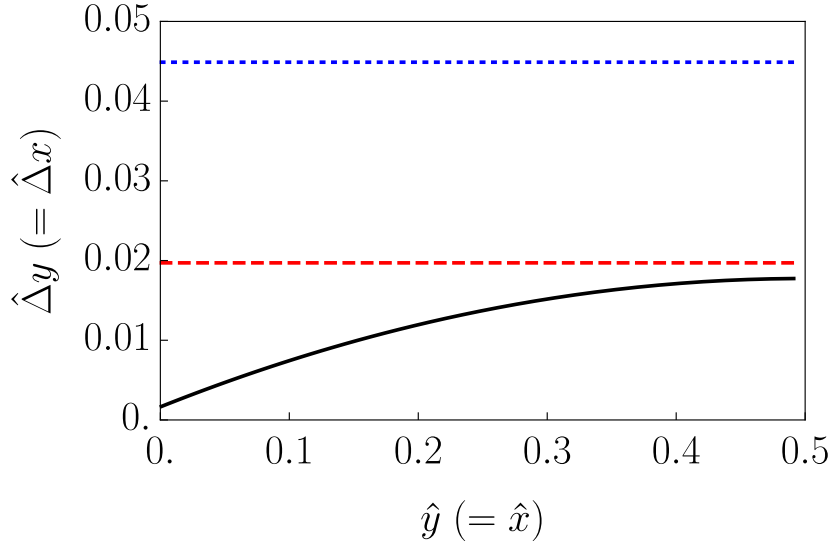


Figure 3.1: Vertical and horizontal grid resolution for the DNS at $Ra = 10^7$: actual resolution (—), global estimation of thermal resolution requirement (---) and global estimation of hydrodynamic resolution requirement (....). Only half the domain is shown due to symmetry.

For the computation of the time increment in our simulations, we set the Courant number equal to 0.25. As discussed in [76] the constraint on the time-step for numerical stability purposes is stricter than that of the Kolmogorov (and Corrsin) timescales; we can therefore assume that the smallest of the flow timescales are well captured.

3.3.2 Large-eddy simulation resolution requirements

As already discussed, the use of LES for the highest Rayleigh numbers investigated is required for reasons of computational limitations. In this study, we first carry out a DNS at $Ra = 10^7$ and then compare statistics with an LES at the same Ra but using a coarse mesh, where cell numbers are reduced by approximately a factor of 3 in each direction. Other methods for assessing the LES refinement quality are also available. For example, Davidson [83] has proposed to verify the grid resolutions on the basis of the computed dissipation spectra. Herein, however, we compare against the resolved DNS to ensure satisfactory results.

Once comparisons of flow statistics confirm satisfactory predictions by the LES at moderate Ra , we apply similar refinement criteria to the meshes at higher Ra . This task is complicated by the further requirement for the minimum number of points in the thermal, N_θ , and hydrodynamic, N_u , boundary layers outlined above. The procedure is summarised in four steps: (i) determine the boundary-layer and bulk resolution requirements for the DNS at the chosen Ra , (ii) reduce by a factor of 3 the number of points in the vertical and horizontal, (iii) increase the hyperbolic-tangent expansion in a manner that guarantees the boundary-layer requirements are met and, finally, (iv)

set $\Delta z = \Delta y_{\max} = \Delta x_{\max}$.

In all LES presented herein the number of points in the boundary layers exceeds the requirement in [77], whereas the bulk resolution requirement is relaxed by approximately a factor of 4. Consequently, the difference between the smallest and largest cells, $\Delta y_{\max}/\Delta y_{\min}$, for the LES is approximately 40.

An alternative LES resolution requirement is to match the filtering cut-off width to the Taylor microscale, which is a characteristic turbulence length-scale related to the mean strain rate. For isotropic turbulence this is defined as $\eta_l = (15\nu\mathbf{u}^2/\epsilon)^{1/2}$ [79], where $\mathbf{u}$ is a representative velocity of the large structures. With appropriate scaling for ϵ , Peng *et al.* [84] used the following relation to find half the Taylor microscale,

$$\frac{\hat{\eta}_l}{2} = \frac{\sqrt{15}\mathbf{u}^*}{\sqrt{Ra(Nu-1)}}, \quad (3.9)$$

$$\hat{\mathbf{u}}^* = \sqrt{0.0027Ra^{1.04} + 0.0312Ra^{0.92}}. \quad (3.10)$$

where (3.10) is found using the turbulent RBC scaling relations of [68].

This procedure gives a good approximation of an *a priori* LES bulk resolution requirement. In-line with [84] we choose to use half the Taylor microscale, $\hat{\eta}_l/2$, as a maximum cell size found in the bulk. The above values are summarised in table 3.4 and an example resolution is shown graphically for $Ra = 10^8$ in figure 3.2, where the maximum bulk cell size lies between that of the hydrodynamic resolution requirement (3.7) and half the Taylor microscale (3.9).

Ra	N_θ	$N_{\mathbf{u}}$	N_x	N_y	N_z	$\frac{\Delta y_{\max}}{\Delta y_{\min}}$	$\frac{\pi\eta_\theta}{\Delta y_{\max}}$	$\frac{N_{\text{DNS}}}{N_{\text{LES}}}$	$\frac{\hat{\eta}_l}{2}$
10^7	6 (4)	7 (5)	40	40	100	40	3.5	37	0.051
10^8	7 (5)	9 (7)	80	80	200	35	3.5	36	0.034
10^9	9 (7)	11 (9)	130	130	300	45	4.5	40	0.023

Table 3.4: LES grid resolution criteria. In the second and third columns, the numbers in parentheses correspond to the minimum resolution requirements according to [77] and those outside correspond to the true values.

Following the above procedure means that the LES is well-resolved at the walls, and hence no wall model is required. However, in the bulk, the LES mesh described above resolves only the large-scale structures. The effects of the unfiltered small scales must therefore be captured by an appropriate subgrid-scale model. These effects can be modelled as subgrid-scale viscous stresses and a subgrid-scale heat flux, respectively, in the momentum and energy equations.

As discussed in section 2.3.3 in regard to the subgrid-scale stresses, the Lagrangian

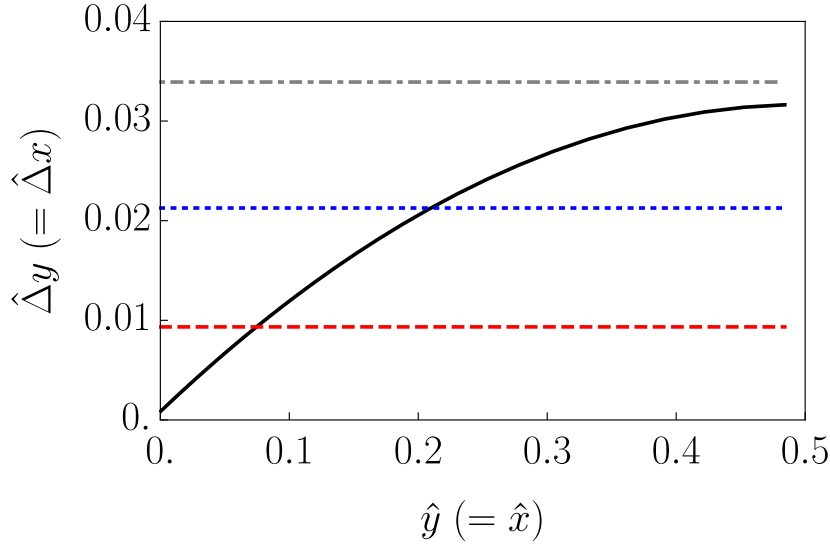


Figure 3.2: Vertical and horizontal grid resolution for the LES at $Ra = 10^8$: actual resolution (—), global estimation of thermal resolution requirement (---), global estimation of hydrodynamic resolution requirement (....) and half the Taylor microscale or $\hat{\eta}_l/2$ (- - -). Only half the domain is shown due to symmetry.

dynamic subgrid-scale model [63] is used to dynamically calculate μ_t . This model allows for the inhomogeneity of the flow within a (partial) container to be captured. Similarly, in this chapter, λ_t is computed from the local μ_t and ρ and by assuming a constant value of the turbulent Prandtl number, $Pr_t = 0.9$ [41].

3.4 Numerical results

The numerical results are presented in two parts. First, the moderate Rayleigh number case, at $Ra = 10^7$, is analysed by looking at the time-averaged flow properties, instantaneous flow structures, comparisons of second-order flow statistics between the LES and DNS and a turbulent kinetic energy budget of the DNS. We then look at the time-averaged flow properties and flow statistics of the LES over increasing Ra and quantify the effects of the free-slip boundary and variable fluid properties. Unless stated otherwise the notation adopted is as follows: the mean of a generic variable ϕ is denoted by $\langle \phi \rangle$ and refers to averaging both in time and over the homogeneous (periodic) z -direction. The fluctuating component is denoted by ϕ' and the rms value by $\phi_{\text{rms}} = \langle \phi' \phi' \rangle^{1/2}$.

3.4.1 Analysis of moderate-Rayleigh-number flow

We start with the presentation and analysis of the flow at the moderate Rayleigh number of 10^7 .

3.4.1.1 Time-averaged flow properties

We first look at the spatial resolution of the DNS. We confirm *a posteriori* that the grid resolution criterion (3.6), $\Delta/\pi\eta_\theta \leq 1$, is appropriately met so that the hydrodynamic and thermal resolution requirements of the flow are satisfied. A resolved DNS means that the comparisons of flow statistics with the LES at the same Ra can be used to test the latter's resolution.

A first understanding of the statistical steadiness of the solution can be obtained from analysis of the heat transfer in the domain. The dimensionless heat transfer across the x - z plane is measured by the local Nusselt number, Nu_y , calculated from time- and area-averaging of the nondimensionalised form of the energy equation (2.27),

$$Nu_y = \underbrace{\sqrt{RaPr} \langle \hat{\rho} \hat{v} \hat{\theta} \rangle_{xzt}}_{Nu_{\text{conv}}} - \underbrace{\langle \hat{\lambda} \frac{\partial \hat{\theta}}{\partial \hat{y}} \rangle_{xzt}}_{Nu_{\text{diff}}}, \quad (3.11)$$

whereas the global Nusselt, Nu_G , is found from volume-averaging the same equation,

$$Nu_G = \sqrt{RaPr} \langle \hat{\rho} \hat{v} \hat{\theta} \rangle_{xyzt} - \langle \hat{\lambda} \frac{\partial \hat{\theta}}{\partial \hat{y}} \rangle_{xyzt}, \quad (3.12)$$

In the above equations, the symbol $\langle . \rangle_{xzt}$ denotes averaging over time and over a given horizontal x - z plane, whereas the symbol $\langle . \rangle_{xyzt}$ denotes averaging over time and volume. For the flow in question, a statistically stationary solution will give Nu_y as constant for $0 \leq y \leq 1$ and further equal to Nu_G . For the DNS at $Ra = 10^7$, $Nu_y = Nu_G = 21.4$. Further, its value changes by less than 0.1% if only the first half of the averaging time is used suggesting that a statistically stationary state has indeed been reached.

For the Large-Eddy Simulations, an effective thermal conductivity, $\lambda_{\text{eff}} = \lambda + \lambda_t$, replaces λ in (3.11) and (3.12) due to the additional turbulent contribution. Regarding the LES at $Ra = 10^7$, we find $Nu_y = 19.9$ and $Nu_G = 20.0$, which corresponds to an underprediction of approximately 7% when compared to the DNS. We note that in previous studies of RBC using LES such as [85], Nu is *over*-predicted when compared to experimental and DNS data. It is known that underresolved boundary layers result in an overprediction of Nu [68, 71]; we therefore postulate that the errors in the prediction of the LES are not due to low resolution, but are most likely related to the use of the Reynolds analogy ($\lambda_t = \mu_t c_p / Pr_t$) and the associated constant turbulent Prandtl number Pr_t used in this study. This is an aspect to be improved in future studies.

The vertical distributions of Nu_y for the DNS and LES at $Ra = 10^7$ are now assessed. The differing contributions of the convective and diffusive components of

Nu_y are shown in figures 3.3a and 3.3b, respectively. Only half of the domain is shown for the convective component which tends to a small non-zero value inside the boundary layers. For the diffusive component, only the boundary layer is shown, as its contribution is negligible in the bulk.

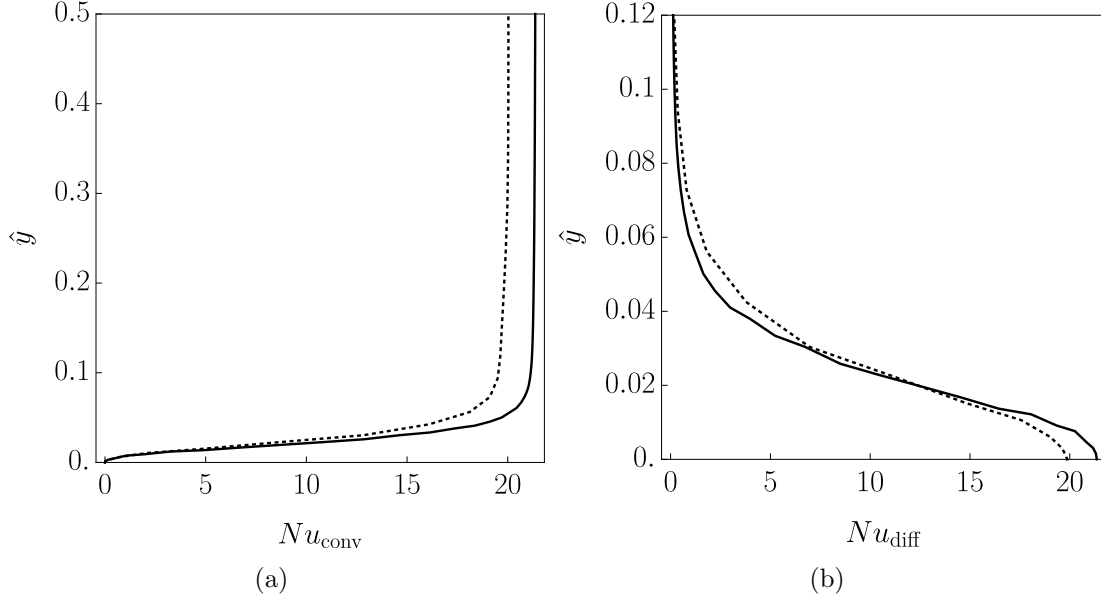


Figure 3.3: Plots of the time- and area-averaged components of Nu_y at $Ra = 10^7$. (a) Nu_{conv} across the lower half of the domain and (b) Nu_{diff} zoom on lower boundary. The legend is as follows: DNS (—) and LES (.....).

We note that a constant Nu is a necessary but not sufficient condition to ensure a statistically stationary solution. A better indication of steadiness is found by looking at the time derivative term of the TKE equation, completed later on in this section.

The DNS at $Ra = 10^7$ is now qualitatively assessed in order to obtain a global understanding of the flow. Time-averaged streamlines are shown in figure 3.4 coloured by the time-averaged vertical velocity $\langle \hat{v} \rangle_t$. The cuboid geometry means that a typical large-scale circulation is observed, such as in [66]. However, due to the extension of the domain in the homogeneous z -direction, multiple large-scale circulation patterns are formed. Three individual large-scale circulations can be identified as contained and the fourth appears across the periodic boundary.

A diagonal plane of the first fully-contained large-scale circulation is shown in figure 3.4 and a zoom is provided of this rotated plane in figure 3.5. The typical large-scale-circulation for RBC in a cubic container is observed in the superimposed velocity vectors, i.e. the large-scale circulation fills the entirety on the vertical domain with recirculation zones in the corners corresponding to peaks in the $\hat{\theta}_{rms}$ [66]. The same pattern is observed over all three contained mean winds except that the direction of the large-scale circulation is reversed between consecutive LSC patterns.

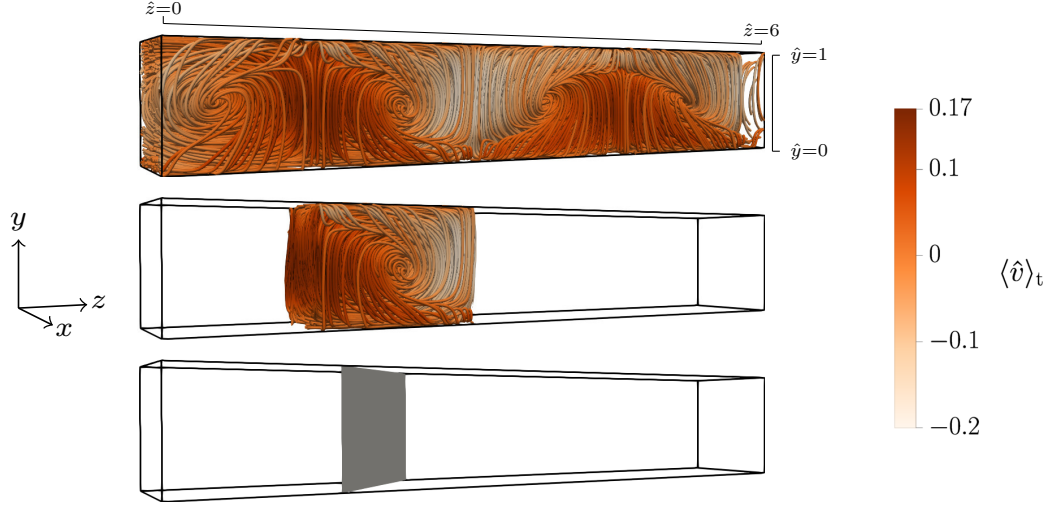


Figure 3.4: Time-averaged streamlines of DNS at $Ra = 10^7$ coloured by dimensionless mean vertical velocity, $\langle \hat{v} \rangle_t$. In the top figure we show the full flow structure with the four LSC patterns, in the middle figure we select a unique LSC pattern, and in the bottom figure we show the diagonal slice that is analysed in figure 3.5.

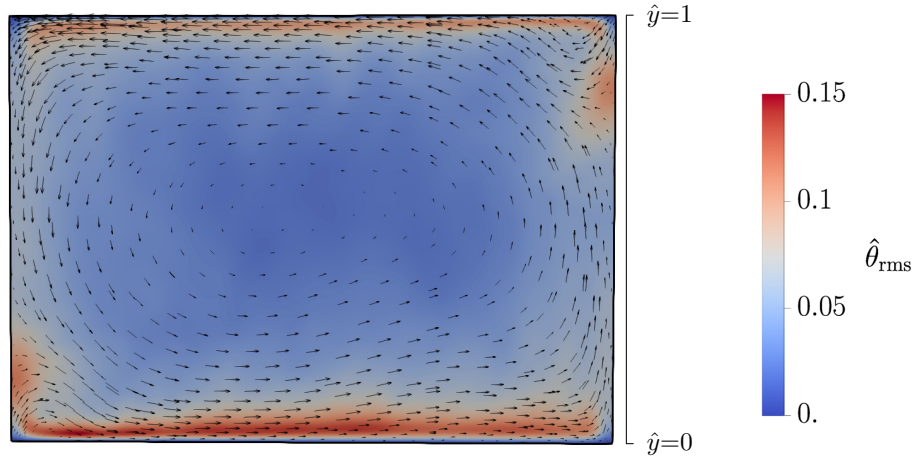


Figure 3.5: Colour plot of $\hat{\theta}_{rms}$ with superimposed velocity vectors of the DNS at $Ra = 10^7$. The location of the diagonal plane is provided in figure 3.4.

3.4.1.2 Instantaneous structures

The instantaneous normalised temperature at the central y - z plane is provided in figure 3.6 where thermal plumes are visible.

A zoom on two such plumes is given in figure 3.7, one warm rising (red) and one cold falling (blue), where both are seen to be extending across the entire vertical domain, i.e. from one thermal boundary layer to the other. This flow behaviour is symptomatic of the soft turbulence regime that still exists for the case of $Ra = 10^7$ [68, 86].

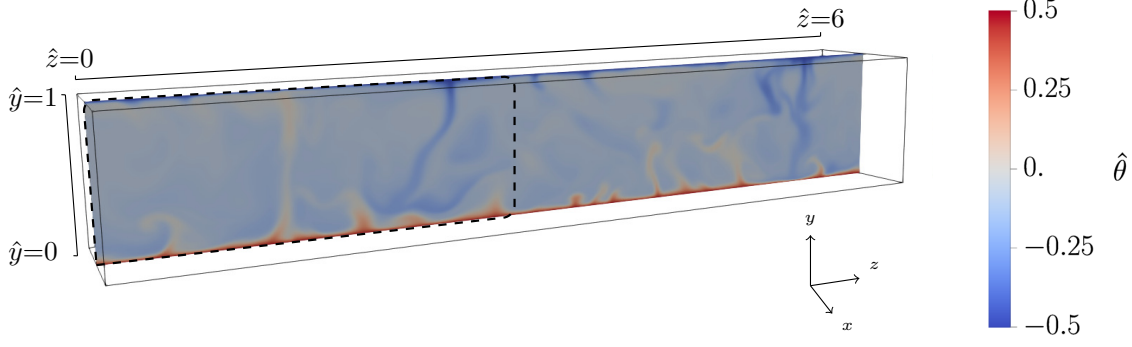


Figure 3.6: Colour plot of the instantaneous normalised temperature $\hat{\theta}$ of the DNS at $Ra = 10^7$. The y - z plane is located at $\hat{x} = 0.5$.

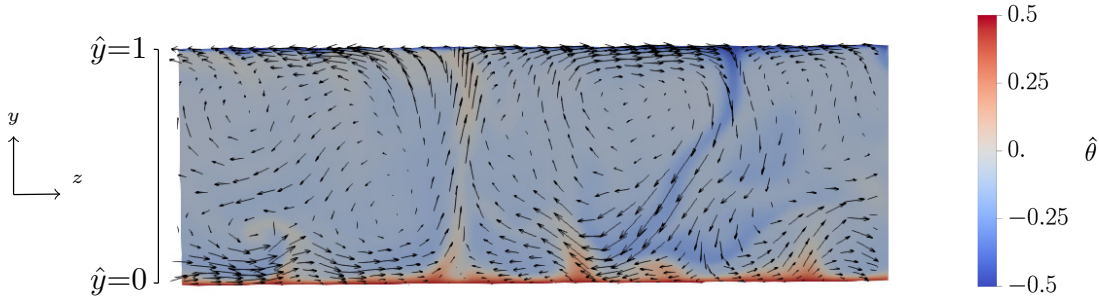


Figure 3.7: Colour plot of the instantaneous normalised temperature $\hat{\theta}$ with superimposed velocity vectors of the DNS at $Ra = 10^7$. The figure shows a zoom on the dashed section from figure 3.6.

3.4.1.3 Flow statistics

In this section, we compare statistics of the velocity and temperature fields at mid-width for the DNS and LES at $Ra = 10^7$. We will often compare our numerical results against those of Kerr [68] for classical turbulent RBC with periodic x - and z -directions. We will also make comparisons against the numerical predictions of Zikanov *et al.* [57] who looked at Oberbeck–Boussinesq thermal convection with a free slip at the upper boundary but with periodic x - and z -directions.

The rms plots of the vertical velocity at mid-width, $\hat{x} = 0.5$, are presented in figure 3.8a. The observed parabolic profile shows zero $\hat{v}_{\text{rms}}$ values at the boundaries which rise steeply towards a maximum in the bulk. Overall, the profiles are similar as those for the flows examined in [57]. However, contrary to the profile in [68], the profile is slightly flatter in the bulk and not fully symmetric with respect to the mid-plane $\hat{y} = 0.5$. This may be attributed to the variation of the fluid transport properties with the temperature, i.e. the non-Oberbeck–Boussinesq conditions. On the other hand, we note that the free-slip condition has no significant effect on the profile of $\hat{v}_{\text{rms}}$ close to the upper boundary. This is due to the zero-Dirichlet condition for the vertical velocity

component that is prescribed at both rigid walls and free-slip boundaries.

With regard to comparisons between LES and DNS, from figure 3.8a we readily deduce that the LES results match closely the DNS data. However, the LES slightly overpredicts the $\hat{v}_{\text{rms}}$ in the bulk of the domain.

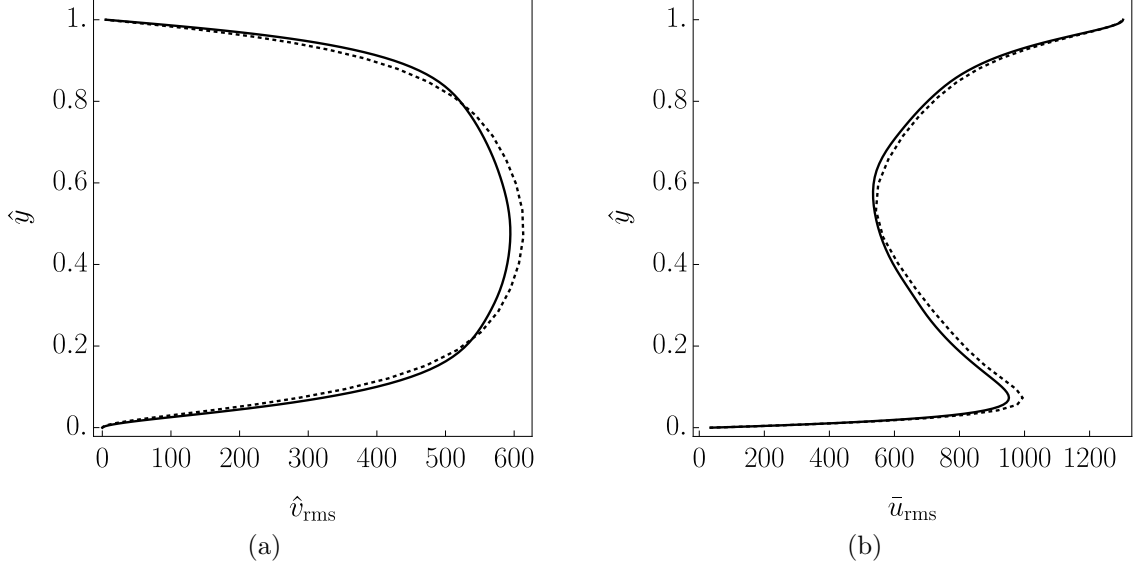


Figure 3.8: Velocity rms plots of $Ra = 10^7$ at mid-width, $\hat{x} = 0.5$. (a) rms of vertical velocity fluctuations, $\hat{v}_{\text{rms}}$ and (b) rms of in-plane velocity fluctuations. The velocity has been nondimensionalised by κ/H . The legend is as follows: DNS (—) and LES (.....).

The rms plots of the in-plane velocity,

$$\bar{u}_{\text{rms}} = \langle \hat{u}'^2 + \hat{w}'^2 \rangle^{1/2}, \quad (3.13)$$

at mid-width, $\hat{x} = 0.5$, are presented in figure 3.8b. According to our simulations, the vertical profile shown first peaks near the lower solid boundary, followed by a significant dip in the core region before a maximum is reached at the free-slip upper boundary. This profile is similar to that in [57] but markedly different from the symmetric profile in [68]. We therefore conclude that the asymmetry in the rms of the in-plane velocity is due to the free-slip condition imposed at the upper boundary.

We see that the LES prediction agrees very well with the DNS results. Nonetheless, it marginally overpredicts the local peak in $\bar{u}_{\text{rms}}$ near the lower boundary. According to [68], the height of a hydrodynamic boundary layer, $\hat{\delta}_u$, is defined as the location of the local peak of the in-plane velocity variance. The DNS and LES predictions of the height of the hydrodynamic boundary layer are given in table 3.5 where the LES predictions are shown to be in very good agreement with our DNS data.

The plots of the mean normalised temperature, $\langle \hat{\theta} \rangle$, across the vertical axis are presented in figure 3.9, alongside a typical profile seen in classical turbulent RBC. For the case of non-Oberbeck–Boussinesq conditions with a free-slip, the bulk value, $\hat{\theta}_{\text{ctr}}$,

is smaller than the average, $\hat{\theta}_{\text{ref}} = \frac{1}{2} (\hat{\theta}_{\text{int}} + \hat{\theta}_{\text{low}}) = 0$, whereas for classical turbulent RBC $\hat{\theta}_{\text{ctr}} = \hat{\theta}_{\text{ref}}$. In other words, the combined effects of the free-slip and variable fluid properties, shift the mean temperature profile towards the temperature at the cold upper boundary. Furthermore, the height of the upper thermal boundary layer is smaller than the height of the lower one.

	Ra	$\hat{\delta}_{\mathbf{u}}$	$\hat{\delta}_{\theta_L}$	$\hat{\delta}_{\theta_U}$	$\frac{1}{2Nu}$
DNS	10^7	0.073	0.027	0.018	0.023
LES	10^7	0.073	0.031	0.017	0.025

Table 3.5: Boundary layer heights at $Ra = 10^7$. In this table, $\hat{\delta}_{\mathbf{u}}$ is the hydrodynamic boundary layer height, and $\hat{\delta}_{\theta_L}$ and $\hat{\delta}_{\theta_U}$ are the thermal boundary layer heights at the lower wall and upper boundary, respectively.

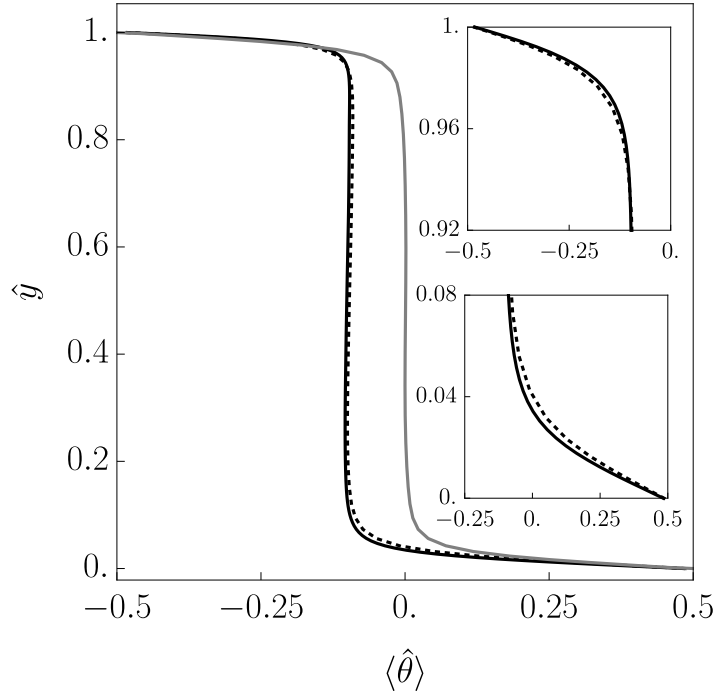


Figure 3.9: Mean normalised temperature, $\langle \hat{\theta} \rangle$, plots of $Ra = 10^7$ at mid-width, $\hat{x} = 0.5$ and across the vertical. The insets show a zoom on the lower wall (below) and a zoom on the upper boundary (above). The legend is as follows: DNS (—) and LES (.....). For comparative purposes we also provide the profile seen in classical RBC (—).

These characteristics are due to the competing influences of the free-slip at the upper boundary and of the variation of the fluid properties with the temperature. In fact, Ahlers *et al.* [75] studied RBC under non-Oberbeck–Boussinesq conditions and attributed an asymmetry to the variable viscosity and thermal diffusivity of water over the temperature range which had the overall effect of increasing the height of the upper

thermal boundary layer and of decreasing the height of the lower one. However, figure 3.9 suggests that the overall effect is to shift $\hat{\theta}_{\text{ctr}}$ in the opposite direction; in other words, in the flow under study, the effect of the free slip on top is more important. The LES prediction agrees very well with the DNS results in the bulk with small deviations in the thermal boundary layers.

The rms plots of the normalised temperature, $\hat{\theta}_{\text{rms}}$, at $\hat{x} = 0.5$ are shown in figure 3.10. The observed profile is that of two peaks in the thermal boundary layers with a minimum value found in the bulk. The most striking feature is the inhomogeneity in the peak values of the two thermal boundary layers and their respective distances from the boundaries. According to [68, 87] the height of a thermal boundary layer is defined as the location of the local peak of the temperature variance. We denote by $\hat{\delta}_{\theta_L}$ and $\hat{\delta}_{\theta_U}$ the thermal boundary layer heights at the lower (hot) and upper (cold) boundaries, respectively. Then, we can readily infer from figure 3.10, that $\hat{\delta}_{\theta_L}$ is larger than $\hat{\delta}_{\theta_U}$, in accordance with the observations made regarding the vertical mean temperature profile at mid-width. The values of $\hat{\delta}_{\theta_L}$ and $\hat{\delta}_{\theta_U}$ are given in table 3.5. We confirm that, at the lower boundary, the hydrodynamic layer is substantially thicker than the thermal one, as expected for $Pr > 1$.

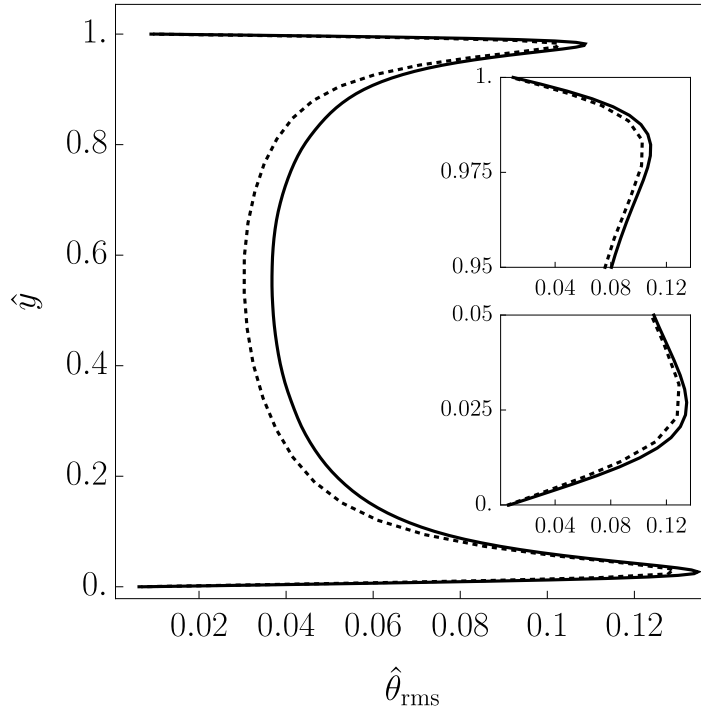


Figure 3.10: Normalised temperature rms, $\hat{\theta}_{\text{rms}}$, plots of $Ra = 10^7$ at mid-width, $\hat{x} = 0.5$ and across the vertical. The insets show a zoom on the lower wall (below) and a zoom on the upper boundary (above). The legend is as follows: DNS (—) and LES (.....).

With regard to the LES predictions of $\hat{\theta}_{\text{rms}}$ we see that they agree well with the DNS results. Most notably, the LES underpredicts $\hat{\theta}_{\text{rms}}$ in the bulk and at the peak locations. Nevertheless, the trend is very well reproduced. Furthermore, the values of

$\hat{\delta}_{\theta_L}$ and $\hat{\delta}_{\theta_U}$ are accurately computed, as expected from a wall-resolved LES.

The last column of table 3.5 represents an estimation of the thermal boundary layer heights in classical turbulent RBC, $\hat{\delta}_{\theta_L} = \hat{\delta}_{\theta_U} = \frac{1}{2}Nu$, so that $\frac{1}{2}(\hat{\delta}_{\theta_L} + \hat{\delta}_{\theta_U}) = \frac{1}{2}Nu$; see e.g. [69]. In other words, this estimate assumes symmetric thermal boundary layers at the upper and lower boundaries for classical turbulent RBC. According to our simulations, the introduction of the free slip at the upper boundary suppresses the symmetry in the heights of the thermal boundary layers. However, despite this asymmetry, the relation $\frac{1}{2}(\hat{\delta}_{\theta_L} + \hat{\delta}_{\theta_U}) = 1/2Nu$ remains valid for the flow under study too.

The plots of the turbulent heat flux $\langle \hat{\theta}'\hat{v}' \rangle$ across the y -direction and at $\hat{x} = 0.5$ are provided in figure 3.11. We observe that the profiles vary in the bulk of the domain. It is further noted that a dip in the turbulent heat flux in the bulk has also been predicted by the LES of classical turbulent RBC presented in [88]. Peng *et al.* [88] attributed this artificial dip to the low resolution of LES. However, in our case, the variation of $\langle \hat{\theta}'\hat{v}' \rangle$ across the vertical direction is observed in our DNS and, consequently, it cannot be a resolution artifact.

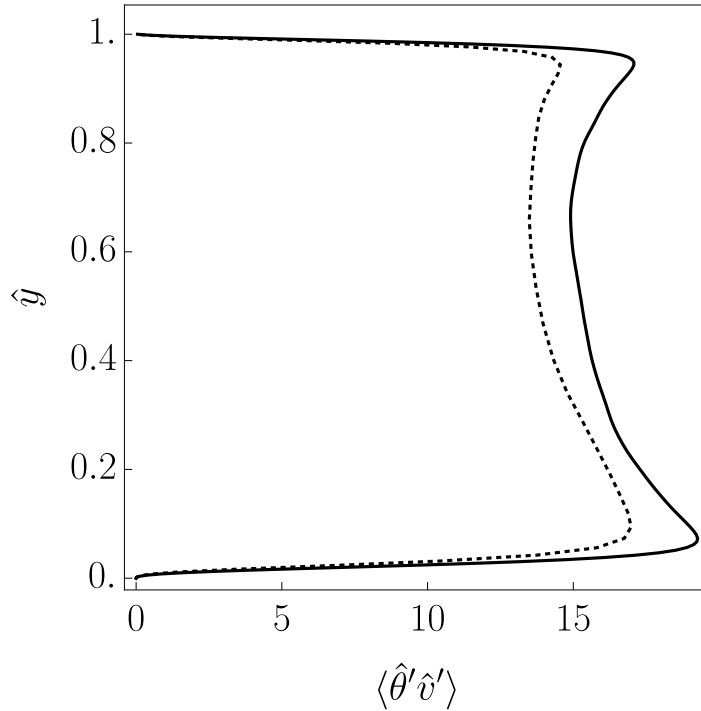


Figure 3.11: Turbulent heat flux, $\langle \hat{\theta}'\hat{v}' \rangle$, plots of $Ra = 10^7$ at mid-width, $\hat{x} = 0.5$. The velocity has been nondimensionalised by κ/H . The legend is as follows: DNS (—) and LES (.....).

In order to explain the observed dip, we first remark that the profiles of $\langle \hat{\theta}'\hat{v}' \rangle_{xzt}$ for classical turbulent RBC [68] are constant in the bulk, where the subscript “ xzt ” denotes time- and area-averaged quantities. Indeed, since convective transfer is dominant in the bulk, a thermal energy balance in a fully developed flow implies that the profile

of $\langle \hat{\theta}\hat{v} \rangle_{xzt}$ is constant in the bulk under Oberbeck–Boussinesq conditions. Moreover, we have that $\langle \hat{\theta}'\hat{v}' \rangle_{xzt} = \langle \hat{\theta}\hat{v} \rangle_{xzt}$ by virtue of the zero divergence of the velocity field. In turn, this implies that $\langle \hat{\theta}'\hat{v}' \rangle_{xzt}$ is constant in the bulk. This has been observed by various authors who studied classical turbulent RBC numerically; see, for example, [84, 85] and references therein.

Under non-Oberbeck–Boussinesq conditions, convective transfer is still dominant in the bulk, i.e. $\langle \hat{\rho}\hat{v}\hat{\theta} \rangle_{xzt}$ is practically constant in the bulk. This is confirmed by our DNS data; see figure 3.3a. However, due to the density fluctuations we have that

$$\langle \hat{\rho}\hat{v}\hat{\theta} \rangle_{xzt} = \langle \hat{\rho} \rangle_{xzt} \langle \hat{\theta}'\hat{v}' \rangle_{xzt} + \langle \hat{v} \rangle \langle \hat{\rho}'\hat{\theta}' \rangle_{xzt} + \langle \hat{\rho}'\hat{v}'\hat{\theta}' \rangle_{xzt} = \text{const} . \quad (3.14)$$

Accordingly, if density fluctuations are significant, this equation implies that $\langle \hat{\theta}'\hat{v}' \rangle_{xzt}$ is no longer constant in the bulk as the second and third terms on the right-hand side are non-zero.

In the flow under study, however, the density fluctuations are sufficiently small that the second and third terms are negligible. In fact, from post-processing of our DNS data we concluded that this is the case and, furthermore, $\langle \hat{\theta}'\hat{v}' \rangle_{xzt}$ is practically constant in the bulk and equal to $\langle \hat{\rho}\hat{v}\hat{\theta} \rangle_{xzt}$.

Therefore, in our case, the observed dip in $\langle \hat{\theta}'\hat{v}' \rangle$, shown in figure 3.11, cannot be attributed to the non-Oberbeck–Boussinesq conditions. We remark however that $\langle \hat{\theta}'\hat{v}' \rangle$ is computed at a given $\hat{x}$ and is time- and z -averaged only, as opposed to the time and x – z averaged equivalent $\langle \hat{\theta}'\hat{v}' \rangle_{xzt}$. In other words, the observed dip of $\langle \hat{\theta}'\hat{v}' \rangle$ is not in contradiction with the fact that $\langle \hat{\theta}'\hat{v}' \rangle_{xzt}$ is constant. Moreover, $\langle \hat{\theta}'\hat{v}' \rangle$ varies along x ; this is not surprising, as this direction is not homogeneous.

Also, from figure 3.11 we see the profile of $\langle \hat{\theta}'\hat{v}' \rangle$ predicted by our LES is similar to the one obtained from our DNS data, but the LES results underpredict the values of the turbulent heat flux in the bulk by approximately 10%. Similarly, the peaks near the top and bottom wall are underpredicted by approximately 15%. Overall, we may conclude that the LES predictions of the first- and second-order statistics of the flow quantities compare quite satisfactorily with the corresponding DNS data.

3.4.1.4 Turbulent kinetic energy budget

In this section, we present the TKE budget based on the DNS data. The TKE balance equation is obtained in three steps. First, the dimensionless momentum equation is multiplied by $\hat{\mathbf{u}}$ and the average is taken to get an equation for $\hat{\mathcal{K}} = (1/2)\langle \hat{\mathbf{u}} \cdot \hat{\mathbf{u}} \rangle$. Second, the dimensionless momentum equation is averaged and then multiplied by $\langle \hat{\mathbf{u}} \rangle$ to give an equation for $\bar{\mathcal{K}} = (1/2)(\langle \hat{\mathbf{u}} \rangle \cdot \langle \hat{\mathbf{u}} \rangle)$. Finally, subtracting the equation for $\bar{\mathcal{K}}$ from the one for $\hat{\mathcal{K}}$ yields the sought-after equation for TKE.

It is noted that the above process removes the term describing the gravitational force

from the TKE balance equation. For variable density flows, the process of carrying out the TKE budget is simplified by introducing density-weighted (Favre averaged) quantities. For any given flow quantity ϕ the Favre-averaged equivalent $\{\phi\}$ is defined as

$$\{\phi\} = \frac{\langle \rho \phi \rangle}{\langle \rho \rangle}. \quad (3.15)$$

The mean and fluctuating values are then related by the Favre decomposition,

$$\phi = \{\phi\} + \phi''. \quad (3.16)$$

The variable $\hat{k}$ then denotes the turbulent kinetic energy of the density-weighted velocity fluctuations,

$$\hat{k} = \frac{1}{2} (\hat{\mathbf{u}}'' \cdot \hat{\mathbf{u}}''). \quad (3.17)$$

By following the procedure outlined above, we arrive at the following equation [41, 89].

$$\begin{aligned} \langle \hat{\rho} \rangle \frac{\partial \{\hat{k}\}}{\partial \hat{t}} = & - \underbrace{\hat{\nabla} \cdot (\langle \hat{\rho} \rangle \{\hat{k}\} \{\hat{\mathbf{u}}\})}_{C_k} - \underbrace{\hat{\nabla} \cdot (\langle \hat{\rho} \rangle \{\hat{k} \hat{\mathbf{u}}''\})}_{T_k} - \underbrace{\langle \hat{\rho} \rangle \{\hat{\mathbf{u}}'' \hat{\mathbf{u}}''\} : \hat{\nabla} \{\hat{\mathbf{u}}\}}_{P_k} \\ & - \underbrace{\hat{\nabla} \cdot (\langle \hat{p} \rangle \langle \hat{\mathbf{u}}'' \rangle)}_{\Phi_k} - \underbrace{\hat{\nabla} \cdot (\langle \hat{p}' \hat{\mathbf{u}}'' \rangle)}_{\phi_k} + \underbrace{\langle \hat{p} \hat{\nabla} \cdot \hat{\mathbf{u}}'' \rangle}_{\Pi_k} + \underbrace{\sqrt{\frac{Pr}{Ra}} \hat{\nabla} \cdot \langle \hat{\boldsymbol{\tau}} \cdot \hat{\mathbf{u}}'' \rangle}_{D_k} - \underbrace{\sqrt{\frac{Pr}{Ra}} \langle \hat{\boldsymbol{\tau}} : \hat{\nabla} \hat{\mathbf{u}}'' \rangle}_{\epsilon_k}. \end{aligned} \quad (3.18)$$

The right-hand-side terms C_k , T_k and P_k represent convection, transport and production of turbulent kinetic energy, respectively. Further, the terms Φ_k and ϕ_k describe, respectively, the work of the mean and fluctuating pressures through fluctuating motions, whereas the term Π_k is interpreted as the correlation between the pressure and the dilatation of the fluctuating velocity. Finally, D_k describes the viscous diffusion, i.e. the work of viscous stresses through fluctuating motions, and ϵ_k describes the viscous dissipation.

When the flow becomes statistically stationary, both sides of equation (3.18) are zero. At the end of our simulation, the computed value of the left-hand side of (3.18) was smaller than 10^{-6} , whereas the sum of the right-hand side was below 20% of the magnitude of the largest term. We therefore consider the flow to be statistically stationary. For the purposes of our study we choose to carry out the above budget at mid-height, $\hat{y} = 0.5$, and mid-width, $\hat{x} = 0.5$. This analysis provides a global picture of the different contributions of each term in (3.18).

The TKE budget across the horizontal axis at $\hat{y} = 0.5$ is shown in figure 3.12 where all terms on the right-hand side of (3.18) are shown, as well as the sum of the rhs terms called, RHS_k . A symmetric profile is observed and we can see that, in the bulk, the mean pressure transport Φ_k is balanced by the viscous dissipation ϵ_k and

the fluctuating transport ϕ_k . The term Φ_k is dominant in the core region due to the hydrostatic component of $\hat{\nabla}\{\hat{p}\}$, as can be evidenced upon expansion of this term,

$$\Phi_k = \hat{\nabla} \cdot (\langle \hat{p} \rangle \langle \hat{\mathbf{u}}'' \rangle) = \langle \hat{p} \rangle \hat{\nabla} \cdot \langle \hat{\mathbf{u}}'' \rangle + \langle \hat{\mathbf{u}}'' \rangle \cdot \langle \hat{\nabla} \hat{p} \rangle. \quad (3.19)$$

We note that due to the large value of the hydrostatic component of $\hat{\nabla}\{\hat{p}\}$, the amplitude of Φ_k is significant. Further, $\langle \hat{\mathbf{u}}'' \rangle$ is quite small (by continuity and due to the fact that the density fluctuations are small), albeit non-zero. Then, this term is multiplied by $\hat{\nabla}\langle \hat{p} \rangle$, whose amplitude is large, thereby resulting in a significant value of Φ_k . The contribution of Φ_k is much more pronounced in turbulent natural convection than in channel flows with thermal mixing [41, 90]. This is due to the dominance of buoyancy effects in natural convection and exemplifies the different characteristics of turbulence between the two types of flow.

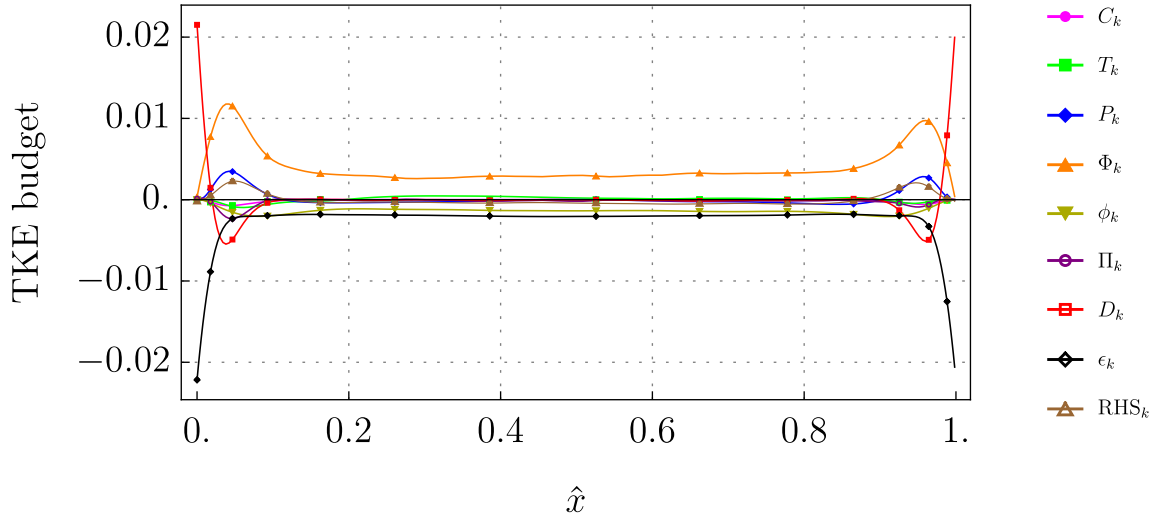


Figure 3.12: Horizontal TKE budget of DNS at $Ra = 10^7$ at mid-height, $\hat{y} = 0.5$.

In figure 3.13 we present a zoom on the side wall. The observed peaks in Φ_k , are predominantly due to the increase in vertical velocity fluctuations $\langle \hat{v}'' \rangle$ in the near-wall regions. The sum of Φ_k and the production term P_k is then balanced by all remaining terms of opposite sign. In fact, the production term P_k is given as the double interior product between $\langle \hat{\rho} \rangle \{ \hat{\mathbf{u}}'' \hat{\mathbf{u}}'' \}$ and $\hat{\nabla}\{\hat{\mathbf{u}}\}$. Upon expansion, we observe that the important components of P_k in the near-wall regions are those involving $\frac{\partial \{ \hat{u} \}}{\partial \hat{y}}$ and $\frac{\partial \{ \hat{v} \}}{\partial \hat{y}}$. Therefore, at these regions it is the velocity gradient in the y direction that contributes the most to the production term. Closer to the walls, all terms go to zero except for D_k and ϵ_k which balance out one another; this behaviour is also observed in turbulent channel flows with thermal mixing [41] where most of the turbulent kinetic energy is also dissipated at the walls.

The TKE budget across the vertical axis at $\hat{x} = 0.5$ is given in figure 3.14, in which the inset shows a zoom on the bulk at $0.4 < \hat{y} < 0.6$. Unlike the TKE budget across the

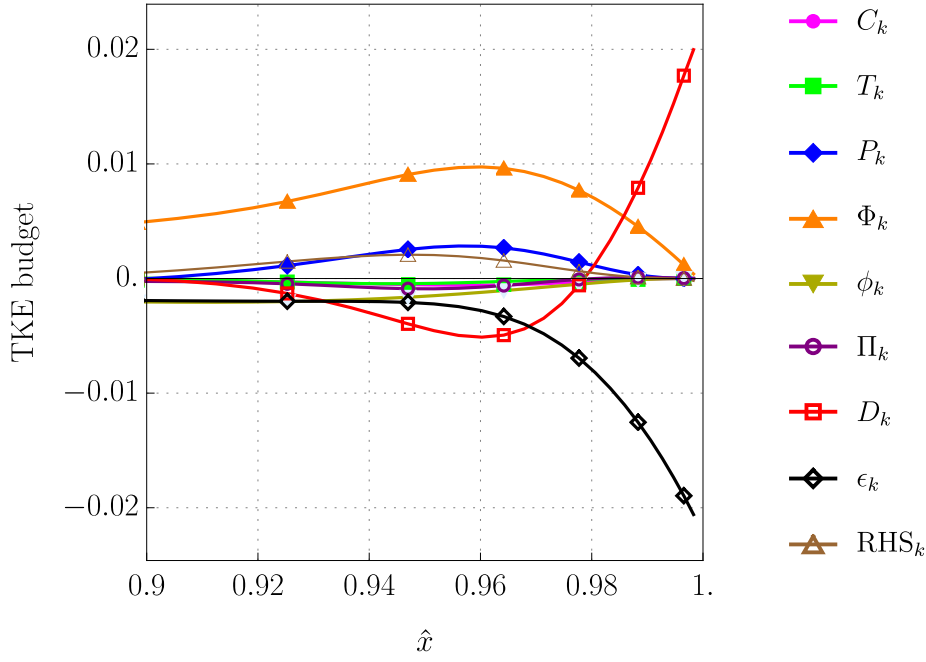


Figure 3.13: Horizontal TKE budget of DNS at $Ra = 10^7$ at mid-height, $\hat{y} = 0.5$. Zoom on the right-hand-side wall of figure 3.12.

horizontal axis, an asymmetric profile is observed. However, Φ_k is still the dominant term in the bulk and is balanced predominantly by ϕ_k and the viscous dissipation ϵ_k . In the bulk, the contribution of the other terms to the TKE budget is negligible. We note that the profile of ϵ_k is flat across the vertical with the exception of the near-boundary regions, this is in-line with the classical experimental observation from Deardroff and Willis [81].

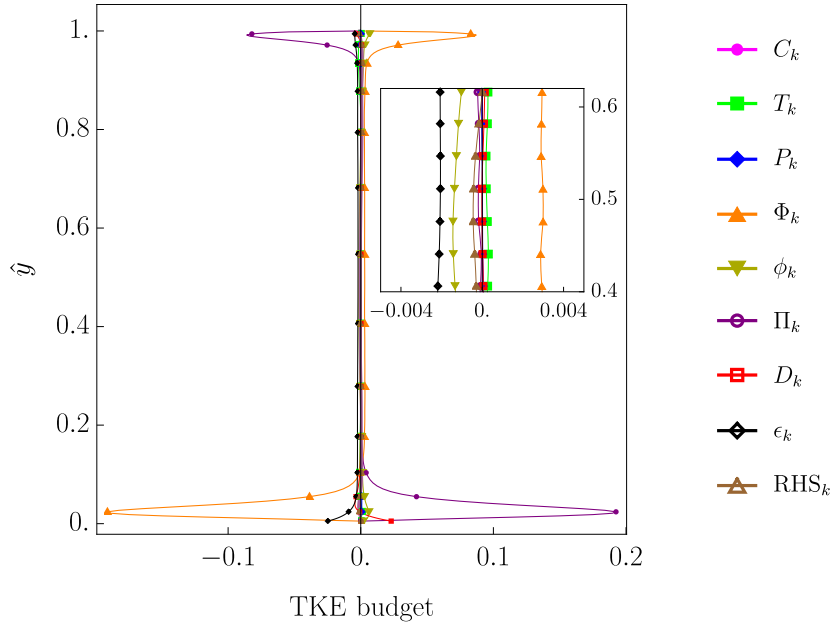


Figure 3.14: Vertical TKE budget of DNS at $Ra = 10^7$ at $\hat{x} = 0.5$. The inset is a zoom on the bulk between $0.4 < \hat{y} < 0.6$.

To analyse the behaviour at the boundaries, we present figure 3.15a for the lower wall and figure 3.15b for the upper free-slip boundary. At the lower wall boundary layer, Φ_k again increases in magnitude but, unlike in the budget in the horizontal direction, is balanced by the term π_k representing the pressure correlation with the dilatation fluctuation. Closer to the wall, we see again that all terms go to zero except that of diffusion and dissipation. At the upper boundary, unlike at the rigid lower wall, the diffusion and dissipation terms take the same sign and their total is predominately balanced by ϕ_k , the fluctuating pressure transport term.

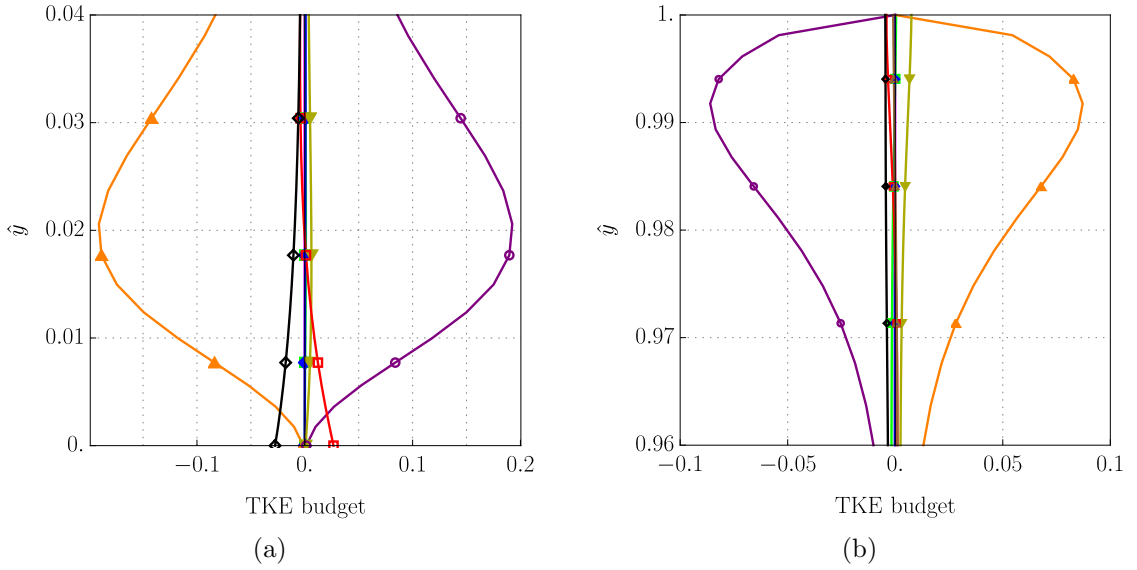


Figure 3.15: Vertical TKE budget of DNS at $Ra = 10^7$ at $\hat{x} = 0.5$. (a) zoom on the lower wall and (b) zoom on the upper boundary. The legend is the same as in figure 3.14.

3.4.2 Analysis of higher-Rayleigh-number flows

We next present and analyse our LES results of the flows at increasing Ra .

3.4.2.1 Time-averaged flow properties

We first look at the effect of increasing Ra on the heat transfer in the domain. In figure 3.16 we plot the profiles of the convective and the diffusive components of Nu . The profiles of Nu_{conv} are flat for all cases except $Ra = 10^9$. The deviation from the flat profile at $Ra = 10^9$ suggests that averaging over 200 free-fall times may not be fully sufficient for this case.

Figure 3.16 also shows the expected trend that increasing Ra will increase Nu . Further, the role of the free-slip upper boundary is to increase Nu in the cavity (see table 3.6 and [51] for comparison at $Ra = 10^7$) as a result of the fewer hydrodynamic boundary layers.

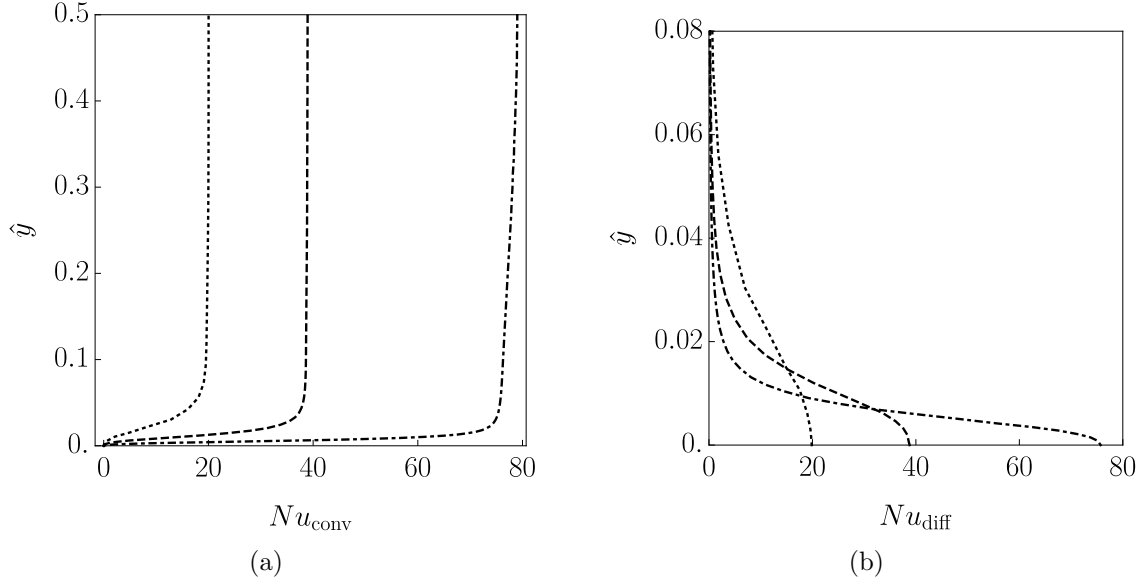


Figure 3.16: LES plots of the time- and area-averaged Nu_y at increasing Ra . (a) Nu_{conv} across the lower half of the domain and (b) Nu_{diff} zoom on the lower boundary. The legend is as follows: LES at $Ra = 10^7$ (.....), $Ra = 10^8$ (- - -) and $Ra = 10^9$ (-.-).

3.4.2.2 Flow statistics

In this section, we again look at the vertical profiles of the flow but this time assess the effect of increasing Ra .

The rms plots of the vertical velocity over increasing Ra are presented in figure 3.17a where the observed trend is for $\hat{v}_{\text{rms}}$ to increase with Ra , i.e. increasing the turbulence results in stronger vertical velocity fluctuations. We also observe that the parabolic profile persists, even at higher Ra , and that the maximum in the bulk is more pronounced at increasing Ra .

With respect to the rms plots of the in-plane velocity over increasing Ra we present figure 3.17b. We can see that the magnitude of the local peak near the lower boundary increases with Ra . We conclude that, globally, the rms velocity profiles follow the same trends independently of the Ra ; the only significant difference is the increase in their magnitude with Ra . In other words, we observe a significant increase in the resolved kinetic energy with Ra , as expected.

It is also worth mentioning that the location of the local peak in $\bar{u}_{\text{rms}}$ near the lower wall, which signifies the height of the local boundary layer, moves closer to the wall as Ra increases. We provide values in table 3.6. This trend is in accordance with the fact that the height of the boundary layer decreases with increasing turbulence intensity.

The normalised temperature plots at increasing Ra are provided in figure 3.18. For the bulk, the same trend is observed in figure 3.18 as in figure 3.9, i.e. $\hat{\theta}_{\text{ctr}} < \hat{\theta}_{\text{ref}}$. Increasing Ra has little effect on the magnitude of this shift. However, at the boundaries the observed trend is for the thermal boundary layers to become thinner with increasing

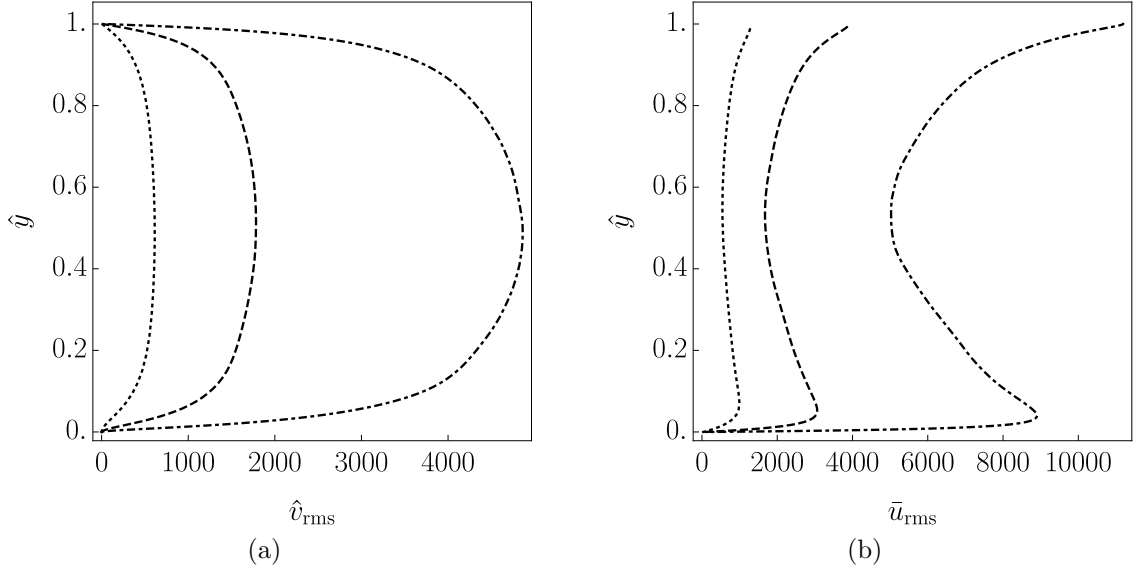


Figure 3.17: LES plots of velocity rms at increasing Ra at mid-width, $\hat{x} = 0.5$. (a) vertical velocity rms, $\hat{v}_{\text{rms}}$ and (b) in-plane velocity rms $\bar{u}_{\text{rms}}$. The legend is as follows: LES at $Ra = 10^7$ (.....), $Ra = 10^8$ (---) and $Ra = 10^9$ (-.-.). Here, the velocities have been nondimensionalised by κ/H .

Ra . This is quantified by looking at the rms of the normalised temperature.

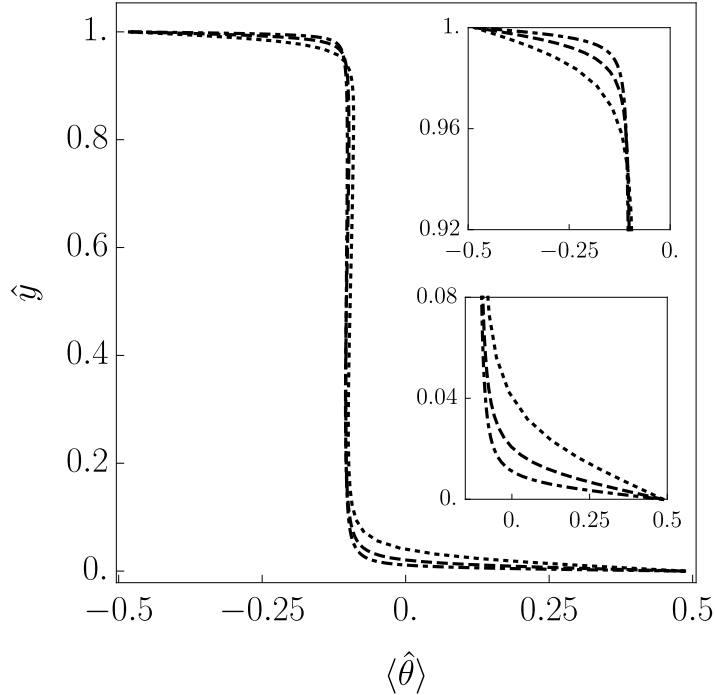


Figure 3.18: LES plots of mean normalised temperature, $\langle \hat{\theta} \rangle$, at increasing Ra at mid-width, $\hat{x} = 0.5$ and across the vertical. The insets show a zoom on the lower wall (below) and a zoom on the upper boundary (above). The legend is as follows: LES at $Ra = 10^7$ (.....), $Ra = 10^8$ (---) and $Ra = 10^9$ (-.-.).

The rms plots of the normalised temperature over increasing Ra are provided in

figure 3.19. As Ra is increased, the magnitude of $\hat{\theta}_{\text{rms}}$ in the bulk is reduced, i.e. the dip in $\hat{\theta}_{\text{rms}}$ becomes more pronounced. A similar trend was observed in [84] over the same range of Ra for classical turbulent RBC. The location of peak temperature variance approaches the boundaries as a result of increasing Ra . This is in accordance with the fact that the thermal boundary layers become thinner with increasing turbulence intensity. The heights of the thermal boundary layers are also provided in table 3.6. It is noted that at both the lower wall and upper boundary, the magnitude of the peak in $\hat{\theta}_{\text{rms}}$ appears to decrease with Ra . This behaviour is similar to that observed at solid boundaries in classical turbulent RBC.

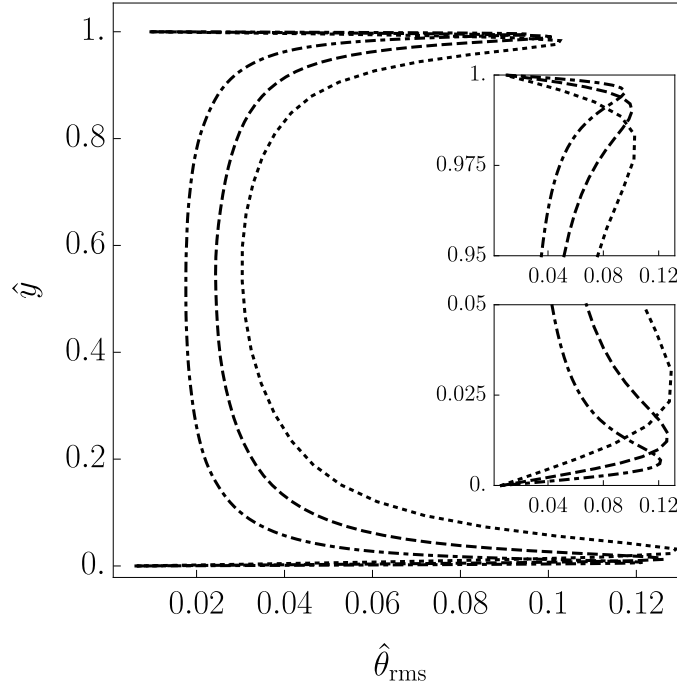


Figure 3.19: LES plots of the rms of normalised temperature fluctuations, $\hat{\theta}_{\text{rms}}$, at increasing Ra at mid-width, $\hat{x} = 0.5$ and across the vertical. The insets show a zoom on the lower wall (below) and a zoom on the upper boundary (above). The legend is as follows: LES at $Ra = 10^7$ (.....), $Ra = 10^8$ (---) and $Ra = 10^9$ (-.-).

Interestingly in [30], it is postulated whether water-side turbulence conditions, governed by the depth of the water tank in their experiments, could influence evaporation rates. Indeed, experimental results confirmed that increasing water-side Ra for the same gas-side conditions tends to increase mass transfer at the free surface. It was hypothesised that an increase in $\hat{\theta}_{\text{rms}}$ at the interface could be the cause. We note, however, that our LES predictions are not in line with this claim because of the isothermal boundary condition employed for the temperature. In the following chapters, where a more representative thermal boundary condition is used, we investigate the Ra -dependence of the rms of temperature fluctuations at the interface.

The plots of the turbulent heat flux over increasing Ra are shown in figure 3.20. As discussed earlier, the profiles are not flat in the core and, moreover, $\langle \hat{\theta}' \hat{v}' \rangle$ varies across

	Ra	Nu_y	Nu_G	$\hat{\delta}_u$	$\hat{\delta}_{\theta_L}$	$\hat{\delta}_{\theta_U}$	$\frac{1}{2Nu}$
DNS	10^7	21.4	21.4	0.073	0.027	0.018	0.023
LES	10^7	19.9	20.0	0.073	0.031	0.017	0.025
LES	10^8	38.9	38.9	0.050	0.015	0.010	0.013
LES	10^9	77.5	78.1	0.039	0.007	0.004	0.006

Table 3.6: Time-averaged results. In this table, Nu_y is an averaged local Nusselt number, Nu_G is the global Nusselt, $\hat{\delta}_u$ is the dimensionless hydrodynamic boundary layer height, $\hat{\delta}_{\theta_L}$ and $\hat{\delta}_{\theta_U}$ are the lower and upper thermal boundary layer heights, respectively.

the inhomogenous x -direction. The dip in the core is accentuated with Ra , i.e. as the turbulence intensity is increased.

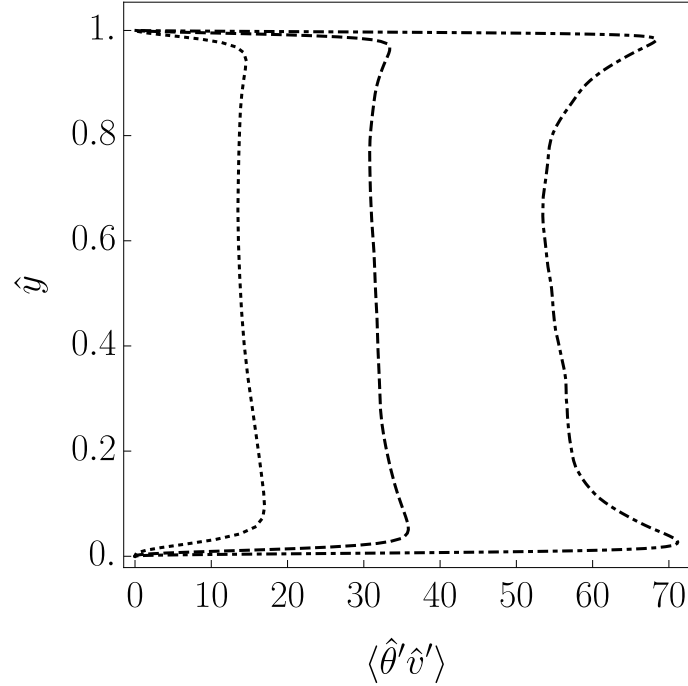


Figure 3.20: LES plots of turbulent heat flux, $\langle \hat{\theta}' \hat{v}' \rangle$, at increasing Ra at mid-width, $\hat{x} = 0.5$. The velocity has been nondimensionalised by κ/H . The legend is as follows: LES at $Ra = 10^7$ (.....), $Ra = 10^8$ (---) and $Ra = 10^9$ (-.-.).

3.5 Conclusions

In this chapter, direct numerical and wall-resolved Large-Eddy Simulations of a thermal convection configuration with a free slip upper boundary have been presented over a range of Ra covering both the soft and hard turbulence regimes. The flow repre-

sents a modified turbulent RBC and we do not implement the Oberbeck–Boussinesq approximation.

As a first attempt to understand the impact of a free surface on turbulent Rayleigh Bénard Convection, a free-slip upper boundary condition has been implemented. Two important consequences of introducing the free-slip upper boundary are an increase in convective heat transfer (or Nu) as a result of the fewer hydrodynamic boundary layers and the removal of the homogeneity in the thermal boundary layer heights at the lower and upper boundaries.

Another consequence of the free slip at the upper boundary is the asymmetry of the vertical profiles of the first- and second-order statistics. As expected, this asymmetry becomes more pronounced with Ra . Further, according to our simulations, the first- and second-order statistics are well produced by the LES when compared to the DNS for the moderate Rayleigh case. However, the LES slightly underpredicts Nu ; this may be, at least partially, attributed to the constant Pr_t presumed in our study.

A turbulent kinetic energy budget was carried out at two locations for the DNS at $Ra = 10^7$; at mid-height and at mid-width. Both profiles showed that, in the bulk, the dominant term was the work of the mean pressure which is balanced by the work of the fluctuating pressure and the turbulent kinetic energy dissipation. Interestingly, the work of the mean pressure is dominant due to the hydrostatic component of the mean-pressure gradient but also depends on the density fluctuations which are small but critically, non-zero. In other words, even though the deviation from the Oberbeck–Boussinesq conditions are small with regard to the fluid density, the effect of this deviation can be significant.

At mid-height, a horizontal TKE profile shows that the equal in magnitude (opposite in sign) terms of TKE diffusion and dissipation terms dominate in the hydrodynamic boundary layers at the vertical side walls; a trend also observed in channel flows. At mid-width, a vertical profile shows the same trend in the hydrodynamic boundary layer at the lower wall. At the free-slip boundary however, all terms approach zero except that of diffusion and dissipation (now of the same sign and different magnitude), their sum being balanced by the fluctuating pressure work term.

Finally, we presented a series of LES at increasing Ra and assessed their first- and second-order statistics. The observed trends were as expected, such as the increase in bulk and maximum velocity variance and reduction in thermal boundary layer heights with increasing Rayleigh number. In the following chapters, we will first implement a representative upper thermal boundary condition for free-surface evaporation and, secondly, perform further simulations at increased Ra . The idea being to develop relevant Ra – Nu scaling for our thermal convection configuration and to further quantify the effect on the thermal boundary layer heights beneath the free surface at very high Ra flows.

Chapter 4

Evaporation-driven thermal convection in water pools

4.1 Introduction

In this chapter, we report on direct numerical simulations of evaporation-driven turbulent thermal convection in a pool. With liquid water as the working medium, we approximate an evaporating free surface by imposing a heat flux at a shear-free upper boundary. The representative thermal boundary condition is a significant improvement on the previous chapter. Rather than assuming a temperature drop across the domain, the prescribed heat flux is representative of the evaporation occurring at an air-water interface. Over a series of simulations, we then investigate the effect of increasing evaporation rates on the flow field below.

High temperature free-surface evaporation is of particular interest. Taking Fukushima 2011 as an example, a loss-of-cooling accident in the spent-fuel pools resulted in fuel uncovering due in part to inventory loss at sub-saturation pool temperatures. In this situation, heat is added to the upper volume of the pool from the fuel assemblies below and is predominantly evacuated via evaporation at the free surface. In the nuclear industry it is imperative to have an understanding of, and the capabilities to predict, the effect of free-surface evaporation on thermal mixing in the pool. An improved understanding will in turn lead to better predictions of the physics in the early-stages of the accident, providing one of the motivations for the work in this chapter.

As a reminder, turbulent convection and free-surface evaporation are the interdependent physical phenomena of interest. With the currently investigated thermal configuration borrowing attributes from both evaporative cooling; see figure 1.3a and turbulent RBC; see figure 1.3b. In this chapter, the problem in hand, shown schematically in figure 1.3c, can be understood as a combination of the well-known thermal

The results of this chapter have been published in *J. Fluid Mech.*, 904:A14, 2020. [91]

convection configurations, turbulent RBC and evaporative cooling.

As discussed in the Introduction, our configuration shares the feature of the LSC with turbulent RBC. This circulation, or mean wind, sweeps across the upper and lower boundaries stabilizing the thermal boundary layers, and simultaneously creating a hydrodynamic boundary layer with its shear [20]. The shape of the container is the final control parameter which plays a particularly important role in determining the structure of the LSC. Experimental work has largely concentrated on cylindrical geometries (Verzicco and Camussi [16], Niemala *et al.* [82], Chavanne *et al.* [92]), however, a significant body of work also exists for the cubic domain.

Turbulent RBC in a cubic domain has been studied experimentally by Daya and Ecke [93]. Therein, measurements of velocity and temperature rms quantities in the bulk of the flow showed differences to that seen in corresponding cylindrical domains at the same Ra and Pr . Foroozani *et al.* [66] carried out Large-Eddy Simulations of turbulent RBC in a cubic domain. The observed scaling for rms fluctuations of velocity and temperature measured in the cell centre were in excellent agreement with Daya and Ecke [93]. The LSC structure in the cubic domain was also evaluated, where peaks in rms fluctuations of temperature were found at the mid-height of the plane orthogonal to the LSC. Kaczorowski and Xia [51] carried out highly resolved DNS of turbulent RBC in a cube for water and air over five decades of Ra , investigating velocity and temperature structure function scaling and heat transfer in the bulk. Later, Foroozani *et al.* [94] used LES over longer time periods to investigate the dynamics of LSC reorientations. They found that all flow reorientations were due to lateral rotations during which the large-scale flow entered a transient state, non-aligned with the diagonal. In this study we do not extend our DNS to such long time periods and choose time-averaging intervals that are representative of a stable LSC.

To our knowledge, the large-scale circulation was first observed by Krishnamurti and Howard [15] for turbulent RBC at $Ra > 2 \times 10^6$. Therein, the LSC is described as being driven by plume formation at both upper and lower boundaries. Therefore, no LSC is observed in the evaporative cooling configuration where plume formation occurs uniquely at a free surface. However, the LSC structure in the present configuration is of interest, given the similarities with turbulent RBC.

In one of the original studies of evaporative cooling, Katsaros *et al.* [24] examined experimentally the thermal boundary layer behaviour below an evaporating water surface. The scaling relationship, $Nu = 0.156Ra^{0.33}$, was found for the evaporative cooling configuration, i.e. with a heat flux across one free boundary, whereas Straus [95] derived Ra – Nu scaling relations for turbulent RBC between two rigid plates and between two free boundaries. The exponent in both power-law scalings was the same but the pre-factor differed. This was later confirmed in Verzicco [96], who looked at contained turbulent RBC between two free boundaries. The presence of the viscous

boundary layers was shown to have no impact on the exponent of the Ra – Nu scaling, which to a good approximation gave $Nu \sim Ra^{0.3}$. Verzicco [96] also stated that the most significant difference between classical turbulent RBC, that is between two rigid boundaries, and that between two free boundaries, was the magnitude of the Nu (pre-factor of Ra – Nu relation) which was approximately twice as large in the latter case.

Much research in the turbulent RBC community has since concentrated on measuring the Nu dependence on Ra ; one example [82] covering a particularly large range of Ra provides $Nu = 0.124Ra^{0.309}$, where we see the relation $Nu \sim Ra^{0.3}$ appear once again. The current configuration shown in figure 1.3c has one rigid plate and one free boundary; it is of interest therefore to find the Ra – Nu scaling for this unique set-up. A comparison of both the heat transfer effectiveness and power-law exponent can then be made with similar thermal convection configurations.

The closest configuration to the one investigated in the present study is that of Zikanov *et al.* [57]. Therein, the authors studied numerically the turbulent convection occurring in warm shallow ocean during adverse weather events. A heat flux was implemented at the free-slip upper boundary to represent evaporation and the lower boundary was a rigid wall. One main difference between Zikanov *et al.* [57] and the study of this chapter is in the geometry of the domain; where Zikanov *et al.* [57] used periodic boundaries in the horizontal directions, we have a wall-bounded domain. Further, Zikanov *et al.* [57] presented results on the initial unsteady phase of the flow from a quiescent state, whereas in this chapter a statistically stationary state is pursued. This produces novel Ra scaling of both Nu and a Reynolds number in the centre of the domain; enabling comparisons with similar thermal convection configurations.

The earlier thermal convection study of the previous chapter [67] assumed a fixed temperature drop across a cuboid domain while enforcing periodicity in one horizontal direction. The impact of both the free-slip and non-Oberbeck Boussinesq conditions were then assessed. The former was shown to play an important role both on Nu and on the mean temperature profile across the domain. The values for Nu were increased when compared to turbulent RBC for the same Ra ; an expected result given the earlier work of Straus [95] and Verzicco [96]. Moreover, the mean temperature profile was shifted towards the colder upper boundary temperature. This was the case even when considering the competing non-Oberbeck Boussinesq effects which, for the case of water as the working fluid, tends to shift the bulk temperature towards the warmer lower wall temperature. The bulk of the domain was therefore significantly cooler than that seen in turbulent RBC.

In summary, the thermal convection set-up investigated in this chapter is novel and characterised by its similarities to the well-known configurations of turbulent RBC and evaporative cooling. The configuration shown in figure 1.3c *has* been investigated

experimentally in the past, however, the aims were to measure gas-side flow and, importantly, evaporation rates [29, 30]. We take results from the latter reference and extend the analysis water-side, to investigate the role of free-surface evaporation on thermal mixing in liquid pools.

This chapter is organised as follows: first, in section 4.2 we present the numerical set-up and governing equations, followed by a detailed discussion on the estimation of evaporation rates in section 4.3. Next, in section 4.4 we outline the boundary conditions and elaborate on the resolution requirements for the DNS. Subsequently, in section 4.6, we analyse the numerical results in two parts. In the first, we provide time-averaged flow properties such as Nu , Re and the LSC structure. We then focus on the flow statistics by plotting vertical profiles of time and horizontally averaged flow properties and analyse the effect of increasing Ra , before drawing conclusions in section 4.7.

4.2 Numerical set-up

As in the previous chapter, we consider only the flow beneath the evaporating surface and as such the working fluid is liquid water, treated as Newtonian. We investigate flows without invoking the Oberbeck–Boussinesq approximation and therefore take into account variations of the density and transport properties with temperature. For this reason, the system of governing equations remains (2.1)–(2.3)

For open domains, the thermodynamic pressure that appears in (2.3), p_0 , is equal to the ambient pressure, whereas for closed domains, p_0 varies with time and can be computed from the equation of state of the working medium. In this study the domain is open. For this reason, p_0 is constant and set to the ambient pressure of one atmosphere. We note that the mass loss leaving the system due to evaporation is not modelled and the surface level is constant throughout. For the highest evaporation case the mass loss through the free surface would be equivalent to 3%. This is considered to have a minor effect on the free surface level over the simulation times considered.

In order to close the system of governing equations, we again introduce the isobaric equation of state for the water density. The ρ – T relation is the fourth-order polynomial fit (2.6) of the tabulated data in Lemmon *et al.* [43] for water density at one atmosphere and over the temperature range of interest. The other fluid thermodynamic properties, λ and μ are also calculated from a quartic polynomial fit of the form (2.6) with data originating from the same reference. In this chapter, we carry out multiple simulations under different thermal boundary conditions, whereas the thermal boundary conditions were fixed in chapter 3. As such, we provide only an example set of coefficients for the fits of ρ/p_0 , λ and μ in table 4.1, for the case at $Ra = 5 \times 10^7$.

For the case with the largest ΔT , the dynamic viscosity and the thermal conductivity vary respectively by 24% and 2% over the temperature range of interest. In

other words, even though the density variations are small, the induced variations in the transport properties of water are non-negligible. On the other hand, c_p varies by a maximum of only 0.4% over the maximum temperature range investigated. It is thus taken as a constant, case-dependent, value in all simulations; see table 4.1. We note that with the aforementioned variations in fluid properties, Pr varies by 26% across the domain for the highest evaporation case.

	c_4	c_3	c_2	c_1	c_0
$\frac{\rho}{\rho_0}$	-5.18×10^{-13}	7.79×10^{-10}	-4.63×10^{-7}	1.21×10^{-4}	-1.53×10^{-3}
μ	6.85×10^{-12}	-1.01×10^{-8}	5.59×10^{-6}	-1.39×10^{-3}	1.32×10^{-1}
λ	-7.96×10^{-11}	1.24×10^{-7}	-7.88×10^{-5}	2.40×10^{-2}	-2.20

Table 4.1: Example polynomial coefficients for water thermodynamic properties at $Ra = 5 \times 10^7$ [43]. The values provided are a fit over the case specific temperature range of interest given in table 4.6. We note that the case-specific c_p is set constant at 4179, 4181, 4190, 4198, and 4202 J/kg/K for cases 1–5, respectively.

For the numerical solution of (2.1)–(2.3) we employ the second-order accurate temporal and spatial discretisation schemes outlined in section 2.3.1. For the pressure-velocity coupling the PISO-type projection method is used from section 2.3.2.

4.3 Estimation of evaporation rates

For specified thermal boundary conditions at the walls of the pool and for given ambient conditions, the evaporation rate depends on the gas-side transport phenomena. In the present chapter however, the focus is not on such phenomena but on the thermal mixing water-side. For this reason, we only solve for the flow field below the free surface (interface). This in turn requires the mean temperature at the interface to be specified, from which the evaporation rates and temperature gradients at the interface can then be estimated. Also for a given mean interface temperature, the bottom-wall temperature is not known in advance and must be estimated *a priori* on a case-by-case basis. As first approximations we take estimations from free-surface evaporation experiments, where data is provided for temperature drops across water domains during evaporation. The thermal boundary conditions are subsequently refined in preliminary simulations until the correct temperature drop is found.

In this section, we obtain realistic approximations of the heat losses at the upper boundary, as well as the corresponding lower wall temperatures. This will enable the assignment of thermal boundary conditions in the following section. To estimate these quantities we start with an energy balance across the interface which provides the

following relation,

$$\dot{q}_{\text{add}}'' = \dot{q}_{\text{conv}}'' + \dot{q}_{\text{evap}}'' . \quad (4.1)$$

Here, the right-hand side terms, $\dot{q}_{\text{conv}}''$ and $\dot{q}_{\text{evap}}''$, represent respectively the convective and latent heat losses per unit surface area to the ambient gas-side environment. The left-hand side term, $\dot{q}_{\text{add}}''$, represents the heat added to the interface from the water-side. By expanding this latter quantity and $\dot{q}_{\text{evap}}''$, we arrive at the following,

$$\overline{\frac{\partial T}{\partial y}} \Big|_{\text{w}} = \frac{1}{\lambda_{\text{w}}} \left(\dot{q}_{\text{conv}}'' + \dot{m}'' h_{\text{lv}} \right) , \quad (4.2)$$

where $\dot{m}''$ is the evaporative mass flux, h_{lv} is the interface-temperature-dependent latent heat of evaporation and $\lambda_{\text{w}} \overline{\partial T / \partial y} \Big|_{\text{w}}$ is the mean heat flux at the water-side of the interface, with λ_{w} as the thermal conductivity of water at the mean interface temperature, T_{int} . The task is then to find approximations for the right-hand side terms in (4.2) which will form the basis of our non-zero Neumann boundary condition.

As a first step in calculating $\dot{q}_{\text{evap}}''$ we fix the gas-side conditions at a distance far from the interface. Here, we take values from the experimental work of Martin and Migot [36] investigating high temperature free surface evaporation from water tanks and provide them in table 4.2.

T_{∞} (K)	p_0 (Pa)	RH (%)	$p_{\text{v},\infty}$ (Pa)	$\rho_{\infty} \left(\frac{\text{kg}}{\text{m}^3} \right)$
298.15	101325	40	1270	1.18

Table 4.2: Gaseous mixture properties far from the interface. In this table, RH is the relative humidity (%), $p_{\text{v},\infty}$ is the water vapour pressure after taking into account RH, and ρ_{∞} is the mass-averaged gaseous mixture density far from the interface.

In table 4.2, T_{∞} is the temperature far from the interface and p_0 is the thermodynamic pressure. The water vapour partial pressure, $p_{\text{v},\infty}$, is calculated from a Wagner equation [97], before taking into account the relative humidity, RH, also provided in table 4.2. The water vapour mass fraction far from the interface, $Y_{\text{v},\infty}$, can then be found from the following relation,

$$Y_{\text{v}} = \frac{p_{\text{v}} M_{\text{w}}}{p_{\text{v}} M_{\text{w}} + (p_0 - p_{\text{v}}) M_{\text{a}}} , \quad (4.3)$$

where M_{w} and M_{a} are respectively the molar masses of water and air. Assuming a binary mixture of water vapour and air, the mass fraction of air at the same location is found from $1 - Y_{\text{v},\infty}$. The gaseous mixture density far from the interface, ρ_{∞} , is calculated from the mass fractions and the ideal-gas equation of state and is given

in table 4.2. Equivalently, we set the conditions *at* the interface to be representative of different evaporation fluxes. First, T_{int} is selected and a corresponding saturation pressure, $p_{\text{v,int}}$, is found. The vapour mass fraction, $Y_{\text{v,int}}$, and mixture density, ρ_{int} , are then calculated as above with values provided in table 4.3.

Case	T_{int} (K)	$p_{\text{v,int}}$ (Pa)	$\rho_{\text{int}} \left(\frac{\text{kg}}{\text{m}^3} \right)$
1	313.15	7400	1.14
2	318.15	9600	1.12
3	338.15	25100	1.06
4	348.15	38600	1.01
5	353.15	47400	0.99

Table 4.3: Gaseous mixture properties at the interface. In this table, $p_{\text{v,int}}$ is the saturation vapour pressure at the mean interface temperature, T_{int} , and ρ_{int} is the interface mass-averaged gaseous mixture density.

We assume that, on the gas side, the transition from the interface conditions to those far away takes place within a layer of finite thickness, referred to herein as a *film*. Finding the mean of the interface values and those at a distance far away allows for an estimation of the film properties. We require the quantities of ρ_{f} , $c_{p\text{f}}$, μ_{f} and λ_{f} , representing respectively the *film* density, specific heat, dynamic viscosity and thermal conductivity. Of these, ρ_{f} is again found from the equation of state and $c_{p\text{f}}$ is mass-averaged using the film mass fraction, $Y_{\text{v,f}}$, whereas the quantities of μ_{f} and λ_{f} are found from the kinetic theory of gases; see [98] and Mason and Saxena [99] respectively. The film diffusion coefficients for momentum, ν_{f} , and energy, κ_{f} , respectively the kinematic viscosity and the thermal diffusivity are then found from a combination of the aforementioned properties. Finally, the film mass diffusivity for the binary mixture of air and vapour, D_{f} , is found from the following relation [100],

$$D_{\text{f}} = 1.87 \times 10^{-10} \frac{T_{\text{f}}^{2.072}}{p_0} \left(\frac{\text{m}^2}{\text{s}} \right), \quad (4.4)$$

where the thermodynamic pressure, p_0 , is in units of atmospheres, i.e. here, equal to one. The film diffusion coefficients are used to find the film Prandtl (Pr_{f}), Schmidt (Sc_{f}) and Lewis (Le_{f}) numbers, all of which are provided in table 4.4. For all cases examined herein, it was assumed that $Le = 1$, implying that the concentration and thermal boundary layer heights above the interface are equal. This allows us to find a gas-side concentration Rayleigh number, Ra_{c} , using properties based on the local water vapour mass fraction and temperature.

As discussed in the Introduction, the most pertinent experimental studies of free-

Case	Pr_f	Sc_f	Le_f	Ra_c	Sh	Ra_θ	Nu_θ
1	0.71	0.61	0.86	1.5×10^5	9.0	1.2×10^5	10.1
2	0.72	0.61	0.85	2.0×10^5	9.8	1.6×10^5	10.8
3	0.74	0.60	0.81	4.0×10^5	12.2	3.0×10^5	12.6
4	0.77	0.59	0.78	5.3×10^5	13.3	3.7×10^5	13.3
5	0.78	0.59	0.75	6.0×10^5	13.8	4.0×10^5	13.7

Table 4.4: Gas-side dimensionless parameters. In this table, $Pr_f = \nu_f/\alpha_f$, $Sc_f = \nu_f/D_f$, and $Le = Sc_f/Pr_f$. The dimensionless groups Ra_c , Sh , Ra_θ and Nu_θ are defined in the text.

surface evaporation include Boelter *et al.* [29] and Bower and Saylor [30]. Both measured evaporation rates into a quiescent air environment, however, Bower and Saylor [30] used an improved set-up, allowing for more realistic air-side natural convection conditions. Moreover, both papers provide Sherwood number (Sh) correlations based on a relationship with the Schmidt number (Sc_f) and Ra_c , defined as follows,

$$Ra_c = \frac{|\mathbf{g}|(\rho_\infty - \rho_{\text{int}})W^3}{D_f\mu_f}. \quad (4.5)$$

Bower and Saylor [30] then proposed the following correlation, used here to find an estimation of the concentration boundary layer height, δ_c ,

$$Sh = 0.23 Sc_f^{\frac{1}{3}} Ra_c^{0.321} \approx \frac{W}{\delta_c}. \quad (4.6)$$

The fact that Sh is inversely proportional to the height of the concentration boundary layer is again an analogy with heat transfer that holds in cases with $Le = 1$. The mass flux can then be estimated with the following relation [101],

$$\dot{m}'' = \frac{\rho_f D_f}{\delta_c} \log(1 + B_m), \quad (4.7)$$

with the mass transfer driving force, B_m , defined as

$$B_m = \left(\frac{Y_{v,\infty} - Y_{v,\text{int}}}{Y_{v,\text{int}} - 1} \right). \quad (4.8)$$

Substituting (4.6) into (4.7) gives the following relation for the mass flux,

$$\dot{m}'' = Sh \frac{\rho_f D_f}{W} \log(1 + B_m). \quad (4.9)$$

The latent heat flux is then found from $\dot{q}_{\text{evap}}'' = \dot{m}'' h_{lv}$ and the final heat and mass

fluxes are provided in table 4.5.

Case	$\dot{m}''$ ($\frac{\text{kg}}{\text{m}^2\text{s}}$)	$\dot{q}_{\text{evap}}''$ ($\frac{\text{W}}{\text{m}^2}$)	$\dot{q}_{\text{conv}}''$ ($\frac{\text{W}}{\text{m}^2}$)	$\overline{\frac{\partial T}{\partial y}} _{\text{w}}$ ($\frac{\text{K}}{\text{m}}$)
1	2.4×10^{-4}	580	90	1000
2	3.6×10^{-4}	860	130	2000
3	1.5×10^{-3}	3420	310	6000
4	2.8×10^{-3}	6480	420	10000
5	3.9×10^{-3}	9040	470	14000

Table 4.5: Fluxes at the interface. In this table, $\dot{m}''$ is the mass flux, $\dot{q}_{\text{evap}}''$ is the evaporative heat flux, and $\dot{q}_{\text{conv}}''$ is the convective heat flux. The prescribed temperature gradient, $\overline{\partial T / \partial y}|_{\text{w}}$, is the dimensional form of the non-zero Neumann upper thermal boundary condition. The values are rounded to the nearest thousand to highlight their approximate nature.

Next, the convective heat loss is estimated by assuming that it is proportional to the difference between the temperature of the interface, T_{int} , and the ambient gas-side temperature, T_{∞} , with the heat transfer coefficient, h , as the proportionality coefficient. Overall we have the following,

$$\dot{q}_{\text{conv}}'' = h (T_{\text{int}} - T_{\infty}) , \quad (4.10)$$

where h is estimated from the following correlation for a horizontal flat surface that is warmer than the ambient air above [102],

$$\frac{h W}{\lambda_{\text{f}}} = Nu_{\theta} = 0.54 Ra_{\theta}^{\frac{1}{4}} . \quad (4.11)$$

In the above relation, Ra_{θ} is the gas-side thermal Rayleigh number,

$$Ra_{\theta} = \frac{|\mathbf{g}| \beta_{\infty} (T_{\text{int}} - T_{\infty}) W^3}{\kappa_{\text{f}} \nu_{\text{f}}} , \quad (4.12)$$

and W is the characteristic length-scale, the width of the domain. We provide values for Ra_{θ} and Nu_{θ} in table 4.4 and $\dot{q}_{\text{conv}}''$ in table 4.5. In this latter table, we note that the evaporative contribution, $\dot{q}_{\text{evap}}''$, is always more important than the convective, $\dot{q}_{\text{conv}}''$. In fact $\dot{q}_{\text{evap}}''$ accounts for a minimum of 87% and a maximum of 95% of heat loss away from the free surface for the cases investigated.

With the upper temperature gradient known, it remains to find an estimate for the corresponding case-dependent lower-wall temperatures, T_{low} . Martin and Migot [36] carried out evaporation experiments of water at high-surface temperatures and measured the temperature drop between the bulk and the interface, $\Delta T_{\text{u}} = T_{\text{bulk}} - T_{\text{int}}$.

They reported that the temperature drop from the interface to the bulk increases in a non-linear manner with increasing evaporation rate. They also observed that the temperature drop between the heated lower wall and the bulk, $\Delta T_l = T_{\text{low}} - T_{\text{bulk}}$, was approximately equal to that between the bulk and the interface. That is, $\Delta T_l \approx \Delta T_u$. Therefore, in our configuration, the total temperature difference across the pool is first approximated as follows,

$$\Delta T = T_{\text{low}} - T_{\text{int}} = 2\Delta T_u, \quad (4.13)$$

with ΔT_u estimated from the experiments of Martin and Migot [36].

This first approximation is updated in preliminary simulations until the correct time- and area-averaged T_{int} is found. As ΔT_u was reported to increase with evaporation rates, the lower wall temperature, T_{low} is case-dependent. A physical explanation for this is seen in (4.1), where a higher evaporation flux is only possible with more heat added to the interface from below. In the current configuration, this energy addition must be via an increase in T_{low} . The lower wall temperatures are provided in table 4.6, alongside the predicted time- and area-averaged T_{int} .

It is worth adding here an observation of Boelter *et al.* [29], that evaporation measurements were invalidated above an upper physical limit. In their experiments boiling at the lower wall began at bulk water temperatures in excess of 361.15 K. In table 4.6, we see that the T_{low} of case 5 exceeds this limit; the results for this case are therefore caveated but are included to explore the parameter space more completely. At the other end of the scale, the smallest Ra investigated herein corresponds to an interface temperature of 40 K. At lower temperatures, the associated evaporation rate produces too small a ΔT to drive turbulent convection below.

Finally, we define the normalised temperature as follows,

$$\hat{\theta} = (T - T_{\text{ref}})/\Delta T, \quad (4.14)$$

with T_{ref} as the mean of the lower wall and interface temperatures. If the estimations of the evaporative heat losses and corresponding lower wall temperatures are correct, we have $\hat{\theta}_{\text{int}} = -0.5$ and $\hat{\theta}_{\text{low}} = 0.5$, at the statistically stationary solution.

4.4 Boundary conditions

The computational domain is a cube of unity aspect ratio. As mentioned in section 4.1, deviations away from the classical turbulent RBC set-up in the current configuration are in both the hydrodynamic *and* thermal boundary conditions prescribed at the upper boundary. Before expanding on this, we provide reference values used for nondi-

Case	Ra	T_{int} (K)	T_{low} (K)	T_{ref} (K)
1	7.5×10^6	313.15	315.25	314.20
2	1.5×10^7	318.15	321.65	319.90
3	5.0×10^7	338.15	345.15	341.65
4	9.0×10^7	348.15	358.15	353.15
5	1.3×10^8	353.15	365.65	359.40

Table 4.6: Thermal boundary conditions. In this table, T_{int} is the predicted interface value, T_{low} is the fixed lower wall temperature, and T_{ref} is the mean pool temperature. The normalised temperature is defined as $\hat{\theta} = (T - T_{\text{ref}}) / \Delta T$, so that the upper and lower boundary values correspond to $\hat{\theta}_{\text{int}} = -0.5$ and $\hat{\theta}_{\text{low}} = 0.5$, respectively for all cases.

mensionalisation purposes in table 4.7. The reference length is the height of the cube, H , and is constant for all cases. With the reference velocity as the free-fall velocity, $U_{\text{ff}} = \sqrt{gH\beta_{\text{ref}}\Delta T}$, we find a reference free-fall time from $t_{\text{ff}} = H/U_{\text{ff}}$. Finally, the reference temperature is the mean in the pool, T_{ref} , with all reference properties then relative to T_{ref} .

Ra	U_{ff}	ΔT	ρ_{ref}	λ_{ref}	$\beta_{\text{ref}} \times 10^{-4}$	$\nu_{\text{ref}} \times 10^{-7}$	$\kappa_{\text{ref}} \times 10^{-7}$	Pr_{ref}
	$\left(\frac{\text{m}}{\text{s}}\right)$	(K)	$\left(\frac{\text{kg}}{\text{m}^3}\right)$	$\left(\frac{\text{W}}{\text{mK}}\right)$	$\left(\frac{1}{\text{K}}\right)$	$\left(\frac{\text{m}^2}{\text{s}}\right)$	$\left(\frac{\text{m}^2}{\text{s}}\right)$	
7.5×10^6	0.019	2.1	991.8	0.63	4.0	6.4	1.52	4.2
1.5×10^7	0.026	3.5	989.5	0.64	4.3	5.8	1.54	3.8
5.0×10^7	0.042	7.0	978.6	0.66	5.6	4.2	1.61	2.6
9.0×10^7	0.051	10.0	971.8	0.67	6.2	3.6	1.63	2.2
1.3×10^8	0.060	12.5	967.8	0.68	6.4	3.4	1.65	2.1

Table 4.7: Reference values for nondimensionalisation purposes. The reference height, H , is 0.045 m for all cases.

The lower wall is located at $\hat{y} = 0$, the upper boundary at $\hat{y} = 1$ and, likewise, the side walls at $\hat{x} = 0$ ($\hat{z} = 0$) and $\hat{x} = 1$ ($\hat{z} = 1$). No-slip velocity boundary conditions are enforced at the side and lower walls. The free-slip condition is prescribed at the upper boundary, i.e. $\frac{\partial \hat{u}}{\partial \hat{y}} = \frac{\partial \hat{w}}{\partial \hat{y}} = 0$ and $\hat{v} = 0$ at $\hat{y} = 1$. This is again considered as a first order approximation of a free surface. For the thermal boundary conditions outlined in the previous section we have adiabatic side-walls with $\frac{\partial \hat{\theta}}{\partial \hat{x}}$ prescribed. At $\hat{y} = 0$ we set $\hat{\theta} = 0.5$ as a Dirichlet boundary condition, whereas at $\hat{y} = 1$ we prescribe the non-zero Neumann conditions provided in table 4.5. For completeness, the dimensionless form of

the prescribed temperature gradients are found by dividing by the case-specific $\Delta T/H$, which gives $\frac{\partial \theta}{\partial y} = 21.4, 25.7, 38.6, 45.0$ and 50.4 for cases 1–5, respectively.

As a result of the aforementioned boundary conditions, five hydrodynamic boundary layers exist, one at each of the vertical side walls and one at the lower wall. On the other hand, there are only two thermal boundary layers, at the cooled upper boundary and heated lower wall. Finally, and with regard to the initial conditions, a linear temperature profile from T_{low} to T_{int} is employed across the vertical direction, whereas for the velocity a quiescent field is enforced to which small random perturbations are applied.

The Rayleigh number is then calculated from (1.1), with the ΔT now specific to our boundaries. We provide values for Ra in table 4.6 and from hereon we refer to cases 1–5 via their corresponding Ra . An instantaneous view of typical temperature isosurfaces are presented in figure 4.1 for the cases of $Ra = 1.5 \times 10^7$ and $Ra = 9 \times 10^7$; smaller flow structures appear as evaporation is increased.

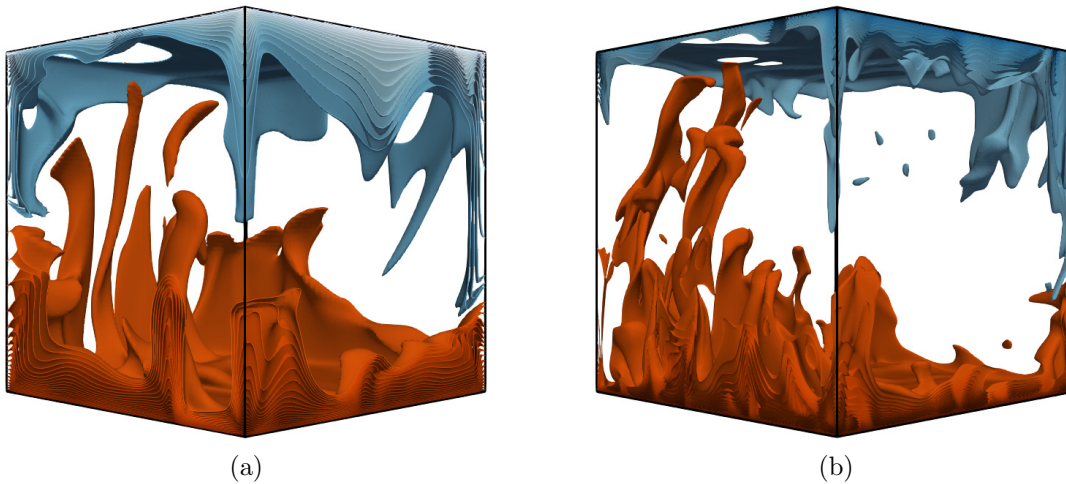


Figure 4.1: Instantaneous isosurfaces of the temperature field: (a) a low evaporation case corresponding to $Ra = 1.5 \times 10^7$ and (b) a high evaporation case corresponding to $Ra = 9.0 \times 10^7$.

4.5 Resolution requirements

In this chapter, we carry out only direct numerical simulations. As such, we must again ensure that the smallest length scales of the flow are everywhere resolved. Much like in chapter 3, the first criterion is to ensure adequate resolution of the hydrodynamic and thermal boundary layers in the vertical direction.

We use the same universal criterion based on the laminar Prandtl-Blasius boundary layer theory [77] which, in fact, is Pr dependent. As we have variable thermal boundary conditions, Pr is variable and the resolution requirements change between the cases

investigated herein. For all cases the thermal boundary layer height is still predicted as $\hat{\delta}_\theta = \frac{1}{2Nu}$.

For the cases where $Pr_{\text{ref}} > 3$, the *a priori* estimate of the dimensionless hydrodynamic boundary layer height, $\hat{\delta}_u$, is still given by (3.1) and the minimum resolution requirements for $\hat{\delta}_u$ and $\hat{\delta}_\theta$, denoted by N_u and N_θ respectively, are (3.2) and (3.3).

Equivalently, where $Pr_{\text{ref}} < 3$, Shishkina *et al.* [77] states that the estimate of $\hat{\delta}_u$ is given by

$$\hat{\delta}_u = \frac{1}{2}Nu^{-1}Pr^{0.357-0.022\log Pr}, \quad (4.15)$$

and the minimum resolution requirements, N_u and N_θ , by

$$N_u = \sqrt{2}aNu^{\frac{1}{2}}Pr^{0.3215+0.011\log Pr}, \quad (4.16)$$

$$N_\theta = \sqrt{2}aNu^{\frac{1}{2}}Pr^{-0.0355+0.033\log Pr}. \quad (4.17)$$

The values of N_u and N_θ are rounded to the next integer and are provided in table 4.8, where they are taken as minimum requirements for the number of points inside the boundary layers. In fact, as can be seen by the difference in values of those in parentheses and those outside, we intentionally over-resolve by a factor of two.

As in chapter 3, it is important to ensure that the grid is adequately refined in the near-wall regions. Accordingly, we choose to refine equally in all directions using a hyperbolic-tangent expansion from a minimum cell size at the boundaries to a maximum in the centre of the pool. This results in $\hat{\Delta}y_{\text{max}} = \hat{\Delta}x_{\text{max}} = \hat{\Delta}z_{\text{max}}$ in the centre of the domain.

Ra	$N_x \times N_y \times N_z$	N_u	N_θ	$\hat{\Delta}y_{\text{min}}$	$\hat{\Delta}y_{\text{max}}$	$\frac{\Delta}{\pi\eta}$	$\frac{\Delta}{\pi\eta_\theta}$
7.5×10^6	$100 \times 100 \times 100$	10 (5)	7 (3)	0.0028	0.0171	0.22	0.65
1.5×10^7	$130 \times 130 \times 130$	12 (6)	8 (4)	0.0016	0.0144	0.25	0.68
5.0×10^7	$180 \times 180 \times 180$	12 (6)	9 (4)	0.0012	0.0104	0.36	0.72
9.0×10^7	$200 \times 200 \times 200$	12 (6)	9 (5)	0.0010	0.0094	0.44	0.76
1.3×10^8	$220 \times 220 \times 220$	12 (6)	10 (5)	0.0009	0.0087	0.46	0.75

Table 4.8: Resolution criteria. In this table, N_y is minimum number of points required in the vertical direction to satisfy both bulk and boundary layer resolution requirements (we then set $N_y = N_x = N_z$), N_θ is the minimum number of points in the thermal boundary layer and N_u is the minimum number of points in the hydrodynamic boundary layer according to [77], $\hat{\Delta}y_{\text{min}}$ and $\hat{\Delta}y_{\text{max}}$ are the minimum and maximum dimensionless cell size, and the penultimate and final columns show the maximum ratio of cell size to the calculated *a posteriori* Kolmogorov and temperature microscales respectively.

The second resolution criterion remains to ensure that the bulk of the domain is

adequately resolved. We use the same method for predicting *a priori* satisfactory refinement as in 3.3.1. That is, the hydrodynamic and thermal resolution requirements are defined as,

$$\Delta \leq \pi\eta \approx \pi H \left(\frac{Pr^2}{Ra Nu} \right)^{\frac{1}{4}}. \quad (4.18)$$

and

$$\Delta \leq \pi\eta_\theta \approx \pi H \left(\frac{1}{Ra Pr Nu} \right)^{\frac{1}{4}}. \quad (4.19)$$

We again note that a prediction of Nu is required in (4.18) and (4.19). Previous studies showed that a first estimate for Nu can be obtained via a classical Ra – Nu correlation from the literature, for example $Nu = 0.124Ra^{0.309}$ [82]. Increasing this value by approximately 30% then allows for the shear-free upper boundary effect to be taken into account.

Preliminary simulations are then performed on a coarse grid, where coarse is defined as reducing the number of cells necessary for a resolved DNS by a factor of two in each direction, whilst still respecting the minimum boundary layer refinements in table 4.8. These preliminary simulations are run until statistically stationary, whereupon we take statistics over 300 free-fall times and assess the time- and area-averaged temperature at the upper boundary. If this value corresponds to the predicted T_{int} provided in table 4.6, then the Ra provided in the same table is accurate and Nu is updated in (4.18) and (4.19). The coarse grid solutions are then used for initialisation purposes for the fully-resolved DNS.

The number of cells in the x , y and z directions for the fully-resolved DNS are then given respectively by N_x , N_y and N_z and are provided in table 4.8. In order to assess this refinement *a posteriori* we find the ratios of grid spacing to the local Kolmogorov (3.4) and temperature (3.5) microscales. The final two columns in table 4.8 show the maximum ratios in the domain, where all refinements are shown to be adequate, that is smaller than unity.

The time-step in our simulations is computed from a Courant number of 0.25. As in Kaczorowski and Wagner [76], the constraint on the time-step for numerical stability purposes is then stricter than that of the Kolmogorov and temperature timescales. The smallest of the flow timescales can therefore be considered well captured.

4.6 Numerical results

The results section is divided into two parts. First, we look at the mean flow characteristics including the structure of the LSC, measurements of the rms of vertical velocity in the bulk of the flow and the dimensionless heat transfer. We then analyse the turbulent statistics across the vertical direction, and in doing so, assess the impact

of increasing Ra on boundary layer behaviour.

The notation adopted in this chapter is subtly different from that in the previous, chapter 3, as we no longer have a homogeneous direction. The mean of a generic variable ϕ is denoted by $\langle\phi\rangle$ and refers to averaging *over time only*, additional averaging over a given horizontal x - z plane is denoted by $\langle\phi\rangle_{xz}$, and over volume by $\langle\phi\rangle_{xyz}$. The fluctuating component is then denoted by ϕ' and the rms value by $\phi_{\text{rms}} = \sqrt{\langle\phi'\phi'\rangle}$. The time averaging in our study was taken over 300 free-fall times which is similar to the time interval used by Kaczorowski and Xia [51] for the range of Ra investigated. We later test the adequacy of this interval.

4.6.1 Mean flow properties

To assess the accuracy of the prescribed heat fluxes at the upper boundary, we first analyse the time- and area-averaged upper boundary temperatures. Figure 4.2 shows the time-averaged normalised temperature at the upper boundary. We note first that in turbulent RBC with fixed temperature boundary conditions the coldest physical temperature is $\hat{\theta} = -0.5$, whereas in the current configuration cold spots appear near the intersection of the upper boundary and side-walls corresponding to twice this value. However, the time- and area-averaged values, $\langle\hat{\theta}_{\text{int}}\rangle_{xz}$, are provided in table 4.9, where they are seen to match well the predicted values in table 4.6. The prescribed heat fluxes are therefore considered accurate.

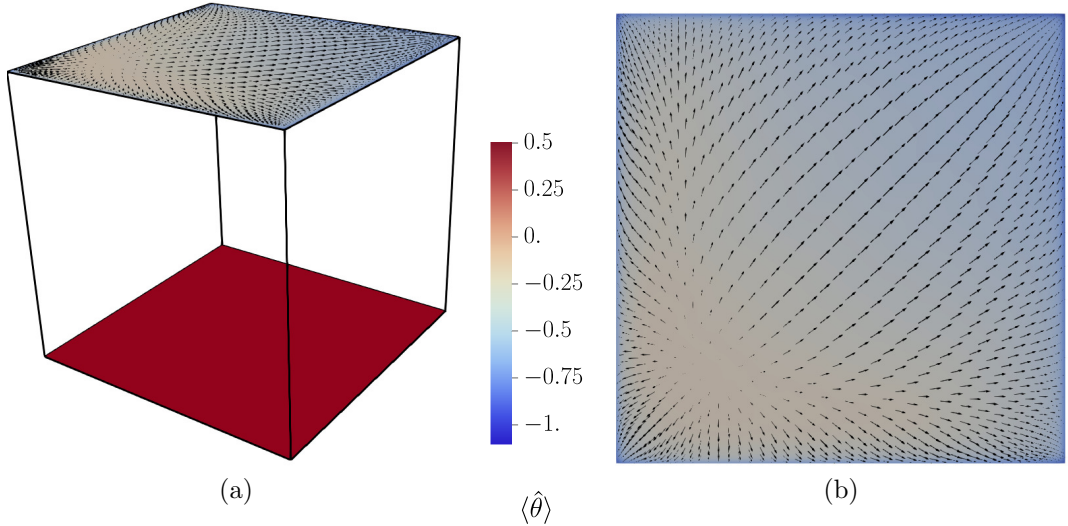


Figure 4.2: Time-averaged normalised temperature, $\langle\hat{\theta}\rangle$, at the interface and lower wall for $Ra = 9.0 \times 10^7$: (a) side-view showing constant $\hat{\theta}_{\text{low}} = 0.5$ on lower wall and spatially-variable $\langle\hat{\theta}_{\text{int}}\rangle$ on upper boundary ($-1.14 < \langle\hat{\theta}_{\text{int}}\rangle < -0.33$) and (b) Top view of upper boundary with superimposed velocity vectors showing LSC impingement and subsequent flow direction.

The impingement point of the LSC can also be identified from the local peak in

temperature seen on the upper boundary in figure 4.2. This is a result of the hot plumes released from the heated lower wall travelling with the mean wind. Further, we note that the direction of the LSC *at* the shear-free boundary following impingement is also visible from the superimposed velocity vectors in figure 4.2b.

Ra	$\langle \hat{\theta}_{\text{int}} \rangle_{xz}$	Nu	$\hat{\delta}_{\theta_{\text{int}}}$	$\hat{\delta}_{\theta_{\text{low}}}$	$\frac{1}{2Nu}$	$\hat{\delta}_{\mathbf{u}}$	$(v_{\text{rms}})_{\text{ctr}}$	Re_{ctr}	$(v_{\text{rms}})_{xyz}$	Re
7.5×10^6	-0.51	21.2	0.017	0.028	0.024	0.048	0.0008	56	0.0015	107
1.5×10^7	-0.49	25.9	0.014	0.021	0.019	0.040	0.0010	76	0.0021	166
5.0×10^7	-0.51	38.3	0.009	0.014	0.013	0.028	0.0016	168	0.0040	428
9.0×10^7	-0.50	44.6	0.008	0.012	0.011	0.025	0.0021	254	0.0052	647
1.3×10^8	-0.51	49.7	0.007	0.011	0.010	0.024	0.0025	326	0.0062	822

Table 4.9: Time-averaged results. In this table, $\langle \hat{\theta}_{\text{int}} \rangle_{xz}$ is the time- and area-averaged normalised interface temperature, Nu is the time- and volume-averaged Nusselt number, $\hat{\delta}_{\theta_{\text{int}}}$ and $\hat{\delta}_{\theta_{\text{low}}}$ are the thermal boundary layer heights at the interface and the lower wall, respectively, whereas $\hat{\delta}_{\mathbf{u}}$ is the hydrodynamic boundary layer height at the lower wall. $Re_{\text{ctr}} = (v_{\text{rms}})_{\text{ctr}} H / \nu_{\text{ref}}$ is the Reynolds number in the centre of the domain, where $(v_{\text{rms}})_{\text{ctr}} = \sqrt{\langle v'v' \rangle}_{\text{ctr}}$ (m/s) is the rms of the vertical velocity in the same location. $Re = (v_{\text{rms}})_{xyz} H / \nu_{\text{ref}}$ is the global Reynolds number where $(v_{\text{rms}})_{xyz} = \sqrt{\langle v'v' \rangle}_{xyz}$ (m/s) is the volume-averaged rms of the vertical velocity.

We next examine the diagonal plane occupied by the large-scale circulation at $Ra = 5 \times 10^7$ shown in figure 4.3a. Similar to turbulent RBC in a cube, the large-scale circulation occupies the entire height of the domain. Further, due to the contained nature of the flow, the LSC creates recirculation zones in opposite top and bottom corners. However, contrary to turbulent RBC in a cube, these recirculation zones are asymmetric in the current configuration. We define the coordinate of the lowest point of the upper recirculation zone as $\hat{y}_{r_1}$. Equivalently, the highest point of the lower recirculation zone is defined as $\hat{y}_{r_2}$. These values represent the $\hat{y}$ at which the vertical component of the mean velocity changes sign nearest the side-wall in figure 4.3a. From the same figure, the recirculation zone at the lower wall visibly occupies a smaller zone than its equivalent in the opposite corner, that is $\hat{y}_{r_2} < 1 - \hat{y}_{r_1}$. The explanation is in the role played by the shear-free boundary, accelerating the large-scale flow in the negative y -direction. The limits of the recirculation zones, $\hat{y}_{r_1}$ and $\hat{y}_{r_2}$, are provided in table 4.10 for the five cases. A general trend is observed where the recirculation zones become taller and thinner as Ra is increased. These zones are pushed towards the corner regions by the increasing strength of the LSC. However, at the highest Ra investigated, small secondary structures were observed in the bottom-left corner of the LSC plane (underneath $\hat{y}_{r_1}$). We believe this to be the cause of the non-monotonic behavior suggested in table 4.10.

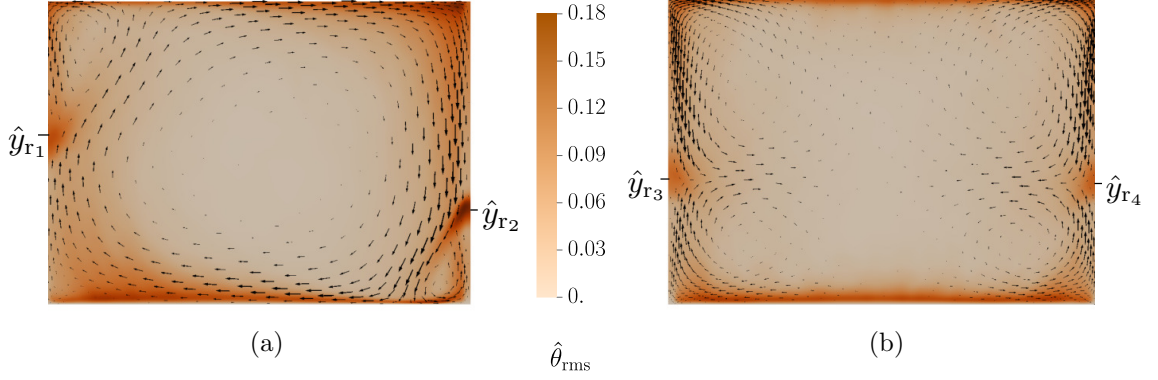


Figure 4.3: Diagonal planes showing $\hat{\theta}_{\text{rms}}$ fields at $Ra = 5.0 \times 10^7$: (a) plane containing the LSC and (b) the plane orthogonal to that shown in (a). The mean velocity vector field is superimposed for clarity. The legend is as follows: $\hat{y}_{r1}$ is the coordinate of the lowest point of the *upper* recirculation zone in the LSC plane, $\hat{y}_{r2}$ is the highest point of the *lower* recirculation zone in the LSC plane and $\hat{y}_{r3} = \hat{y}_{r4}$ is the coordinate at which the counter-rotating vortex structures in the orthogonal plane interact.

Figure 4.3b shows the orthogonal plane to that given in 4.3a. We observe four counter-rotating vortical cells, similar again to previous observations in wall-bounded turbulent RBC. However, contrary to turbulent RBC in a box [66], the counter-rotating vortical cells occupy more space in the upper volume of the pool than in the lower. Their size can be qualitatively inferred by the locations of the peak $\hat{\theta}_{\text{rms}}$ on the side-walls. We again find the vertical coordinate at which the upper and lower counter-rotating vortical cells interact, from the first $\hat{y}$ at which the vertical component of the mean velocity changes sign nearest the side-wall in figure 4.3b. For turbulent RBC in a box, this occurs at $\hat{y} = 0.5$, whereas for the current configuration this location is found closer to the lower wall; see $\hat{y}_{r3} = \hat{y}_{r4}$ in table 4.10. The explanation is the same as for the LSC plane; the rotating vortical cells accelerate towards the boundaries after impingement at the shear-free surface. This is visible from the vector field in figure 4.3b, showing stronger downward motion than upward. The structure of the LSC is thus visibly impacted by the presence of the free surface. We again provide values for the recirculation zone limits, $\hat{y}_{r3}$ and $\hat{y}_{r4}$, in table 4.10 and note that the counter-rotating vortical cells near the shear-free surface occupy an increasingly larger zone as Ra is augmented. To better visualise the LSC and the location of the points $\hat{y}_{ri}$, $i = 1-4$, we plot in figure 4.4, the time-averaged streamlines coloured by the mean vertical velocity, $\langle \hat{v} \rangle$, for the $Ra = 5.0 \times 10^7$ case.

One consequence of the asymmetry is that the upper recirculation zone extends towards the mid-plane of the domain at $\hat{y} = 0.5$. To better understand the LSC, we therefore plot, in figure 4.5, the mean vertical velocity, $\langle \hat{v} \rangle$, across the diagonal containing the LSC at $\hat{y} = 0.4$. Therein, we observe the near-zero (vertical) velocity region in the centre of the LSC, also visible in figure 4.3a. The peaks near the sidewalls corre-

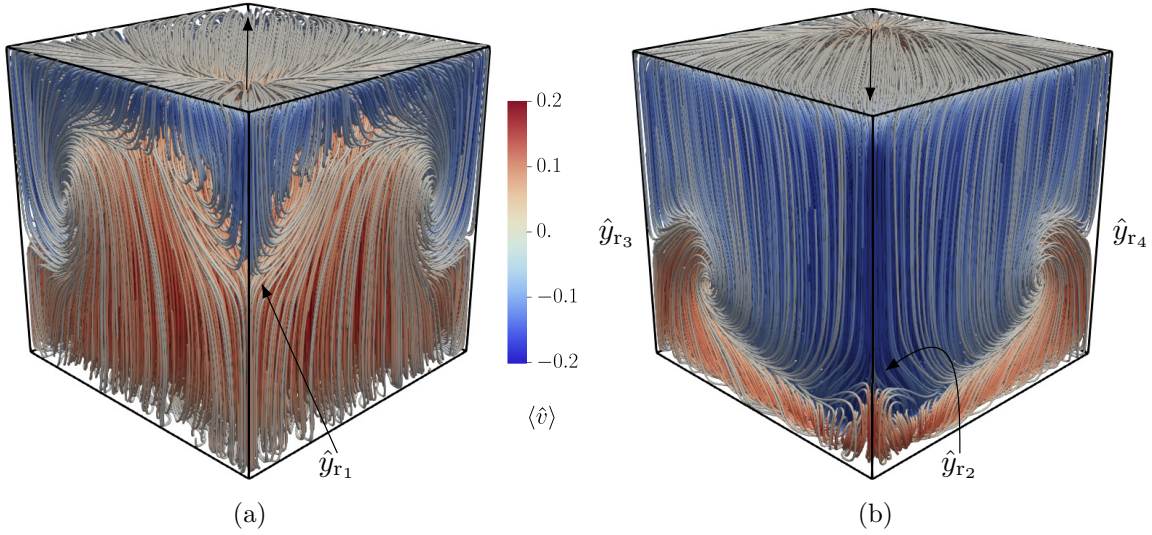


Figure 4.4: Time-averaged streamlines coloured by the mean vertical velocity, $\langle \hat{v} \rangle$, for the $Ra = 5.0 \times 10^7$ case. We annotate the figure with the direction of the LSC on the free-slip upper boundary as well as the vertical limits of the recirculation zones.

Ra	$\hat{y}_{r1}$	$\hat{y}_{r2}$	$\hat{y}_{r3} = \hat{y}_{r4}$
7.5×10^6	0.55	0.26	0.42
1.5×10^7	0.52	0.27	0.42
5.0×10^7	0.51	0.35	0.41
9.0×10^7	0.50	0.38	0.40
1.3×10^8	0.53	0.37	0.40

Table 4.10: Vertical limits of the recirculation zones. The coordinates $\hat{y}_{r1}$ to $\hat{y}_{r4}$ are shown in figures 4.3 and 4.4.

spond respectively to the upward, $\frac{x}{\sqrt{2}H} \approx 0.03$, and downward, $\frac{x}{\sqrt{2}H} \approx 0.97$, motions of the LSC. Instead of the symmetric peaks observed in the equivalent plot of Foroozani *et al.* [94] (at $\hat{y} = 0.5$), here the shear-free boundary accelerates the fluid following impingement. This results in the magnitude of the downward velocity exceeding that of the upward. This is clearly observed also in the vector field superimposed onto figure 4.3a. The insets in figure 4.5 show how the LSC is pushed towards the corner walls as Ra is increased; a trend also noted in both Cioni *et al.* [23] and Foroozani *et al.* [94] for confined turbulent RBC.

It is worth adding that LSC reorientations are a known phenomenon in thermal convection configurations such as turbulent RBC [23, 94, 103]. We also observed such events in our simulations. However, since the study does not concentrate on LSC reorientations, all results presented herein are from simulations whose time-averaging periods correspond to a stable LSC.

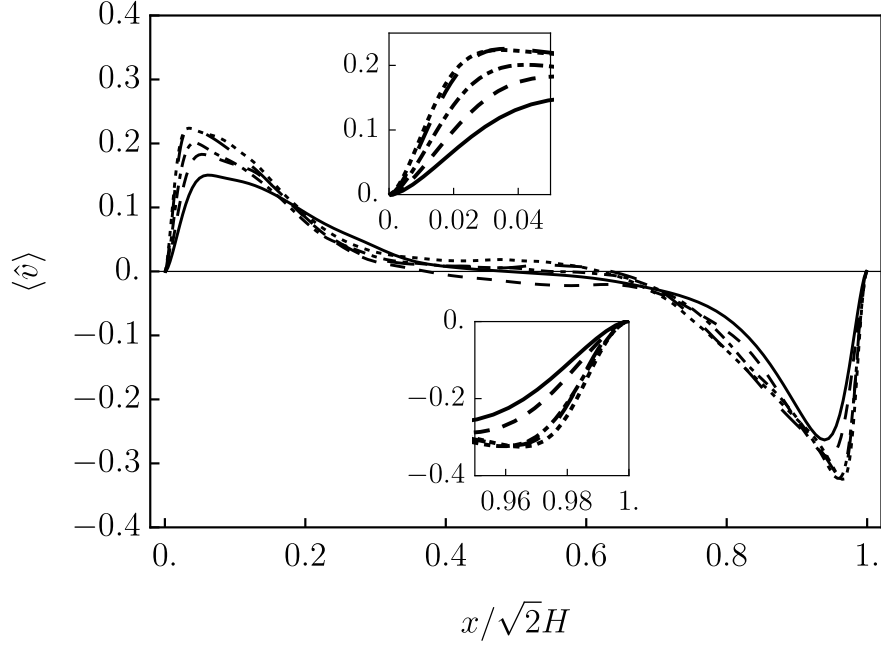


Figure 4.5: Plot of the mean dimensionless vertical velocity, $\langle \hat{v} \rangle$, along the diagonal line containing the LSC at $\hat{y} = 0.4$. The insets show zooms near the corner regions. The legend is as follows: $Ra = 7.5 \times 10^6$ (—), $Ra = 1.5 \times 10^7$ (---), $Ra = 5.0 \times 10^7$ (-.-.), $Ra = 9.0 \times 10^7$ (- -), and $Ra = 1.3 \times 10^8$ (.....).

We next present analysis of the rms of the vertical velocity fluctuations in the centre of the domain, $(v_{\text{rms}})_{\text{ctr}} = \sqrt{\langle v'v' \rangle}_{\text{ctr}}$. Nondimensionalising by ν_{ref}/H , provides the following local Reynolds number,

$$Re_{\text{ctr}} = \frac{(v_{\text{rms}})_{\text{ctr}} H}{\nu_{\text{ref}}}, \quad (4.20)$$

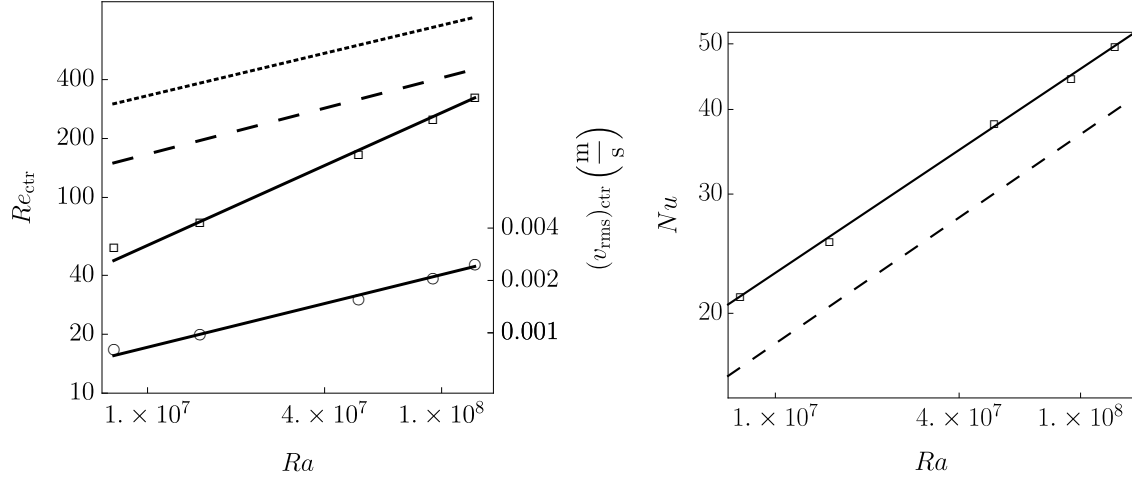
Values of Re_{ctr} are provided in table 4.9 and are plotted in figure 4.6a, where the associated power-law fit,

$$Re_{\text{ctr}} = 1.0 \times 10^{-3} Ra^{0.68}, \quad (4.21)$$

merits further discussion.

The turbulent RBC experiments of Daya and Ecke [93] measured Re_{ctr} over 1.3 decades of Ra for cubic geometries and provided the power-law fit, $Re_{\text{ctr}} = Ra^\beta$, with $\beta = 0.36 \pm 0.05$, whereas Foroozani *et al.* [66] found numerically $Re_{\text{ctr}} = 0.31 Ra^{0.39}$ over an increased range of Ra . Importantly, in both these studies the mean temperature in the domain remained constant as Ra was increased. As a result, the viscosity used for the nondimensionalisation in (4.20) was also constant between experiments (or simulations).

In contrast, the Rayleigh numbers investigated in this study are updated via changes in thermal boundary conditions. As such, both T_{ref} and ν_{ref} vary significantly between cases, as shown in tables 4.6 and 4.7. We know this to be the cause of the discrepancy



(a) Ra scaling of Re_{ctr} and $(v_{\text{rms}})_{\text{ctr}}$. The legend is as follows: Re_{ctr} data ($\square$), $(v_{\text{rms}})_{\text{ctr}}$ data ($\circ$), the fits to the present data: $Re_{\text{ctr}} = 1.0 \times 10^{-3} Ra^{0.68}$ (—) above and $(v_{\text{rms}})_{\text{ctr}} \propto Ra^{0.41}$ (—) below, the fit of Daya and Ecke [93]: $Re_{\text{ctr}} = Ra^{0.36}$ (.....), the fit of Foroozani *et al.* [66]: $Re_{\text{ctr}} = 0.31Ra^{0.39}$ (- -).

(b) Ra scaling of Nu . The legend is as follows: Nu data ($\square$), power-law fit to the present data: $Nu = 0.178Ra^{0.301}$ (—) and the power-law fit of Niemala *et al.* [82]: $Nu = 0.124Ra^{0.309}$ (- -).

Figure 4.6: Ra -scaling plots

in the exponents because, according to our simulations, a power-law fit of the $(v_{\text{rms}})_{\text{ctr}}$ data reads,

$$(v_{\text{rms}})_{\text{ctr}} \propto Ra^{0.41}, \quad (4.22)$$

see also figure 4.6a. The exponent in (4.22) is in good agreement with Daya and Ecke [93] and Foroozani *et al.* [66] for turbulent RBC.

We also provide in table 4.9 the rms of the vertical velocity based on the combined volume-time averages; $(v_{\text{rms}})_{xyz} = \sqrt{\langle v'v' \rangle}_{xyz}$, as well as the associated global Reynolds number, Re . We see the same trend in the power-law fits for the global data where we have

$$Re = 1.0 \times 10^{-3} Ra^{0.73} \quad \text{and} \quad (v_{\text{rms}})_{xyz} \propto Ra^{0.49}. \quad (4.23)$$

Our fit of $(v_{\text{rms}})_{xyz}$ matches well that of Scheel and Schumacher [104] for turbulent RBC in cylindrical domains, according to which Re scales as Ra^β , with $\beta = 0.49 \pm 0.01$. Please note that, since $(v_{\text{rms}})_{\text{ctr}}$ and $(v_{\text{rms}})_{xyz}$ are dimensional quantities, only the exponents of the corresponding power laws are of interest here.

Similarly to Daya and Ecke [93], the explored parameter space is limited to a rather short range of 1.25 Ra decades, what is of interest, however, is the similar scaling for the v_{rms} observed both globally and in the centre of the domain. Of course, the current set-up differs from turbulent RBC due to the free-slip upper boundary. The similar scaling for the rms of vertical velocity fluctuations in the bulk suggests that, away from the boundaries, the behavior of this fluctuating quantity is similar for the two configurations.

The dimensionless heat transfer across any x - z plane is measured by the local Nusselt number, Nu_y , and is calculated from the sum of the Nu_{conv} and Nu_{diff} contributions as in (3.11), we provide the relations here again for clarity,

$$Nu_y = \underbrace{\sqrt{RaPr} \langle \hat{\rho} \hat{v} \hat{\theta} \rangle_{xz}}_{Nu_{\text{conv}}} - \underbrace{\langle \hat{\lambda} \frac{\partial \hat{\theta}}{\partial \hat{y}} \rangle_{xz}}_{Nu_{\text{diff}}} . \quad (4.24)$$

The volume-averaged (global) Nusselt, Nu , is then given as

$$Nu = \sqrt{RaPr} \langle \hat{\rho} \hat{v} \hat{\theta} \rangle_{xyz} - \langle \hat{\lambda} \frac{\partial \hat{\theta}}{\partial \hat{y}} \rangle_{xyz} . \quad (4.25)$$

For the flow in question, a statistically stationary solution gives Nu_y as constant and further equal to Nu . Indeed, for all examined cases, our simulations predicted constant Nu_y and in excellent agreement with Nu , the values of which are provided in table 4.9. Moreover, for all cases investigated, the global value after 150 free-fall times, or half the averaging time, changed by less than 1%. This finding suggests that the time-averaging interval is indeed sufficient.

The contributions of the convective and diffusive components of Nu_y are shown in figures 4.7a and 4.7b respectively. The convective component, Nu_{conv} , tends to a non-zero, albeit very small, value inside the thermal boundary layers and is the dominant contribution away from the walls. For the diffusive component, Nu_{diff} , only the near-wall contribution is shown, as it is negligible in the bulk. The definitions (4.24) and (4.25) take into account the variable density and thermal conductivity of the working fluid. However, these thermodynamic properties vary by a maximum of only 1.5% and 2% respectively and hence the non-Oberbeck–Boussinesq effect on Nu is very small for the flow considered.

With respect to the scaling with Ra we provide figure 4.6b where we find a power-law fit of

$$Nu = 0.178 Ra^{0.301} , \quad (4.26)$$

over 1.25 decades of Ra . Again, although the explored parameter space could be considered limited, what is of interest here is the excellent agreement with the exponent of Niemala *et al.* [82] who obtained $Nu = 0.124 Ra^{0.309}$ for turbulent RBC. As Nu is a measure of the total (convective plus diffusive) heat transfer to diffusive heat transfer, the increased prefactor in our scaling is a result of the reduced number of hydrodynamic boundary layers present [95].

Verzicco [96] looked at turbulent RBC between two free boundaries and two rigid walls. Therein, it was found that the heat transfer in the flow with the free-slip boundary conditions was twice as large as that of the analogous flow with no-slip velocity

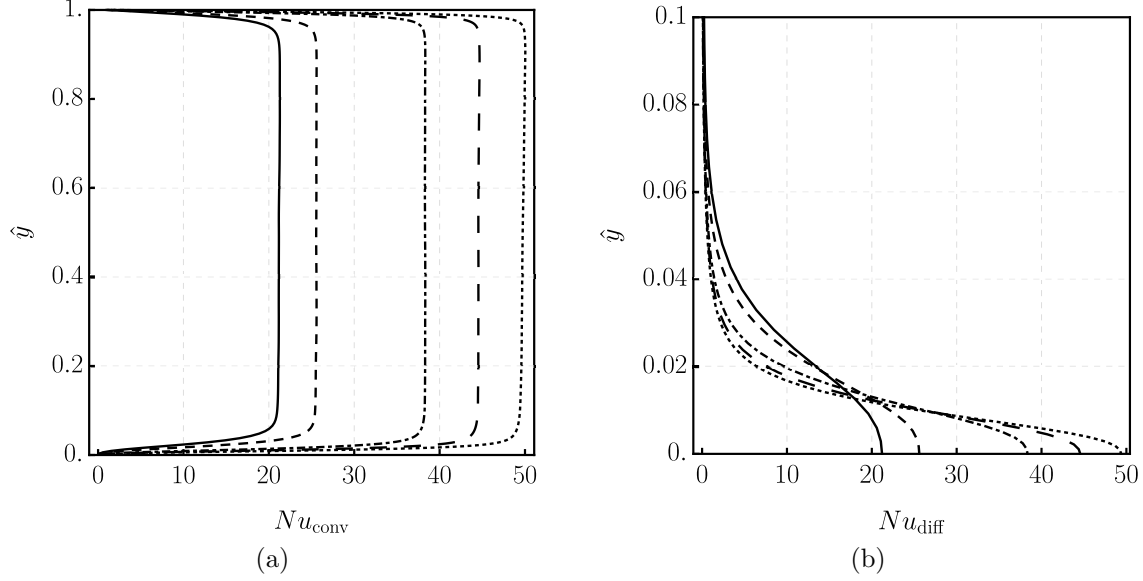


Figure 4.7: Plots of the time- and area-averaged components of Nu_y . (a) Nu_{conv} across the vertical direction and (b) Nu_{diff} zoom on lower boundary. The legend is as follows: $Ra = 7.5 \times 10^6$ (—), $Ra = 1.5 \times 10^7$ (---), $Ra = 5.0 \times 10^7$ (-.-.), $Ra = 9.0 \times 10^7$ (- -), and $Ra = 1.3 \times 10^8$ (.....).

boundary conditions. Nevertheless, the power-law fit gave the same exponent, that is $Nu \propto Ra^{0.3}$. Using this information, and taking the prefactor from Niemala *et al.* [82] as ~ 0.12 , we can estimate a prefactor of ~ 0.24 for the case of turbulent RBC between two free boundaries. The relation, (4.26), then fits well within these correlations, with the prefactor being about half as large again as that of Niemala *et al.* [82]. The following then provides an approximation of Nu for the different RBC configurations,

$$Nu \approx \alpha Ra^{0.3} \text{ with } \alpha = \begin{cases} 0.12 & \text{RBC between two rigid boundaries,} \\ 0.18 & \text{Current thermal configuration,} \\ 0.24 & \text{RBC between two free boundaries.} \end{cases} \quad (4.27)$$

4.6.2 Flow statistics

In this section, we compare vertical profiles of time- and area-averaged flow fields. For comparison against the more general thermal convection configuration of evaporative cooling, figure 1.3a, we use the experimental references of Katsaros *et al.* [24] and Flack *et al.* [27]. Equivalently, for turbulent RBC, figure 1.3b, we use the DNS results of Kerr [68]. Finally, for comparisons against the set-up most similar to ours, we select Zikanov *et al.* [57]. In this latter paper, numerical experiments of turbulent convection driven by surface cooling were carried out in a domain with periodicity in the x and z directions.

The profiles of the rms of the velocity components are presented in figure 4.8.

Concerning the rms of the vertical velocity fluctuations, $\hat{v}_{\text{rms}}$, an almost parabolic profile is observed in figure 4.8a with zero values at the boundaries rising steeply towards a maximum in the bulk. Overall, the profiles are similar to those for the flows seen in turbulent RBC of Kerr [68] and also to those reported by Zikanov *et al.* [57], which had a shear-free upper boundary. However, contrary to the profile in Kerr [68], which simulated turbulent RBC in a periodic domain, the profile is not fully symmetric with respect to the mid-plane $\hat{y} = 0.5$. The slight asymmetry is due to stronger descending plumes than those ascending, as a result of the free surface [57]. On the other hand, we note that the free-slip condition has no significant effect on the profile of $\hat{v}_{\text{rms}}$ close to the upper boundary. This is due to the fact that the vertical velocity component prescribed at both rigid walls and free-slip boundaries is zero.

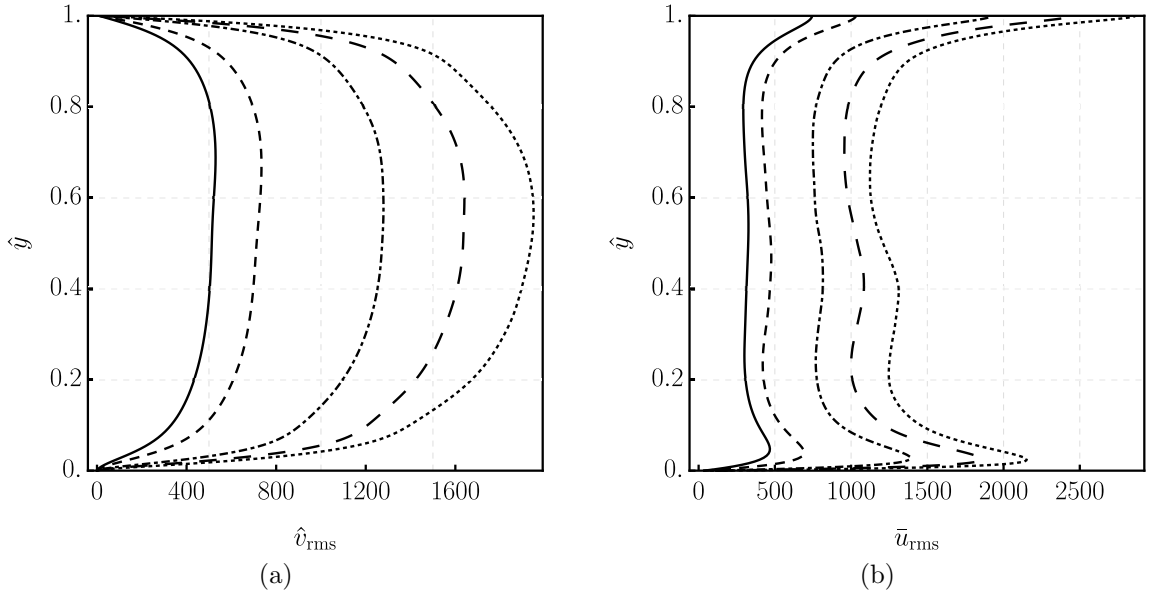


Figure 4.8: Plots of the rms of velocity fluctuations across the vertical direction: (a) rms of vertical velocity fluctuations, $\hat{v}_{\text{rms}}$, (b) rms of in-plane velocity fluctuations, $\bar{u}_{\text{rms}}$. The velocities have been made dimensionless using κ_{ref}/H . The legend is as follows: $Ra = 7.5 \times 10^6$ (—), $Ra = 1.5 \times 10^7$ (---), $Ra = 5.0 \times 10^7$ (-.-.), $Ra = 9.0 \times 10^7$ (- - -), and $Ra = 1.3 \times 10^8$ (.....).

In figure 4.8b we observe the profile of the fluctuating component of the in-plane velocity defined as follows,

$$\bar{u}_{\text{rms}} = \sqrt{\langle \hat{u}'^2 + \hat{w}'^2 \rangle_{xz}}. \quad (4.28)$$

There is a clear asymmetry observed in the profile of the rms of in-plane velocity fluctuations, where a hydrodynamic boundary layer is visible near the lower wall only. The shear-free upper boundary results in the maximum in-plane velocity being found at the surface, in line with figure 4.2b showing the presence of strong surface currents. This observation has also been made experimentally by Flack *et al.* [27] investigating turbulent structures in evaporative cooling. The near-flat bulk profile observed in the current configuration is different to the bulk profile seen by Kerr [68] and later Zikanov

et al. [57], where both noted a characteristic dip in the bulk. This feature of our configuration is attributed to the container geometry, with its side-wall boundaries leading to the formation of the counter-rotating vortical cells seen in figure 4.3b. This flow structure results in higher values for the rms of in-plane velocity fluctuations in the bulk. In fact, the maximum bulk value seen in figure 4.8b corresponds to the vertical position at which the counter-rotating vortical cells interact, $\hat{y}_{r3} = \hat{y}_{r4}$, provided in the last column of table 4.10.

The hydrodynamic boundary layer created by the shear of the large-scale circulation has a height, $\hat{\delta}_u$. According to Kerr [68] and Xin and Xia [105] this height can be estimated from the local peak in $\bar{u}_{\text{rms}}$, for which we provide values in table 4.9. It is confirmed that, at the lower boundary, the hydrodynamic boundary layer is substantially thicker than the thermal one, as expected for $Pr > 1$. Further, as a result of the increasing shear generated by the LSC, $\hat{\delta}_u$ is negatively correlated with Ra .

The profiles of the mean normalised temperatures are presented in figure 4.9, with the insets showing the boundary layers at the upper boundary and lower wall. We first observe that the normalised temperature in the bulk (or centre) of the flow, $\hat{\theta}_{\text{ctr}}$, is smaller than the reference (or mean), $\hat{\theta}_{\text{ref}} = (\hat{\theta}_{\text{int}} + \hat{\theta}_{\text{low}})/2 = 0$. In other words, the mean temperature profile is shifted towards the temperature of the cold upper boundary. Conversely, Ahlers *et al.* [75] showed that with water as the working fluid, the non-Oberbeck–Boussinesq effect in turbulent RBC results in $\hat{\theta}_{\text{ctr}} > \hat{\theta}_{\text{ref}}$. That is, if variable thermodynamic properties are taken into account in turbulent RBC, the result is a mean bulk temperature shifted towards that at the hotter lower wall.

These two statements taken together suggest that the free-slip and non-Oberbeck–Boussinesq effects are competing with the former being dominant. A similar observation was made in section 3.4.1.3 for flows with a shear-free boundary under non-Oberbeck Boussinesq conditions but with a fixed upper boundary temperature. We can therefore confirm that a shear-free upper boundary plays an important role in the thermal mixing in the pool, irrespective of whether the upper boundary temperature is fixed or spatially-variable. Further, the temperature drop from the bulk to the interface, ΔT_u , is shown to be 45% smaller than the temperature drop between the lower wall and the bulk, ΔT_l . This observation merits future experimental validation.

The rms plots of the normalised temperature fluctuations, $\hat{\theta}_{\text{rms}}$, are provided in figure 4.10. The observed profile shows a single peak at the lower wall, a minimum value in the bulk and a maximum at the upper boundary. This profile is in contrast to turbulent RBC, and indeed to the results from the previous chapter, where fixed temperature boundary conditions ensure zero $\hat{\theta}_{\text{rms}}$ values *at* the boundaries, and maximums defining the thermal boundary layer heights are found in the top and bottom near-wall regions. In our configuration, at the lower wall, the thermal boundary layer is contained within its hydrodynamic equivalent.

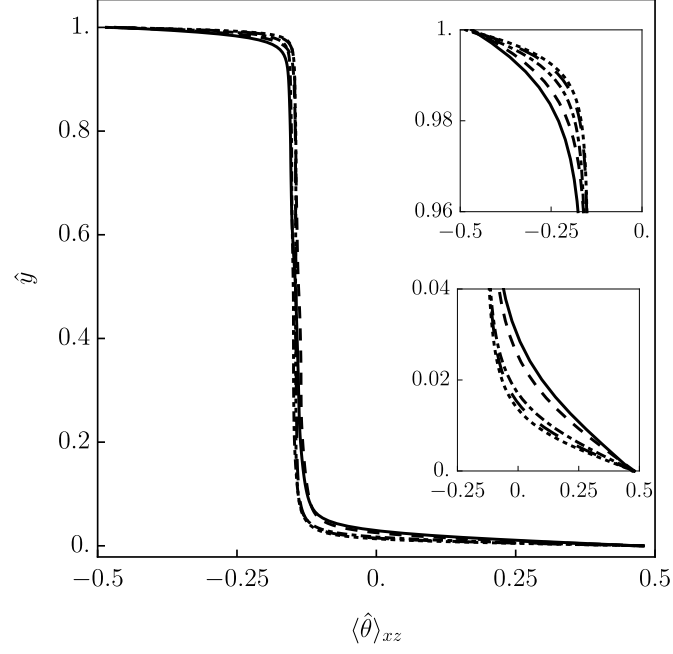


Figure 4.9: Plots of the mean normalised temperature, $\langle \hat{\theta} \rangle_{xz}$, across the vertical direction. The top and bottom insets are zooms on the upper and lower boundaries, respectively. The legend is as follows: $Ra = 7.5 \times 10^6$ (—), $Ra = 1.5 \times 10^7$ (---), $Ra = 5.0 \times 10^7$ (-.-.), $Ra = 9.0 \times 10^7$ (- -), and $Ra = 1.3 \times 10^8$ (.....).

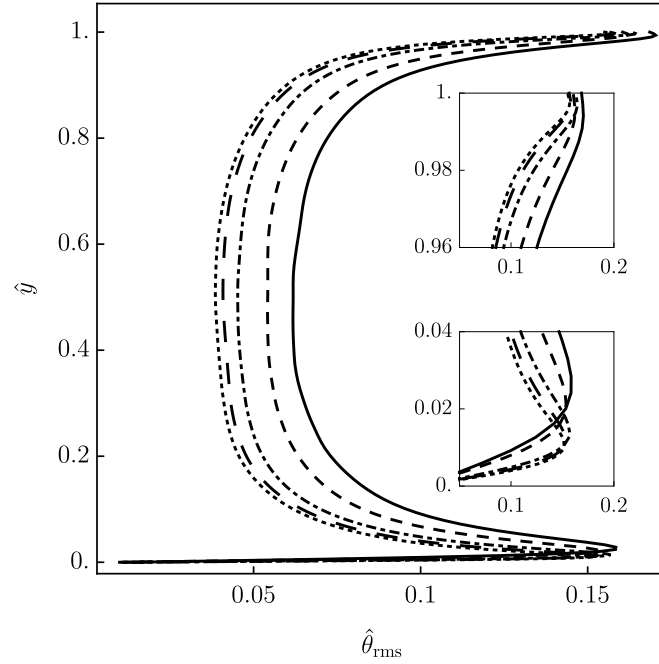


Figure 4.10: Plots of the rms of the normalised temperature fluctuations, $\hat{\theta}_{rms}$, across the vertical direction. The top and bottom insets are zooms on the upper and lower boundaries, respectively. The legend is as follows: $Ra = 7.5 \times 10^6$ (—), $Ra = 1.5 \times 10^7$ (---), $Ra = 5.0 \times 10^7$ (-.-.), $Ra = 9.0 \times 10^7$ (- -), and $Ra = 1.3 \times 10^8$ (.....).

Within the thermal boundary layer, the rms of the temperature fluctuations increase

with distance from the lower wall, as a result of the velocity fluctuations also increasing and more effectively stirring the fluid. The dip in the bulk is due to the ejected plumes losing their temperature contrast with the core fluid as they move through the domain [106]. The maximum $\hat{\theta}_{\text{rms}}$ at the shear free boundary can be explained by the peak in $\bar{u}_{\text{rms}}$ at the same location; water is increasingly stirred up to the interface.

We denote by $\hat{\delta}_{\theta_{\text{low}}}$ and $\hat{\delta}_{\theta_{\text{int}}}$ the thermal boundary layer heights at the hot wall and cold interface, respectively. The height of the thermal boundary layer on the lower wall can be defined as the location of the local peak in temperature variance [68]. We then readily find $\hat{\delta}_{\theta_{\text{low}}}$ from figure 4.10 and provide values in table 4.9. We observe, however, that the maximum $\hat{\theta}_{\text{rms}}$ across the vertical direction appears *at* the upper boundary; we must then estimate $\hat{\delta}_{\theta_{\text{int}}}$ by another means. An alternative method is proposed by Katsaros *et al.* [24], where the thermal boundary layer height at an evaporating interface is defined as follows,

$$\delta_{\theta_{\text{int}}} = -\lambda_w \frac{T_{\text{int}} - T_{\text{bulk}}}{\dot{q}_{\text{tot}}''}, \quad (4.29)$$

with $\dot{q}_{\text{tot}}''$ as the total heat flux, i.e. the sum of the convective and latent contributions, applied at the interface and λ_w as the thermal conductivity of water at the interface. Note that this quantity is calculated from equation (4.2) and the rounded values of $\overline{\partial T / \partial y}|_w$ from table 4.5. The dimensional T_{bulk} is interpreted from figure 4.9 and we provide values for $\hat{\delta}_{\theta_{\text{int}}}$ in table 4.9. A similar approach is used in the turbulent RBC literature for calculating a boundary layer thickness scale based on the local temperature gradients at the hot and cold walls [71, 75, 104].

We next focus on the inhomogeneities between the upper and lower thermal boundary layers. In particular, $\hat{\delta}_{\theta_{\text{low}}}$ is larger than $\hat{\delta}_{\theta_{\text{int}}}$, in accordance with the observations made regarding the vertical mean temperature profile. This observation was also made in section 3.4.2.2 but for a fixed temperature upper boundary, as opposed to the spatially-variable interface temperature investigated here. A similar result was also found in Verzicco [96], where the thermal boundary layer heights in free-boundary turbulent RBC were always smaller than their rigid boundary simulation counterparts.

We attribute the inhomogeneities to the presence of the shear-free boundary. Sun *et al.* [20] state that the thermal boundary layers in turbulent RBC are not isolated from but modified (and stabilised) by the viscous shear of the LSC. This same shear also produces the hydrodynamic boundary layers which are dynamically coupled to their thermal equivalents. The asymmetry introduced by the differing hydrodynamic boundary conditions results in an asymmetric LSC whose modifying (and stabilizing) capacity on the thermal boundary layers is, of course, impacted. The thinner thermal boundary layer above is therefore a result of the increase in LSC velocity. Further, and with similar reasoning, the thermal boundary layer thinning effect with increasing Ra

is confirmed from table 4.9.

We also provide in table 4.9 the estimation for thermal boundary layer heights in RBC between two rigid plates, $\frac{1}{2Nu}$, which assumes symmetry between the upper and lower boundaries. We find that despite the asymmetry introduced by the shear-free surface, the relation $(\hat{\delta}_{\theta_{\text{low}}} + \hat{\delta}_{\theta_{\text{int}}}) \approx \frac{1}{Nu}$ still holds.

In terms of third-order statistics we provide in figure 4.11 the skewness of the normalised temperature,

$$\hat{S}_\theta = \frac{\langle \hat{\theta}^3 \rangle_{xz}}{\hat{\theta}_{\text{rms}}^3}. \quad (4.30)$$

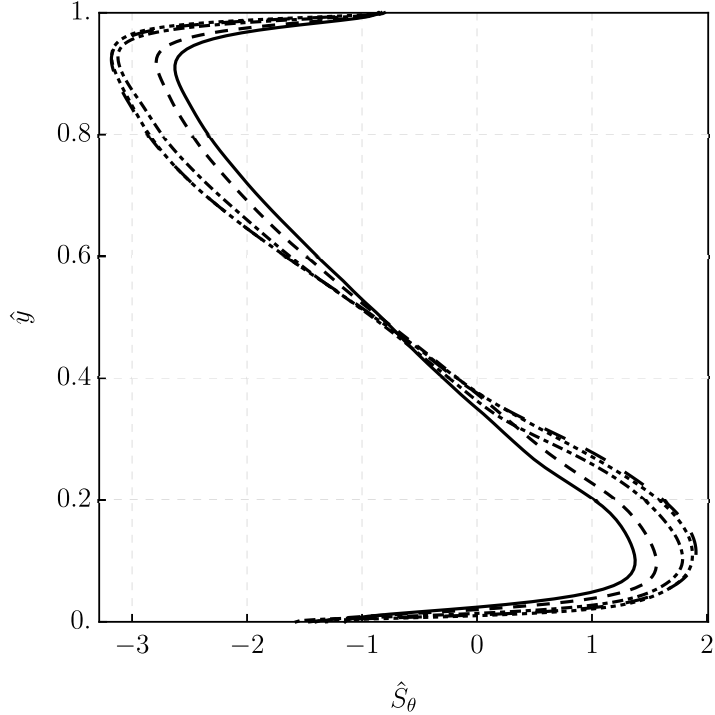


Figure 4.11: Plots of the normalised temperature skewness, $\hat{S}_\theta$, across the vertical direction. The legend is as follows: $Ra = 7.5 \times 10^6$ (—), $Ra = 1.5 \times 10^7$ (---), $Ra = 5.0 \times 10^7$ (-.-.), $Ra = 9.0 \times 10^7$ (- -), and $Ra = 1.3 \times 10^8$ (.....).

We observe a negative skewness profile near the lower wall inside the thermal boundary layer turning positive just outside, similar to that seen in turbulent RBC [19]. There is then a change in sign at $\hat{y} \approx 0.4$ and contrary to the situation at the lower wall, the upper boundary skewness is never positive. This is in contrast to turbulent RBC between rigid plates where the profile is symmetric and where the change in sign occurs at the mid-height, i.e. $\hat{y} = 0.5$ [68]. The uniquely negative skewness underneath the evaporating surface is a feature of evaporative cooling and seen experimentally in Katsaros *et al.* [24]. Further, the predominantly negative skewness profile represents more intense and frequent plume formation at the shear-free surface, which then travel in the negative direction, similar to the observation reported by Zikanov *et al.* [57]. In

summary, the skewness profile in figure 4.11 shows unique traits of the current turbulent convection configuration, which borrows characteristics from both turbulent RBC and evaporative cooling.

4.7 Conclusions

In this chapter, direct numerical simulations have been carried out of a thermal convection set-up with similarities to both turbulent Rayleigh-Bénard convection and evaporative cooling. The flow is a simplified model of the water-side thermal mixing occurring beneath an air-water interface during high temperature evaporation of spent-fuel pools.

Five cases have been evaluated with the heat fluxes applied at the upper boundary approximating the evaporative heat loss. For the geometry chosen, a sixteenfold increase in evaporation rate induces a 1.25 decade change in Rayleigh number for the convective flow beneath the interface. For each case investigated, the time-averaged temperature at the upper boundary has significant spatial variation, but the time- and area-averaged value matches well with the predicted temperatures corresponding to the prescribed heat fluxes.

The upper boundary is also shear-free and as such, is an approximation of a free surface. One consequence of the free slip at the upper boundary is the asymmetric large-scale circulation. The large-scale circulation impinges the upper surface near one corner, where it is subsequently accelerated, suggesting the presence of strong surface currents, before falling back down in the opposite corner. This acceleration leads to inhomogeneous recirculation zones in the cubic geometry, which become taller and thinner with increasing Ra . As a result, the structure of the large-scale circulation is effected by the presence of the free surface.

Another impact of the shear-free surface is an increase in convective heat transfer, Nu . The provided power-law fit for this novel configuration, $Nu = 0.178Ra^{0.301}$, shows a similar exponent to turbulent RBC but with an increased prefactor due to the reduced number of hydrodynamic boundary layers. Our definition of Nu takes into account the variable density and thermal conductivity, however, these thermodynamic properties vary by a maximum of only 1% and 2% respectively and hence the non-Oberbeck-Boussinesq effect on Nu is very small for the flow considered.

Further, a shear-free upper boundary is shown to introduce inhomogeneities in the heights of thermal boundary layers between the lower wall and upper boundary. This is in spite of taking into account the variable thermodynamic properties of water which tend to have the opposite effect. Such an observation is novel for the current set-up with a spatially-variable temperature boundary condition on the upper surface.

The modelled flow is an idealised system whereby the evaporation rate at the interface, although representative in an overall sense, is applied uniformly; the evaporation

rate is constant in time and space. For a more realistic dynamic boundary condition based on local surface temperatures, a similar time- and area-averaged interface temperature is expected to emerge and is the focus of the next chapter.

Chapter 5

Thermal convection driven by dynamic evaporation in domains of different aspect ratios

5.1 Introduction

In this chapter, we dynamically calculate the evaporation rate at the free surface and present a series of Large-Eddy Simulations of evaporation-driven turbulent thermal convection. With liquid water as the convecting fluid, a dynamically calculated inhomogeneous temperature gradient at a shear-free upper boundary serves as an approximation of an evaporating free surface. We first propose and validate an evaporation algorithm before investigating whether the aspect ratio of a cuboidal domain has an influence on large-scale circulation structure, evaporation rates, mean flow properties or statistics. Building on the previous chapter, the non-zero Neumann thermal boundary condition is calculated dynamically and locally so that there is no longer a requirement for iterative simulations.

The evaporation-driven thermal convection investigated in this chapter is again represented by figure 1.3c. However, with the spatially variable temperature and temperature gradient, we approach a modelling strategy that is much closer to reality than the two previous chapters. The evaporation-driven thermal convection here has plume formation at both the lower wall and upper free surface, hence also the presence of a LSC [91], which is an attribute shared with turbulent RBC, and a flow feature that we explore in more detail in this chapter.

Our motivation remains to better understand the combined effects of turbulent convection and free surface evaporation in the early stages of a loss-of-cooling accident in an SFP. Wherein, heat is added to the upper volume of the pool from the fuel

The results of this chapter have been published in *Phys. Fluids*, 33(1), 2021. [107].

assemblies below and free-surface evaporation is the main mode of phase change that leads to heat evacuation and water inventory loss. During an accident, an SFP will experience both low and high free-surface evaporation mass transfer regimes.

Post-Fukushima 2011, efforts have been made to create [35] and validate [36] models for predicting evaporative mass-transfer rates across the free surface in this high evaporation regime. Prior to this, most models were based on observations and measurements from nature, such as the evaporation taking place at the surface of lakes or oceans. Typically, the mass-transfer rate in these models was, inaccurately, a function of *bulk* water temperature and, accurately, a function of ambient air conditions, that is relative humidity and temperature.

One source of error, is that in reality the mass-transfer rate depends on the free-surface temperature. It has long been known that interfacial and bulk temperatures differ as a result of free-surface evaporation [108, 109], with recent research showing this difference to be substantial in the high-mass-transfer regime [30, 36]. The experimental study of Boelter et al. [29] investigated evaporation in tanks up to a maximum bulk temperature of 361.15 K, and hence under high-mass transfer conditions. Importantly however, due to limitations of the experimental techniques at the time, no distinction was made between free-surface and bulk temperatures. We utilise the more recent data [36] to validate our proposed algorithm for predicting evaporation rates at a free surface. To the authors knowledge, the algorithm presented in this chapter represents the first validated model of dynamic and local free-surface evaporation in a single-phase CFD code.

The container shape, and in particular its aspect ratio, $\Gamma = W/H$ where W is the width of the cuboidal domain, plays an important role in determining the structure of the LSC. In the literature for turbulent RBC, the LSC has previously been shown to be either in a single-roll, dual-roll or transitory state. In the single-roll state, the LSC occupies the entirety of the domain as we observed in the previous chapter, whereas under certain Ra , Pr and Γ conditions, the single-roll breaks down into a dual-roll state. In turbulent RBC in a cylinder, this latter state resembles one unit-aspect-ratio recirculation roll, stacked on top of another counter-rotating one[16]. One explanation for this breakdown is that the LSC is driven by plumes of the same size as the thermal boundary layers. As Ra is increased, this thickness decreases and eventually a critical Ra exists, for a given Γ and Pr , whereby hot plumes emitted from the lower wall become so thin and elongated that they lose their excess heat, and thus buoyancy, to the bulk fluid before reaching the cool upper boundary. At such a point the LSC sinks somewhere in the middle of the domain in order to regain heat from the lower wall [110]. The opposite is true if the starting point is considered as the cool upper boundary and we focus instead on the cold plumes.

In this chapter, we fix the upper boundary surface area, so that the depth equals

the width, and vary the aspect ratio via the height. In cuboidal domains of aspect ratio $\Gamma = 1$, and seemingly over a large range of Pr , the single-roll state of the LSC is dominant in thermal convection flows [66, 91, 94]. With respect to turbulent RBC in cylindrical domains of aspect ratio $\Gamma = 1/2$ and with water as the working fluid, the single-roll state is again dominant, whereas the dual-roll state is observed only as a transitory state, such as during a reorientation event. In Xi and Xia [111] it was shown that the most likely state of the LSC for aspect ratios $\Gamma = 1$ and $1/2$ is the a single-roll state, where it exists for $\sim 90\%$ and $\sim 70\%$ of the time, respectively. On the other hand, at still smaller aspect ratios, specifically $\Gamma = 1/3$, the single-roll state was shown to be present $\sim 25\%$ of the time. For the remainder, the LSC is in transition to, or actually occupying the dual-roll state. This trend suggests that any further decrease in Γ is likely to reduce further the likelihood of the single-roll state.

The single-roll state has been shown to be marginally more efficient for heat transfer than the dual-roll equivalent [111, 112] when working in 3D geometries and with water as the working fluid. Although the difference is limited to a few percent in domains of aspect ratio $\Gamma = 1/2$ at high Ra [113, 114]. In this chapter, we investigate the role played by the aspect ratio on the LSC state, evaporation rates, mean flow properties and statistics. To the best of our knowledge, this work is the first study of its kind to assess the aforementioned subjects in slender 3D cuboidal geometries.

The rest of the chapter is structured as follows: in section 5.2, we outline the governing equations and the subgrid-scale modelling. In section 5.3, we provide the algorithm for calculating the temperature gradient at the upper boundary based on evaporative heat losses. Next, in section 5.4 we present the numerical set-up and resolution criteria. In section 5.6 we present the results, where we first focus on the validation process. Therein, the evaporation model predictions are compared with experimental results, before comparing the flow statistics from a direct numerical and a large-eddy simulation at moderate Ra . We then present a study of the aspect ratio before drawing conclusions in section 5.7.

5.2 Numerical set-up

We again consider only the flow beneath the evaporating surface, as such the working fluid is again liquid water, treated as Newtonian. In this chapter, we carry out Large-Eddy Simulations of variable density flows. Hence, the system of governing equations is the Favre filtered low-Mach number approximation of the compressible NSF equations [38, 40], (2.25)–(2.27). Furthermore, in this chapter, the domain is considered open to atmosphere so that p_0 is constant and equal to the ambient pressure. We add that mass loss due to evaporation is not modelled and consequently the surface level is constant throughout.

In order to close the system of governing equations, an isobaric equation of state for the water density is required. More specifically, a $\bar{\rho}$ - $\tilde{T}$ relation is introduced. This relation is a fourth-order polynomial fit, see (2.6), of tabulated data for water density at the ambient pressure and over the temperature range of interest [43]. The other fluid thermodynamic properties, λ and μ are also calculated from a quartic polynomial fit, with data originating from the same reference. For certain simulations with large ΔT , the dynamic viscosity and the thermal conductivity can vary considerably. On the other hand, c_p variations are negligible and it is taken as a constant, case-dependent, value in all simulations. We provide an example set of coefficients for the fits of ρ/p_0 , λ and μ in table 5.1, for the highest evaporation case at $Ra = 1.3 \times 10^8$.

	c_4	c_3	c_2	c_1	c_0
ρ/p_0	-3.93×10^{-13}	6.07×10^{-10}	-3.74×10^{-7}	1.00×10^{-4}	2.73×10^{-4}
μ	4.19×10^{-12}	-6.38×10^{-9}	3.67×10^{-6}	-9.50×10^{-4}	9.34×10^{-2}
λ	-4.33×10^{-11}	7.34×10^{-8}	-5.26×10^{-5}	1.80×10^{-2}	-1.68

Table 5.1: Example polynomial coefficients for variable water thermodynamic properties over the temperature range of interest [43] in the $Ra = 1.3 \times 10^8$ case. We note that the c_p is set constant at 4202 J/kg/K.

For the numerical solution of (2.1)–(2.3) we employ the second-order accurate temporal and spatial discretisation schemes outlined in section 2.3.1 and for the pressure-velocity coupling the PISO-type projection method is used from section 2.3.2.

5.2.1 Sub-grid scale modelling

In this chapter, we seek the higher Rayleigh number flows pertinent to industrial applications. As a result, we adopt the LES approach, which offers a computationally cheaper alternative to fully-resolved DNS. According to it, only the large, energy containing eddies are resolved and the effects of the unresolved scales on the flow are modelled. Many LES studies of thermal convection [55–58] have used the eddy-viscosity model of Smagorinsky [59]. Wherein, the influence of the filtered-out eddies are approximated as a viscous contribution on the resolved fields. Lilly [61] extended the model, to account for the turbulence owing to buoyancy caused by the temperature gradients of the large-scale flow. The inclusion of a buoyancy production term gives (2.34) as the relation for the turbulent viscosity with the Richardson number, Ri , valid for low-Mach number flows, and given by (2.35).

In this chapter, we employ the Lagrangian dynamic model [63] adapted for variable density flows. As such, the resolved scales are used to compute C_s locally and at

each time-step. This model employs the dynamic procedure [65], where the numerator and denominator of (2.36) are averaged over streamlines. This averaging procedure therefore requires the solution of two further transport equations; see (2.37) and (2.38). Any negative viscosity is removed and the correct behaviour of C_s is found near the walls. Indeed, although some clipping is required in our simulations it is always limited to a few percent. Finally, we use the Reynolds analogy ($\lambda_t = \mu_t c_p / Pr_t$) to compute the eddy conductivity. We take Pr_t , also present in (2.34), as constant and equal to 0.4 as recommended in Eidson [55].

5.3 Evaporation model

In the previous chapter, on evaporation-driven thermal convection (see also [91]), we investigated different evaporation rates which formed the basis of a temperature gradient assigned as a non-zero Neumann boundary condition at a shear-free upper boundary. Over a series of simulations, the lower (bottom) wall temperature was then iteratively refined until the statistically stationary solution for the time- and area-averaged upper-boundary temperature matched the predicted mean value.

In what follows, we present an improved dynamic and inhomogeneous version of this evaporation model. The new algorithm removes the requirement for iterative simulations and results in significant computational savings. The non-zero Neumann thermal boundary condition is calculated at each time-step and is dependent only on the cell temperature nearest the interface and on fixed ambient conditions. Many of the equations provided below are repeated from the previous chapter for clarity. The algorithm that follows is then easier to follow for the reader.

We find both the evaporative ($\dot{q}_{\text{evap}}''$) and convective ($\dot{q}_{\text{conv}}''$) heat losses at the water-side of the interface and use them to apply a non-zero-Neumann thermal boundary condition of the following form,

$$\frac{\partial \tilde{T}}{\partial y} = \frac{1}{\lambda_{\text{int}}} (\dot{q}_{\text{conv}}'' + \dot{q}_{\text{evap}}'') = \frac{1}{\lambda_{\text{int}}} (\dot{q}_{\text{conv}}'' + \dot{m}'' h_{\text{lv}}), \quad (5.1)$$

where $\dot{m}''$ is the evaporative mass flux, h_{lv} is the latent heat of evaporation, and $\lambda_{\text{int}} \partial \tilde{T} / \partial y$ is the heat flux at the water-side of the interface, with λ_{int} as the thermal conductivity of water at T_{int} .

Beginning with the evaporative heat losses, the first step in finding $\dot{m}''$ is to fix the gas-side conditions, where we use the same values from the previous chapter. Table 4.2 then provides the temperature (T_∞), ambient pressure (p_0) and relative humidity at a distance far from the interface.

The water vapour partial pressure, $p_{v,\infty}$, is calculated from a Wagner equation [97]

of the following form,

$$p_v = p_c \exp((a\tau + b\tau^{1.5} + c\tau^3 + d\tau^6)/T_r), \quad (5.2)$$

where p_c and T_c are respectively the critical pressure and temperature, $T_r = \tilde{T}/T_c$ is the reduced temperature and $\tau = 1 - T_r$, with the constants available in the literature [115]. The vapour mass fraction far from the interface, $Y_{v,\infty}$, is then found from,

$$Y_v = \frac{p_v M_w}{p_v M_w + (p_0 - p_v) M_a}, \quad (5.3)$$

where M_w and M_a are respectively the molar masses of water and air. Assuming a binary mixture of water vapour and air, the mass fraction of air far from the interface is then equal to $1 - Y_{v,\infty}$. The gaseous mixture density far from the interface, ρ_∞ , is calculated from the ideal-gas equation of state,

$$\rho_g = \frac{M_w p_v}{RT} + \frac{M_a (p_0 - p_v)}{RT}, \quad (5.4)$$

where ρ_g is the gaseous mixture density, $R = 8314 \text{ J/kmol/K}$ is the universal gas constant and T is the relevant temperature.

Equivalently, we find the conditions *at* the interface; this requires the local T_{int} , from which we find the local properties of saturation pressure, $p_{v,\text{int}}$, the vapour mass fraction, $Y_{v,\text{int}}$, and mixture density, ρ_{int} , all calculated in the same manner as above.

Transition from the interface conditions to those far away is assumed to occur over a layer of finite thickness, or a *film*. Film properties are estimated from mean values of the interface and those at ∞ . The quantities ρ_f and μ_f representing respectively the *film* density and dynamic viscosity are required. This latter quantity is found from the kinetic theory of gases assuming a two-component mixture [98],

$$\mu_f = \sum_{i=1}^2 \frac{x_i \mu_i}{x_1 \phi_{i1} + x_2 \phi_{i2}}, \quad (5.5)$$

with

$$\phi_{ij} = \frac{[1 + (\mu_i/\mu_j)^{1/2} (M_j/M_i)^{1/4}]^2}{\sqrt{8} [1 + (M_i/M_j)]^{1/2}}. \quad (5.6)$$

where x_i is the molar fraction of component i and values for air and vapour dynamic viscosities are found from polynomial fits. The film kinematic viscosity, ν_f is then inferred from the above quantities. On the other hand, the film mass diffusivity for the

binary mixture of air and vapour, D_f , is found from [100],

$$D_f = 1.87 \times 10^{-10} \frac{T_f^{2.072}}{p_0} \left(\frac{\text{m}^2}{\text{s}} \right), \quad (5.7)$$

where the thermodynamic pressure, p_0 , is in units of atmospheres, i.e. equal to 1 atm. The film diffusion coefficients are used to find the Schmidt number, Sc_f , and we evaluate the concentration Rayleigh number, Ra_c , as

$$Ra_c = \frac{|\mathbf{g}| (\rho_\infty - \rho_{\text{int}}) W^3}{D_f \mu_f}, \quad (5.8)$$

with W being the characteristic length-scale, the width of the domain. We again use a Sherwood number, Sh , correlation for natural convection flows [30], to find the concentration boundary layer height, δ_c ,

$$Sh = 0.23 Sc_f^{\frac{1}{3}} Ra_c^{0.321} \approx \frac{W}{\delta_c}. \quad (5.9)$$

The mass flux can then be estimated from [101],

$$\dot{m}'' = \frac{\rho_f D_f}{\delta_c} \log(1 + B_m), \quad (5.10)$$

with the mass transfer driving force, B_m , defined as

$$B_m = \left(\frac{Y_{v,\infty} - Y_{v,\text{int}}}{Y_{v,\text{int}} - 1} \right). \quad (5.11)$$

Substituting (5.9) into (5.10) gives the final mass flux relation,

$$\dot{m}'' = Sh \frac{\rho_f D_f}{W} \log(1 + B_m). \quad (5.12)$$

Finally, we find h_{lv} from a Watson relation [116],

$$h_{\text{lv}} = 2256.4 \left(\frac{T_c - T_{\text{int}}}{T_c - 373.15} \right)^n \quad (5.13)$$

with the exponent $n = 0.283$.

Next, we concentrate on the convective heat losses away from the free-surface. We estimate this by assuming that heat transfer away from the interface is proportional to the difference between the temperature of the interface, T_{int} , and the ambient gas-side temperature, T_∞ , with the heat transfer coefficient, h , as the proportionality coefficient. Overall we have the following,

$$\dot{q}_{\text{conv}}'' = h (T_{\text{int}} - T_\infty), \quad (5.14)$$

where h is estimated from the following correlation for a horizontal flat surface, warmer than the ambient air above [102],

$$\frac{h}{\lambda_f} W = Nu_t = 0.54 Ra_t^{0.25}. \quad (5.15)$$

In the above relation we obtain λ_f in an equivalent manner [99] to μ_f from (5.5). The film thermal diffusivity, κ_f is again found from aforementioned quantities, and we define Ra_t as the gas-side thermal Rayleigh number,

$$Ra_t = \frac{|\mathbf{g}|\beta_\infty (T_{\text{int}} - T_\infty) W^3}{\kappa_f \nu_f}. \quad (5.16)$$

Regarding the initial conditions, the water is quiescent and a linear temperature profile from T_{low} to a first approximation of T_{int} (from previous simulations [91]) is imposed across the vertical direction. At the first time-step, the temperature gradient at the upper boundary is assumed to be zero, that is $\partial \tilde{T} / \partial y = 0$, so that the boundary faces have the same value as their cell-centre neighbour. A flowchart for the above algorithm which finds the temperature gradient at the upper boundary for the following time-step, $\left. \frac{\partial \tilde{T}}{\partial y} \right|^{n+1}$, is provided as figure 5.1.

The thermal boundary conditions for the simulations in the cubic ($\Gamma = 1$) domain are presented in table 5.2. The given T_{low} is fixed, whereas the remaining columns are the values from the statistically stationary solution. For the study of the aspect ratio in section 5.6.2 we use the same T_{low} as in the highest evaporation case in cubic ($\Gamma = 1$) domain, that is LES5. We then assess the influence, or lack thereof, of the aspect ratio on the other values. The lowest and highest Ra , which are here representative of low and high mass transfer regimes, correspond to temperature drops across the domain of approximately 3 K and 13 K respectively. With this temperature drop occurring over two thermal boundary layers, one can infer the large discrepancy between bulk and interface temperatures at high evaporation rates discussed in the Introduction.

5.4 Boundary conditions

Before elaborating on the remaining details of the numerical set-up we first provide nondimensionalisation reference values in tables 5.3 and 5.4. The reference velocity is the free-fall velocity, $U_{\text{ff}} = \sqrt{|\mathbf{g}|H\beta_{\text{ref}}\Delta T}$, from which the reference free-fall time is found, $t_{\text{ff}} = H/U_{\text{ff}}$. Further, the reference temperature, T_{ref} , is the mean of the lower wall and (time- and area-averaged) interface temperatures, with all reference properties then relative to T_{ref} . With this in mind, the normalised temperature is defined as,

$$\hat{\theta} = (\tilde{T} - T_{\text{ref}}) / \Delta T, \quad (5.17)$$

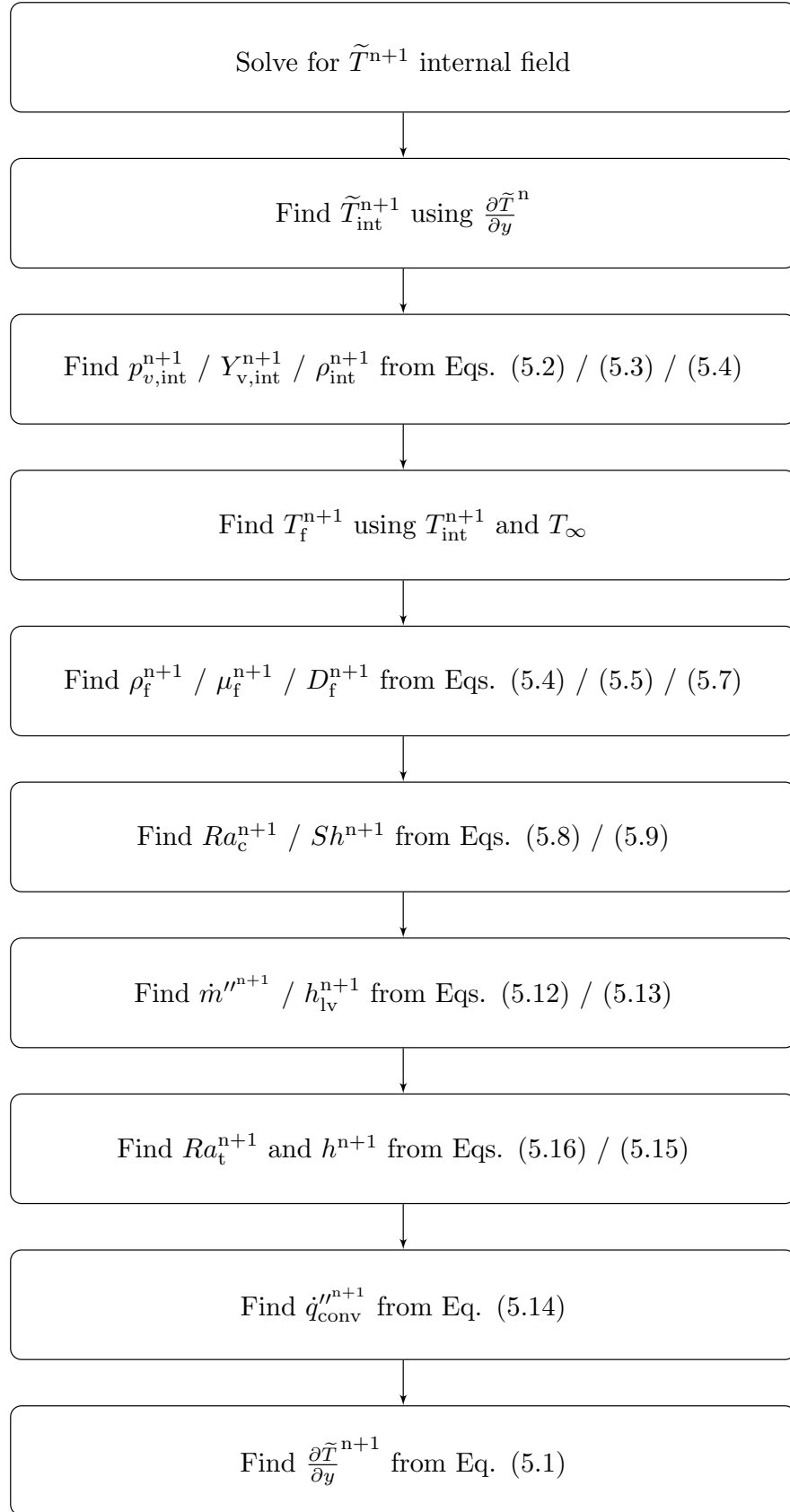


Figure 5.1: A flowchart of the free-surface evaporation algorithm.

Case	Ra	T_{low} (K)	$\frac{\partial \tilde{T}}{\partial y}$ ($\frac{\text{K}}{\text{m}}$)	T_{int} (K)	$\dot{m}''$ (g/s/m ²)
DNS1	1.2×10^7	320.95	-1555	318.20	0.36
LES1	1.2×10^7	320.95	-1550	318.05	0.36
LES2	3.1×10^7	335.15	-3480	330.15	0.86
LES3	5.1×10^7	345.15	-5670	338.25	1.46
LES4	8.4×10^7	355.15	-8875	345.75	2.36
LES5	1.3×10^8	365.65	-13725	352.95	3.77

Table 5.2: Thermal boundary conditions for the simulations of the cubic ($\Gamma = 1$) domain. In this table, T_{low} is the fixed lower wall temperature, and $\partial \tilde{T} / \partial y$, T_{int} and $\dot{m}''$ are respectively the time- and area-averaged temperature gradient, temperature and evaporative mass flux at the upper boundary. For all cases the time- and area-averaged normalised interface temperature, $\langle \hat{\theta}_{\text{int}} \rangle_{xz} = -0.5$.

and the Rayleigh number, found from the reference values as,

$$Ra = \frac{g \beta_{\text{ref}} (T_{\text{low}} - T_{\text{int}}) H^3}{\nu_{\text{ref}} \kappa_{\text{ref}}} . \quad (5.18)$$

Case	Γ	Ra	U_{ff} ($\frac{\text{m}}{\text{s}}$)	ΔT (K)	T_{ref} (K)	ρ_{ref} ($\frac{\text{kg}}{\text{m}^3}$)	$\beta_{\text{ref}} \times 10^{-4}$ ($\frac{1}{\text{K}}$)	$\nu_{\text{ref}} \times 10^{-7}$ ($\frac{\text{m}^2}{\text{s}}$)	$\kappa_{\text{ref}} \times 10^{-7}$ ($\frac{\text{m}^2}{\text{s}}$)	Pr_{ref}
LES1	1	1.2×10^7	0.023	2.9	319.5	989.6	4.3	5.84	1.54	3.8
LES2	1	3.1×10^7	0.034	5.0	332.6	983.5	5.1	4.76	1.5	3.0
LES3	1	5.1×10^7	0.041	6.9	341.7	978.6	5.6	4.20	1.61	2.6
LES4	1	8.4×10^7	0.051	9.4	350.5	973.5	6.1	3.75	1.63	2.3
LES5	1	1.3×10^8	0.060	12.7	359.3	967.9	6.5	3.40	1.65	2.1

Table 5.3: Nondimensionalisation reference values for the cubic ($\Gamma = 1$) domain. In this table, Ra is increased between simulations via the thermal boundary conditions. The reference length for all cases in the above table is the height of the domain, $H = 0.045\text{m}$. The nondimensionalisation reference values for the DNS are not provided as they are equal to those for LES1.

The current configuration differs from a turbulent RBC set-up in its upper hydrodynamic and thermal boundary conditions. The lower wall is located at $\hat{y} = 0$, the upper boundary at $\hat{y} = 1$ and, likewise, the side walls at $\hat{x} = 0$ ($\hat{z} = 0$) and $\hat{x} = 1$ ($\hat{z} = 1$). No-slip velocity boundary conditions are enforced at the side and lower walls. The free-slip condition is prescribed at the upper boundary, so that $\frac{\partial \hat{u}}{\partial \hat{y}} = \frac{\partial \hat{w}}{\partial \hat{y}} = 0$ and $\hat{v} = 0$ at $\hat{y} = 1$. This acts as a first order approximation of a free surface. For the thermal boundary conditions we have adiabatic side-walls with $\frac{\partial \hat{\theta}}{\partial \hat{x}}$ prescribed. At

Case	Ra	Γ	H (m)	$U_{ff} \left(\frac{m}{s} \right)$
LES5	1.3×10^8	1	0.045	0.060
LES6	1.1×10^9	1/2	0.09	0.086
LES7	8.8×10^9	1/4	0.18	0.120

Table 5.4: Nondimensionalisation reference values for the study of the aspect ratio. For all cases in this table, T_{low} is the same as that of LES5 (see table 5.2) and Ra is increased between simulations via the height of the domain. In table 5.7, we provide the remaining thermal boundary conditions for LES5–LES7, where we see that they remain steady as Ra is increased (aspect ratio is decreased).

$\hat{y} = 0$ we set $\hat{\theta} = 0.5$ as a Dirichlet boundary condition, whereas at $\hat{y} = 1$ we calculate and prescribe at each time step the non-zero Neumann condition explained in detail in section 5.3. For completeness, the statistically stationary dimensionless temperature gradients at the interface for LES1–LES5 are 24.1, 31.3, 37.0, 41.6 and 49.0. Similarly, for the aspect ratio study the equivalent values for LES6 and LES7 are 94.9 and 180.7; the increase being due to the change in the height of the domain.

As a result of the aforementioned boundary conditions, five hydrodynamic boundary layers exist, one at each of the vertical side walls and one at the lower wall. On the other hand, there are only two thermal boundary layers, at the cooled upper boundary and heated lower wall.

5.5 Resolution criteria

In this section, we present the resolution criteria for the fully resolved DNS and the LES. The accuracy of a DNS is ensured only when the smallest length scales of the flow are everywhere resolved. The first criterion is therefore to ensure adequate resolution of the hydrodynamic and thermal boundary layers in the vertical direction. Here, we use the criterion based on the Prandtl-Blasius boundary layer theory [77], which assumes the boundary layers to be laminar at the Ra investigated herein. The number of cells in the hydrodynamic, N_u , and the thermal, N_θ , boundary layers for all simulations are provided in table 5.5 with the numbers inside the parentheses representing the minimum requirements and those outside the true values. We note that the boundary layers are over-resolved by a factor of three for the DNS, whereas only the minimum requirements are met for the LES. We use a hyperbolic tangent expansion function to cluster cells near the walls and expand into the bulk.

The second criterion is the maximum cell size in the bulk of the domain. Here, we assume homogenous isotropic turbulence exists away from the walls and that, for the

DNS, all eddies down to the Kolmogorov length-scale, η , must be resolved. On the basis of the discussion in chapter 3, and for fluids with $Pr > 1$, which is the case in all simulations investigated here, the temperature microscale, η_θ , is limiting. With respect to the DNS we therefore ensure that all cells are smaller than the *a priori* estimation of the temperature microscale given as follows [71, 78],

$$\Delta \leq \pi \eta_\theta \approx \pi H \left(\frac{1}{Ra Pr Nu} \right)^{0.25}. \quad (5.19)$$

Clearly we require an estimation of the global Nusselt number, Nu , for (5.19). To this end we first define a local Nusselt number, Nu_y , as the sum of convective, diffusive and turbulent contributions as follows,

$$Nu_y = \underbrace{\sqrt{Ra Pr} \langle \hat{\rho} \hat{v} \hat{\theta} \rangle_{xz}}_{Nu_{\text{conv}}} - \underbrace{\langle \hat{\lambda} \frac{\partial \hat{\theta}}{\partial \hat{y}} \rangle_{xz}}_{Nu_{\text{diff}}} - \underbrace{\langle \hat{\mathbf{q}}^r \rangle_{xz}}_{Nu_{\text{turb}}}, \quad (5.20)$$

with the turbulent contribution estimated via the dimensionless version of (2.32). The global Nusselt is then defined as above except that volume-averaging is carried out, i.e. $\langle \cdot \rangle_{xyz}$. Specifically, for Nu in (5.19) we can now use the relation from the previous chapter, $Nu = 0.178 Ra^{0.301}$, based on the similar thermal configuration [91]. Thanks to this scaling, no iterative preliminary simulations are required to update the refinement, which can be a computationally expensive task.

On the other hand, the maximum cell size in the bulk for the LES is less stringent. The mesh plays the role of the filtering cut-off length, which must be in the inertial subrange. An *a priori* estimation can be found using the Taylor microscale, η_l . For isotropic turbulence this is given [79] by $\eta_l = (15 \nu \mathbf{u}^{*2} / \epsilon)^{1/2}$, where $\mathbf{u}^*$ is representative of the velocity in the bulk. Here, we use the square root of the bulk turbulent kinetic energy given as,

$$\mathbf{u}^* = \sqrt{K_{\text{bulk}}} = \sqrt{\frac{(v_{\text{rms}})_{\text{bulk}}^2 + (\bar{u}_{\text{rms}})_{\text{bulk}}^2}{2}}, \quad (5.21)$$

with $(v_{\text{rms}})_{\text{bulk}}$ as the rms of vertical velocity fluctuations in the bulk and $(\bar{u}_{\text{rms}})_{\text{bulk}}$ as the rms of the in-plane velocity fluctuations, also found in the bulk. It is noted that the rms of the in-plane velocity fluctuations is defined as

$$\bar{u}_{\text{rms}} = \sqrt{\langle u'^2 + w'^2 \rangle_{xz}}. \quad (5.22)$$

From the similar thermal convection configuration investigated in the previous chapter (see also [91]), we find the relation $(v_{\text{rms}})_{\text{bulk}} H / \kappa = 0.37 Ra^{0.454}$. Similarly, for the rms of in-plane velocity fluctuations we find the relation $(\bar{u}_{\text{rms}})_{\text{bulk}} H / \kappa = 0.16 Ra^{0.479}$. With appropriate scaling [84] for the dissipation of the turbulent kinetic energy, ϵ , the

following relation can then be used to find the Taylor microscale,

$$\eta_l = \frac{H\sqrt{15}\hat{\mathbf{u}}^*}{\sqrt{Ra(Nu-1)}}, \quad (5.23)$$

with $\hat{\mathbf{u}}^*$ now given by,

$$\hat{\mathbf{u}}^* = \frac{\mathbf{u}^*H}{\kappa} = \sqrt{0.068Ra^{0.91} + 0.012Ra^{0.96}}. \quad (5.24)$$

For all LES presented herein, the largest cell size in the bulk is defined as the smallest of either half the Taylor length-scale or a relaxed temperature microscale, taken here as $4\pi\eta_\theta$. Preliminary simulations conducted in the course of this study showed that this latter relaxed criterion in the bulk serves as a bounding value. We find that meshes with cells of size greater than $4\pi\eta_\theta$ in the bulk, that still satisfy boundary layer requirements for a wall-bounded domain, tend to demand a very large expansion and result in unacceptably high aspect ratios in near-wall cells. We present the final grid resolution criteria in table 5.5.

In order to assess the DNS refinement *a posteriori* we find the ratios of local grid spacing to the local temperature microscale with this latter quantity defined as before,

$$\eta_\theta = (\kappa^3/\epsilon)^{0.25}, \quad (5.25)$$

The maximum ratio in the domain is 0.46, as this value is smaller than unity the DNS refinement is considered as adequate. Finally, in all simulations the time-step is calculated from a Courant number of 0.25.

5.6 Numerical results

The results section is divided into two parts, with the first assessing the validity of both the LES strategy and the evaporation model. In the second part, we decrease the aspect ratio and assess the impact on the LSC state, evaporation rates, mean flow properties and flow statistics. We adopt the same notation as in the previous chapter: the mean of a generic variable ϕ is denoted by $\langle\phi\rangle$ and refers to time averaging, additional averaging over a given horizontal x - z plane is denoted by $\langle\phi\rangle_{xz}$, and over volume by $\langle\phi\rangle_{xyz}$. The fluctuating component is then denoted by ϕ' and the rms value by $\phi_{\text{rms}} = \sqrt{\langle\phi'\phi'\rangle}$.

5.6.1 Validation of the modelling approach

In this section, we focus on the cubic ($\Gamma = 1$) domain and compare flow statistics of the fully resolved DNS against an LES at a moderate $Ra = 1.2 \times 10^7$. We then compare a series of LES predictions of evaporative mass loss at the free surface against

Case	Γ	Ra	$N_x \times N_z$	N_y	N_u	N_θ	$\hat{\Delta}y_{\min}$	$\hat{\Delta}y_{\max}$	$\frac{\eta}{2}$	$4\pi\eta_\theta$	t_{avg}
DNS1	1	1.2×10^7	130×130	130	14 (5)	10 (3)	1.6×10^{-3}	0.014	/	/	300
LES1	1	1.2×10^7	40×40	40	6 (5)	5 (3)	2.4×10^{-3}	0.059	0.059	0.069	300
LES2	1	3.1×10^7	48×48	48	6 (5)	5 (4)	1.9×10^{-3}	0.050	0.052	0.057	300
LES3	1	5.1×10^7	54×54	54	6 (6)	5 (4)	1.6×10^{-3}	0.044	0.044	0.047	300
LES4	1	8.4×10^7	60×60	60	6 (6)	5 (4)	1.5×10^{-3}	0.040	0.041	0.042	300
LES5	1	1.3×10^8	64×64	64	6 (6)	5 (5)	1.4×10^{-3}	0.037	0.037	0.037	400
LES6	1/2	1.1×10^9	64×64	128	8 (8)	6 (6)	6.4×10^{-4}	0.019	0.025	0.019	600
LES7	1/4	8.8×10^9	64×64	256	9 (11)	7 (9)	6.2×10^{-5}	0.009	0.017	0.010	800

Table 5.5: Resolution criteria. In this table, N_x , N_z and N_y are respectively the number of cells in the x , z and y directions, N_u and N_θ are the number of cells inside the hydrodynamic and thermal boundary layers with numbers in parentheses providing the minimum requirement and those outside the true values. The terms $\hat{\Delta}y_{\min}$ and $\hat{\Delta}y_{\max}$ are respectively the smallest and largest cell size, $\frac{\eta}{2}$ is half the Taylor microscale and $4\pi\eta_\theta$ is the relaxed *a priori* temperature microscale prediction. We add for the DNS that $\pi\eta_\theta = 0.017$ so that (5.19) is satisfied as $\hat{\Delta}y_{\max} = 0.014$. Finally, t_{avg} is the averaging time for statistics in free-fall time units.

experimental data as a means of testing the accuracy of the implemented evaporation model.

We first compare DNS and LES predictions of the “convective plus turbulent” and diffusive contributions to Nu_y in figures 5.2a and 5.2b respectively. The convective component is the dominant contribution in the bulk but tends to a very small value inside the thermal boundary layers. For the diffusive component, Nu_{diff} , only the near-wall contribution is shown, as it is negligible in the bulk. We observe that the LES underpredicts Nu_y everywhere by approximately 3%. The improvement over the LES carried out in chapter 3 is due to the inclusion of the buoyancy production term.

For all flows considered herein, a statistically stationary state is achieved when Nu_y is constant along the vertical and further equal to Nu . For all cases investigated, the final Nu differed by a maximum of 1.5% from the Nu found after half the averaging time. The time-averaging interval can therefore be considered adequate.

We now compare the DNS and LES predictions of the rms of velocity fluctuations in figure 5.3. In figure 5.3a, we note a near parabolic profile for $\hat{v}_{\text{rms}}$ with zero values at the boundaries. The profiles are similar to those of other thermal convection set-ups with shear-free upper boundary conditions [57, 67, 91]. The profile is not symmetric with respect to the mid-plane $\hat{y} = 0.5$ as a result of the different strengths in ascending and descending plumes [57], the latter being stronger. We find that the LES predictions are very close to those of the DNS, but slightly underpredict the peak in the upper half of the domain.

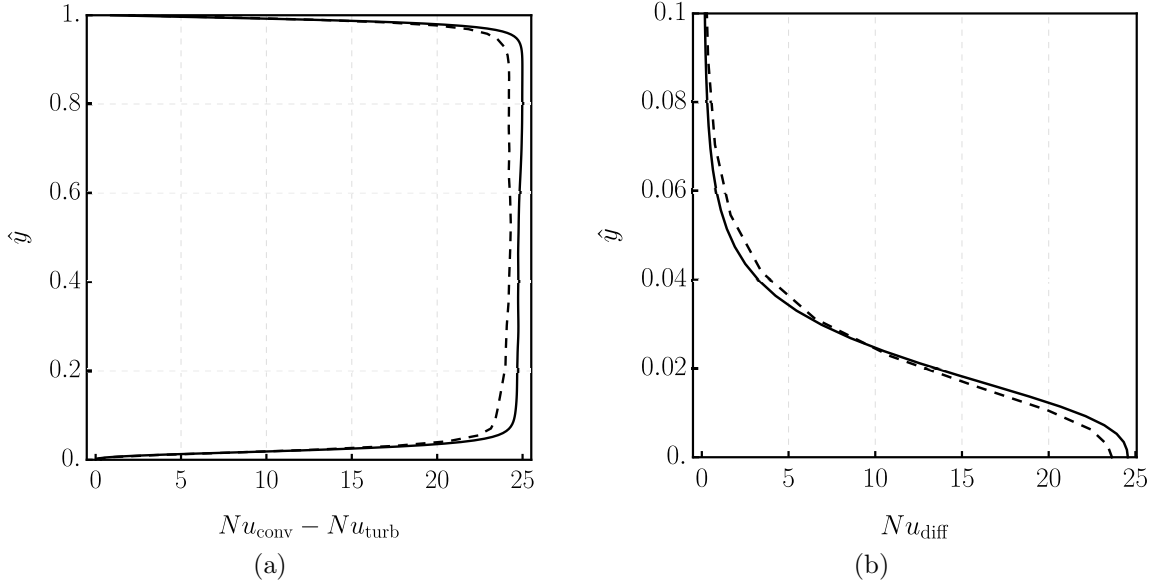


Figure 5.2: Plots of the time- and area-averaged components of Nu_y at $Ra = 1.2 \times 10^7$. (a) $Nu_{\text{conv}} - Nu_{\text{turb}}$ across the vertical direction and (b) Nu_{diff} zoom on lower boundary. We note that the negative sign in (a) results in a positive contribution as per the definition of Nu_{turb} in (5.20). The legend is as follows: DNS (—), LES (---).

The $\bar{u}_{\text{rms}}$ profile is presented in figure 5.3b. We observe a unique hydrodynamic boundary layer at the lower wall and a maximum in the rms of in-plane velocity fluctuations found at the surface. This feature has been observed experimentally [27] for evaporative cooling and numerically [57, 91] for thermal convection configurations with a shear-free upper boundary. The profile in the bulk of figure 5.3b is different to that seen in similar thermal convection flows with periodic boundaries [57, 68] where the bulk profile is flat. This feature of the profile is attributed to the side-wall boundaries leading to counter-rotating vortical cells. For the DNS, the maximum bulk value seen in figure 5.3b corresponds approximately to the vertical position at which the counter-rotating vortical cells interact. The same is true for the LES, however, due to the coarseness of the mesh, the peak is less pronounced.

Finally, the hydrodynamic boundary layer created by the shear of the large-scale circulation has a height, $\hat{\delta}_{\text{u}}$, estimated from the local peak in $\bar{u}_{\text{rms}}$ [68, 105]. The LES predicts a boundary layer height very close to that of the DNS, as seen in table 5.6, suggesting that the hydrodynamic boundary layer is well-resolved in the LES. We add that, in table 5.6 we observe the expected hydrodynamic boundary layer thinning as Ra is increased.

We next compare the DNS and LES predictions of the mean temperature and rms of temperature fluctuations respectively in figures 5.4a and 5.4b. Firstly, in figure 5.4a we note that boundary layers exist at both the upper and lower boundaries and that the bulk temperature gradient is essentially zero. We further note that the bulk temperature is shifted towards the cooler upper boundary value, as also seen in similar

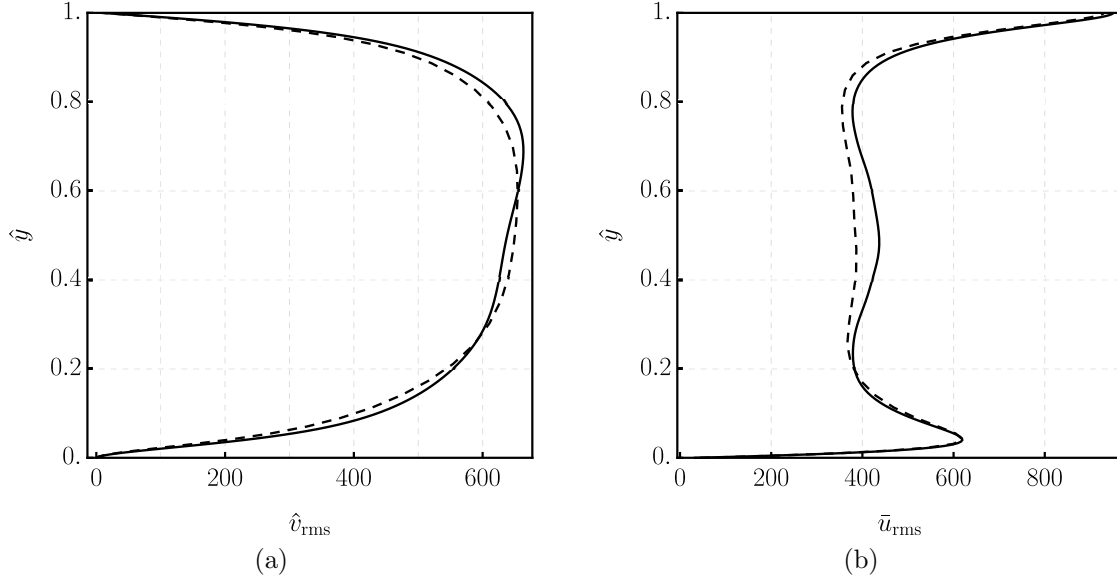


Figure 5.3: Plots of the rms of velocity fluctuations at $Ra = 1.2 \times 10^7$. (a) $\hat{v}_{rms}$ and (b) dimensionless $\bar{u}_{rms}$. The velocities have been made dimensionless by κ_{ref}/H . The legend is as follows: DNS (—), LES (---).

configurations with a shear-free upper boundary (see figures 3.9, 3.18, and 4.9). This is in contrast to turbulent RBC [68] where the bulk temperature is the mean of the upper and lower boundaries. We present also a zoom on the upper and lower boundaries as insets, where we see that the LES reproduces well the profile.

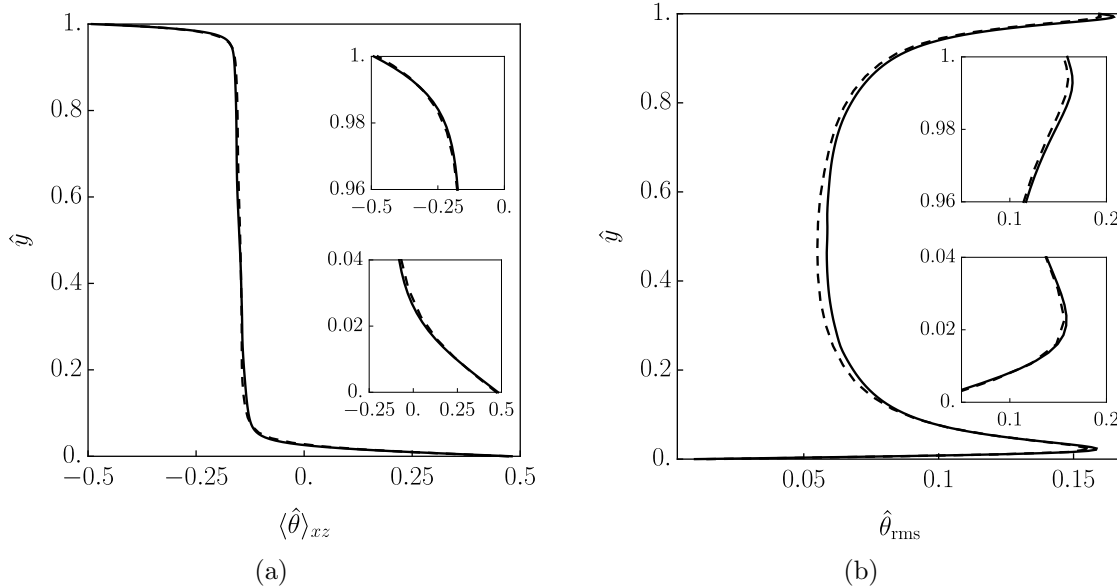


Figure 5.4: Plots of the temperature at $Ra = 1.2 \times 10^7$. (a) Mean, $\langle \hat{\theta} \rangle_{xz}$, and (b) rms, $\hat{\theta}_{rms}$. The legend is as follows: DNS (—), LES (---).

In figure 5.4b, we note a local peak near the lower wall representing the location of the thermal boundary layer, $\hat{\delta}_{\theta_{low}}$, before dropping in the bulk and increasing to a maximum at the upper boundary. We again show insets, which suggest that the LES

Case	Ra	Nu	$\hat{\delta}_{\theta_{\text{int}}}$	$\hat{\delta}_{\theta_{\text{low}}}$	$\hat{\delta}_{\mathbf{u}}$	Re
DNS1	1.2×10^7	24.9	0.014	0.024	0.040	205
LES1	1.2×10^7	24.2	0.015	0.023	0.042	210
LES2	3.1×10^7	31.7	0.011	0.017	0.029	410
LES3	5.1×10^7	36.8	0.0094	0.013	0.028	600
LES4	8.4×10^7	41.7	0.0086	0.011	0.023	840
LES5	1.3×10^8	47.4	0.0074	0.010	0.022	1150

Table 5.6: Time-averaged results for cubic ($\Gamma = 1$) domain. In this table, Nu is the global Nusselt number, $\hat{\delta}_{\theta_{\text{int}}}$ and $\hat{\delta}_{\theta_{\text{low}}}$ are the thermal boundary layer heights at the interface and the lower wall, respectively, whereas $\hat{\delta}_{\mathbf{u}}$ is the hydrodynamic boundary layer height at the lower wall. Finally, we provide the global Reynolds number, Re , defined in the text.

reproduces well the DNS results. In particular, we note that the height of the lower thermal boundary layer appears well predicted. The upper thermal boundary layer height, $\hat{\delta}_{\theta_{\text{int}}}$, on the other hand is estimated as follows,

$$\delta_{\theta_{\text{int}}} = -\lambda_{\text{int}} \frac{T_{\text{int}} - T_{\text{bulk}}}{\dot{q}''}, \quad (5.26)$$

with T_{int} and $\dot{q}''$ respectively as the time- and area-averaged temperature and heat flux at the interface and where the dimensional T_{bulk} is interpreted from figure 5.4a. Table 5.6 confirms that the LES reproduces well the DNS predictions of both $\hat{\delta}_{\theta_{\text{low}}}$ and $\delta_{\theta_{\text{int}}}$, suggesting that the thermal boundary layers are well-resolved in the LES.

We note that $\hat{\delta}_{\theta_{\text{low}}}$ is larger than $\hat{\delta}_{\theta_{\text{int}}}$ and attribute the inhomogeneity to the presence of the shear-free upper boundary [67, 91]. This feature of the flow remains even with the non-uniform interface temperature (see later figure 5.12), and indeed temperature gradient at the interface, investigated herein. We add that table 5.6 shows boundary layer thinning as a result of increasing Ra in the cubic ($\Gamma = 1$) domain, however, the inhomogeneities in the thermal boundary layer heights remain.

Finally, we compare the predictions of the third order statistics of the DNS and LES in figure 5.5. The profile of the third central moment of the temperature is provided as figure 5.5a where we again see an asymmetry introduced by the shear-free upper boundary. The normalised third central moment, the temperature skewness, is defined as $\hat{S}_{\theta} = \langle \hat{\theta}^3 \rangle_{xz} / \hat{\theta}_{\text{rms}}^3$. Figure 5.5b shows that the temperature is predominantly negatively skewed owing to the more intense plume formation at the shear-free surface [57]. We can see in both aforementioned figures that the third-order statistics are well approximated by the LES, although the peaks are underestimated near the boundaries and, in particular, the LES exaggerates the negative skewness in the upper half of the

domain. Overall, considering that the LES mesh is over 30 times coarser than that of the DNS, we find that the LES predictions of first, second and third order statistics compare satisfactorily with the DNS data.

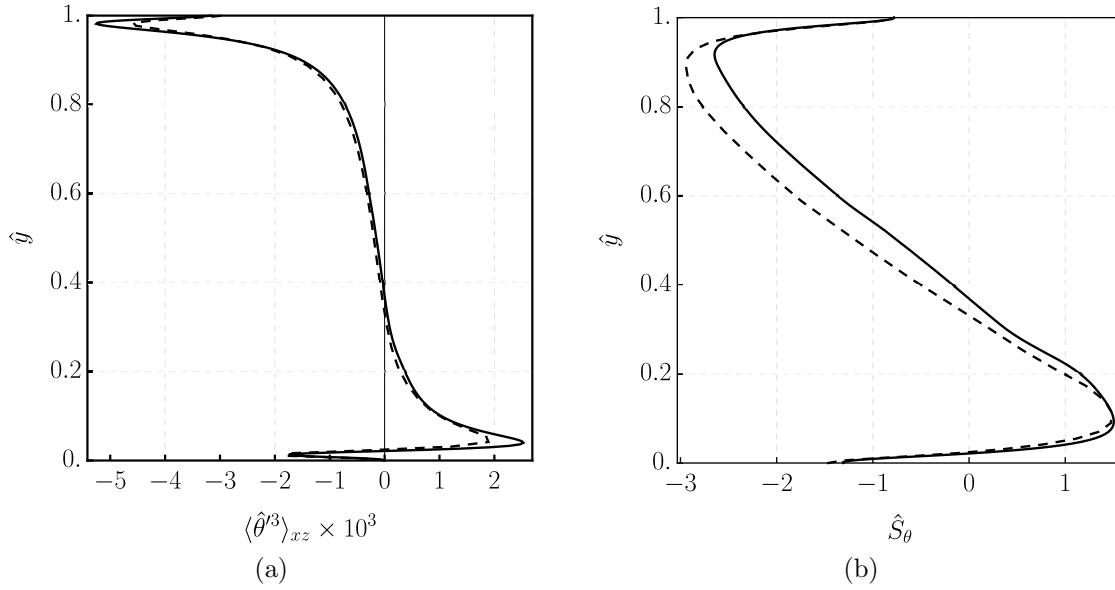


Figure 5.5: Plots of third-order statistics at $Ra = 1.2 \times 10^7$. (a) Third central moment of temperature and (b) skewness of temperature. The legend is as follows: DNS (—), LES (---).

We next present the validation exercise for the evaporation model where we start by discussing the experimental set-up [36] in the Institut de Radioprotection et de Sûreté Nucléaire (IRSN) of France. The experiments were conducted using a set of insulated stainless steel tanks of differing shapes (cylindrical and cuboidal) and aspect ratios. During the tests, the tanks were filled with water and heated from below. The water mass and free-surface temperatures were then measured simultaneously, the latter using an infrared camera. The ambient gaseous conditions, i.e. the relative humidity and temperature, were also recorded above the experimental device.

Importantly, the tanks were heated up towards, but never arriving at boiling point, so as to avoid initiating any nucleation. At which point, the heating was stopped and the water allowed to cool. During both the heat-up and cool-down stages, the following parameters were measured: the mass of water in the tank, the bulk water temperature, the interface temperature T_{int} , the ambient air temperature T_∞ , and the relative humidity. The collated data allowed for a plot of evaporative mass flux against free-surface temperature with error bars representative of the measurement device accuracy. In figure 5.6, we replot this data and superimpose the time- and area-averaged evaporative mass flux predictions for cases LES1–LES5. We observe that the predicted evaporative mass fluxes are an excellent fit with the best estimate from the experimental measurements and are easily within the limits of experimental error indicated by the shaded grey area. We can therefore assume that the evaporation

model is valid.

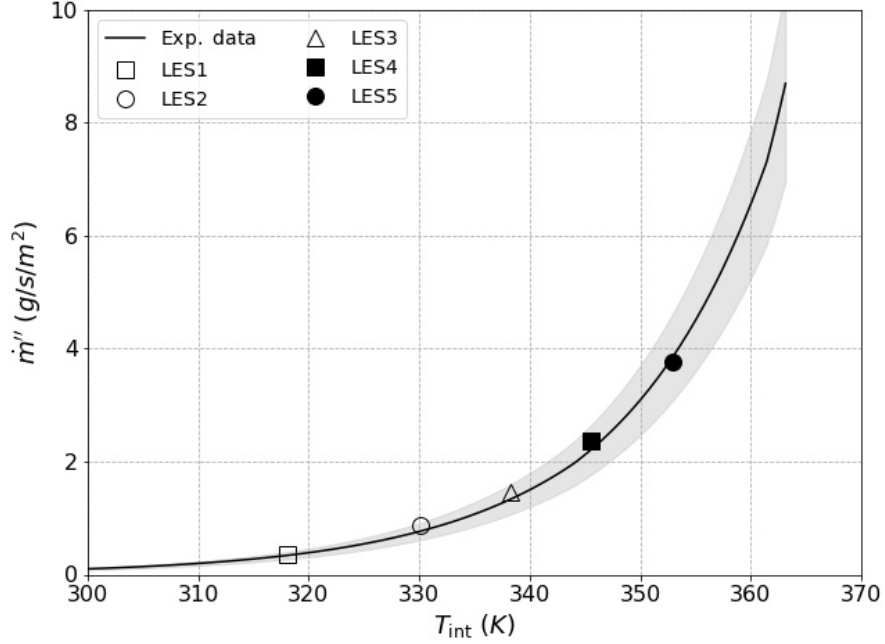


Figure 5.6: Comparisons between LES predictions and experimental measurements of the evaporative mass flux, $\dot{m}''$, and interface temperature, T_{int} , at an evaporating air-water interface. The shaded area represents the accumulated experimental error ($\sim \pm 20\%$ of the measured flux). All experimental runs, regardless of the ambient conditions or tank geometry lie within the shaded area. The solid line represents a best estimate from all experimental data.

It is worth noting that discrepancies in experimental results due to variable ambient conditions, tank geometry and the stage of heat transfer (i.e. heat-up or cool-down) were smaller than the margin of errors in the experimental measurement devices. This suggests that the aspect ratio should not play an important role in the rate of evaporation, a result which we confirm in the next section.

Finally, table 5.6 shows the global Reynolds number, $Re = (\mathbf{u}_{\text{rms}})_{xyz}H/\nu$ where $(\mathbf{u}_{\text{rms}})_{xyz} = \sqrt{\langle u^2 + v^2 + w^2 \rangle}_{xyz}$ (m/s) is the time- and volume-averaged rms of the velocity fluctuations. Using this data, we obtain the power-law fit over the parameter space as, $Re = 2.7 \times 10^{-3} Ra^{0.69}$. We note that, for the cubic domain, Ra is updated between simulations via the thermal boundary conditions. Consequently, there exists large variations in T_{ref} and hence in the kinematic viscosity, ν , between the cases. For this reason, we also provide a power-law fit of the time- and volume-averaged rms of the velocity fluctuations, as $(\mathbf{u}_{\text{rms}})_{xyz} \propto Ra^{0.47}$. This latter fit of the dimensional rms velocity, matches well that of Scheel and Schumacher [104] for turbulent RBC at $Pr = 0.7$ in cylindrical domains of aspect ratio $\Gamma = 1$, according to which Re scales as Ra^β , with $\beta = 0.49 \pm 0.01$.

5.6.2 Study of the effect of the aspect ratio

The purpose of this section is to investigate the role of aspect ratio on the structure of the LSC, evaporation rates, mean flow properties and flow statistics. In relation to the latter, the common technique of increasing Ra in turbulent RBC experiments is to maintain both T_{ref} and Γ and increase Ra via thermal boundary conditions, specifically ΔT . In this section, however, we maintain the thermal boundary conditions and Ra is updated between simulations by reducing the aspect ratio Γ via the height of the domain.

We start by presenting the time-averaged LSC flow structure in the cubic ($\Gamma = 1$) domain at $Ra = 1.3 \times 10^8$ in figures 5.7 and 5.8. The streamlines of figure 5.7 suggest a steady single-roll state of the LSC that occupies the entirety of the domain. From figure 5.7a we note that the impingement point of the LSC is aligned in one corner, with the lower wall impingement point (not shown) found in the opposite corner. This is characteristic of a steady LSC in cubic geometries where the single-roll state dominates [91, 94]. The same global observations of the LSC are made in all $\Gamma = 1$ simulations. Further, asymmetries are observed in both the recirculation zones of figure 5.8a and in the counter-rotating vortices of figure 5.8b. These are a result of the free-slip upper boundary condition accelerating fluid following impingement [91].

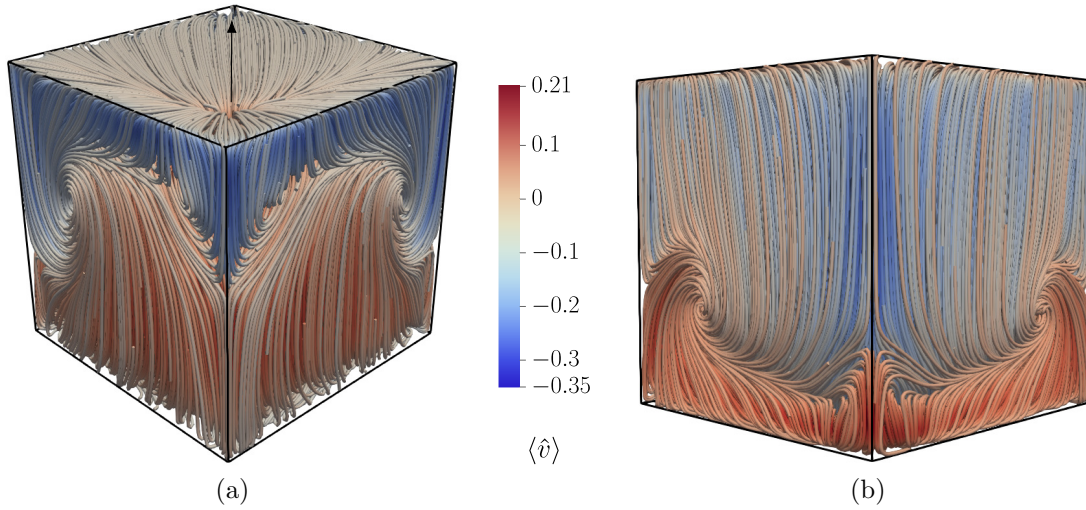


Figure 5.7: Time-averaged streamlines in the aspect ratio $\Gamma = 1$ domain at $Ra = 1.2 \times 10^8$, coloured by mean vertical velocity, $\langle \hat{v} \rangle$. (a) Top-view from the front showing LSC direction after impingement and (b) side-view from the back.

We next present the LSC structure in the domain of aspect ratio $\Gamma = 1/2$ at $Ra = 1.1 \times 10^9$ in figures 5.9 and 5.10. The same single-roll LSC state exists as seen in the $\Gamma = 1$ case (shown in figures 5.7 and 5.8); this LSC structure remained unchanged during the simulation. Further, the asymmetries in recirculation zones and counter rotating vortices persist in figures 5.10a and 5.10b respectively. As discussed in the Introduction to this chapter, the transition from a single to a dual-roll state

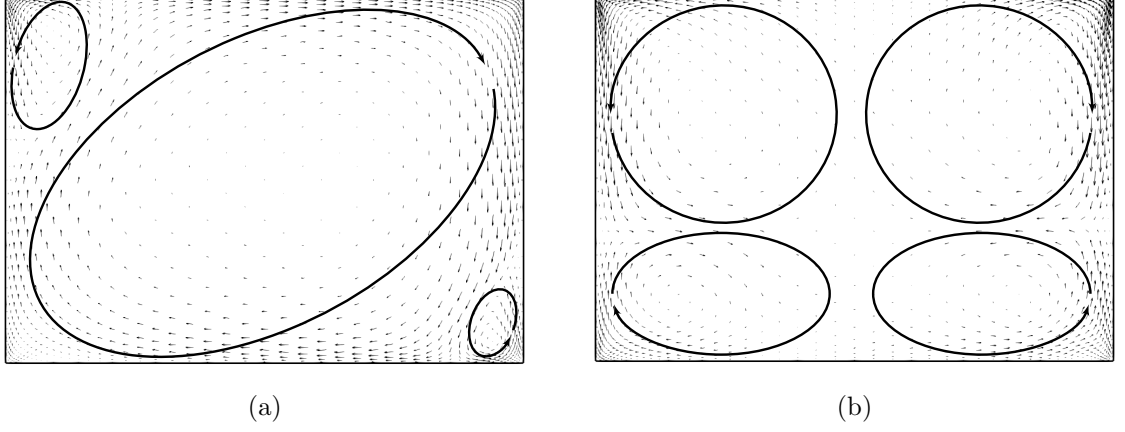


Figure 5.8: Time-averaged velocity vectors scaled by magnitude with superimposed large-scale structures in the cubic ($\Gamma = 1$) domain (a) LSC plane and (b) orthogonal plane. The same global LSC structure is seen across all simulations in the cubic domain.

is dependent on Ra , Pr and Γ . A Ra – Pr phase diagram was previously proposed [110] for determining whether the mean flow structure is a single or dual-roll states in cylindrical domains of aspect ratio $\Gamma = 1/2$. For the parameter space investigated here, that is $Ra \approx 10^9$ and $Pr \approx 2$, the phase diagram [110] predicts a single-roll state like that observed in figure 5.10a. This result suggests that the experimental studies into the role of aspect ratio of the LSC state using cylindrical domains could still be relevant for cuboidal applications.

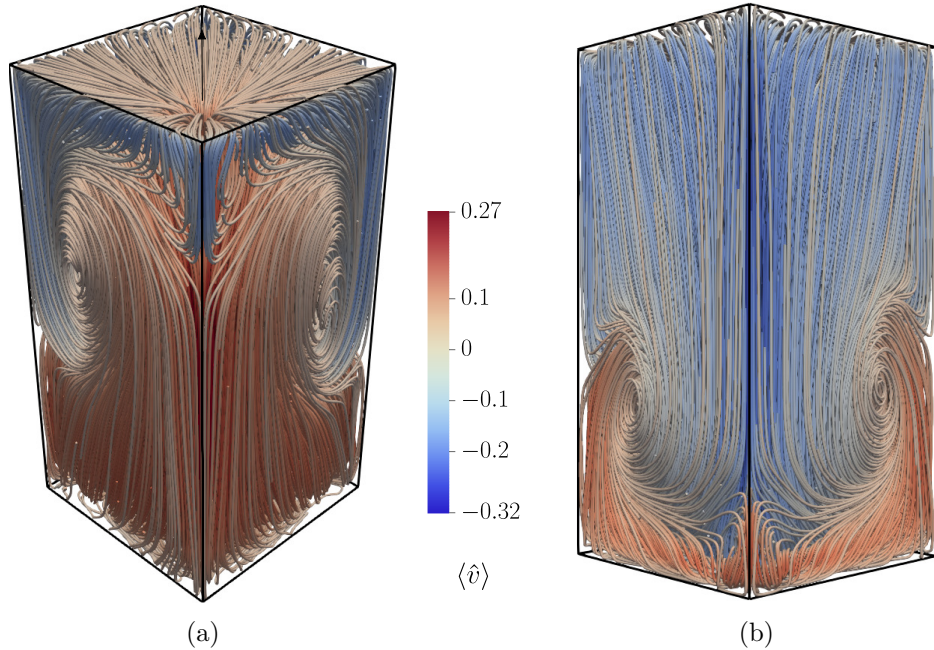


Figure 5.9: Time-averaged streamlines in the domain of aspect ratio $\Gamma = 1/2$ at $Ra = 1.1 \times 10^9$, coloured by mean vertical velocity, $\langle \hat{v} \rangle$. (a) Top-view from the front showing LSC direction after impingement and (b) side-view from the back.

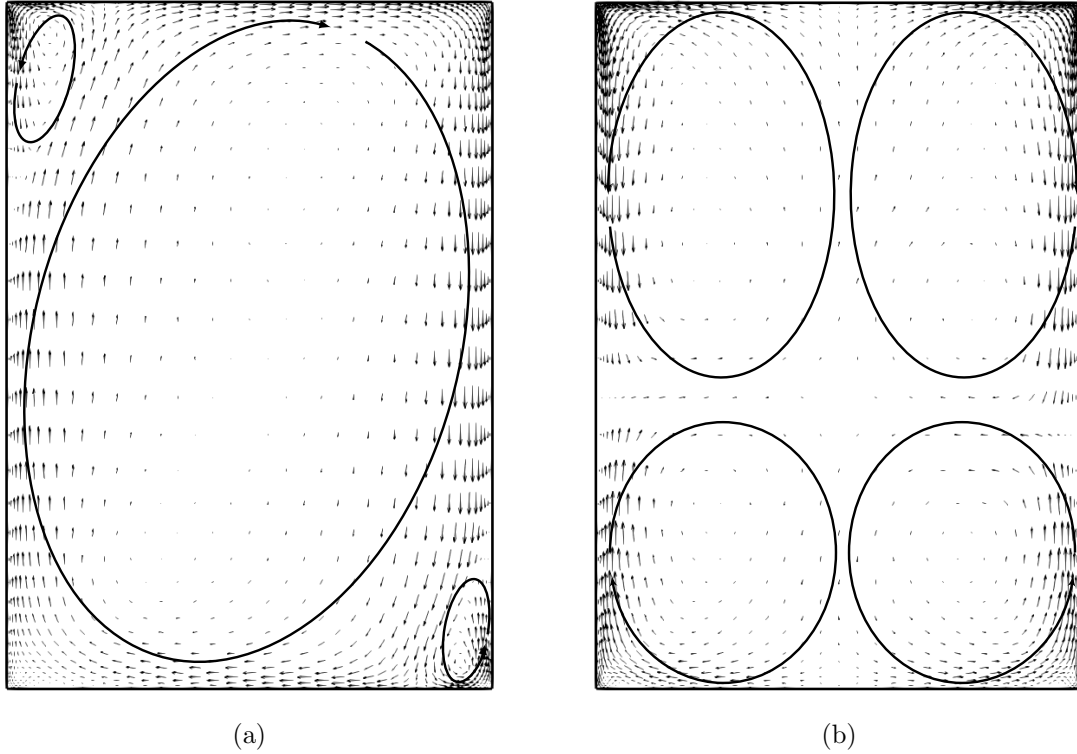


Figure 5.10: Time-averaged velocity vectors scaled by magnitude with superimposed large-scale structures for aspect ratio $\Gamma = 1/2$ (a) LSC plane and (b) orthogonal plane.

A long lifetime dual-roll state has previously been inferred (but not observed) in a cylindrical domain of aspect ratio $\Gamma = 1/2$ with water as the convecting fluid [117]. However, this observation was later questioned by Weiss and Ahlers [113] who investigated a similar set-up. Therein, it was found that the dual-roll state existed only as a transitional state between reorientation events of the single-roll LSC (such as drifting, cessations, or torsional oscillations), and as such for very short lifetimes. Their research was again based on a slender cylindrical domain, but the same conclusion can be inferred from figure 5.10 for the cuboidal domain where we see a steady single-roll LSC state.

In figures 5.11a and 5.11b we present the time-averaged streamlines in the domain of aspect ratio $\Gamma = 1/4$ at $Ra = 8.8 \times 10^9$. In terms of the flow structure we see that the LSC is in a dual-roll or transitional state. Such a dual-roll or transitional state is expected to be dominant in low aspect ratio (slender) domains [111], however, to the authors knowledge, no experimental observations are available in the literature for comparison at the aspect ratio $\Gamma = 1/4$, be that in cylindrical domains or otherwise.

In figure 5.11c we show both the “LSC” plane and a rotated orthogonal plane together and again superimpose the large-scale structures. Here, we confirm that the LSC is in a dual-roll state. However, we note that the terminology of large-scale circulations in cuboidal domains may require some clarifications. The symmetric flow structures observed in 5.11c, are in fact similar to the orthogonal plane structures we

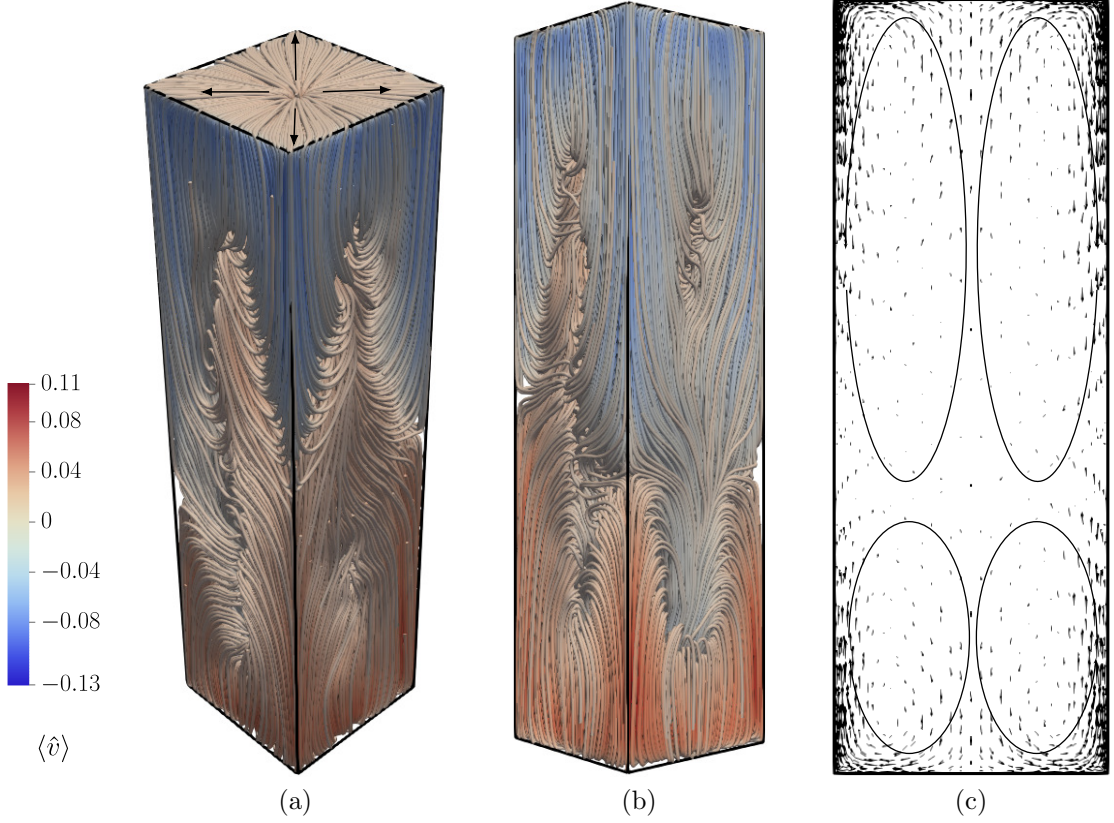


Figure 5.11: Time-averaged flow structure in the domain of aspect ratio $\Gamma = 1/4$ at $Ra = 8.8 \times 10^9$. (a) Top-view from the front of streamlines at $Ra = 8.8 \times 10^9$, coloured by mean vertical velocity, $\langle \hat{v} \rangle$. Here we see the LSC impingement in the middle of the free surface due to the dual-roll state, (b) same as in (a) but a side-view from the back is shown and (c) velocity vectors scaled by magnitude with superimposed large-scale structures, as the LSC and orthogonal planes are now almost symmetric we show them together, with the latter rotated to be on the same axis. A dual-roll state is then observed in both planes, where the dual-roll state is seen to have the same structure as the orthogonal plane in figures 5.8b and 5.10b.

observed earlier in figures 5.8b and 5.10b. One could therefore consider that the earlier definitions of an LSC plane and an orthogonal plane, are actually better described as coexisting single-roll and dual-roll LSC planes.

Regarding the simulation of the domain of aspect ratio $\Gamma = 1/4$, the impingement point above is no longer aligned with a corner, as was the case in figures 5.7a and 5.9a, but in the centre of the surface, similar to observations made in another aspect ratio study [118].

Theoretically, reorientation events of the dual-roll LSC are possible during the averaging time of the aspect ratio $\Gamma = 1/4$ simulation. Indeed, such events become more likely as Γ is reduced [114] and the LSC becomes less stable. Unlike in figures 5.8a and 5.10a, where reorientation events are absent, it is possible that figures 5.11a and 5.11b represent a time-averaged flow in which reorientation events have occurred. However, we note that the observed flow structure in figure 5.11c appears to remain

steady throughout.

We next discuss whether the aspect ratio has an influence on the free surface parameters, and notably on the evaporative mass flux. We first present figure 5.12 showing the mean normalised temperature at the interface, where we observe that $\langle\hat{\theta}\rangle$ varies in space. There is a clear role of the LSC in determining this spatial variation. As the LSC is driven by the hot buoyant plumes released from the lower wall, the warmest locations on the free surface coincide with the impingement point of the LSC.

Remarkably, however, table 5.7 shows that the time- and area-averaged interface temperature remain steady as Ra is increased by almost two orders of magnitude. Consequently, the evaporative mass flux at the free-surface also remains steady and can be considered independent of the water-side Ra . At the same time, the reduction in aspect ratio to $\Gamma = 1/4$ and subsequent transformation of the LSC to a non-single-roll state clearly changes the velocity field on the interface; see figure 5.12c. The LSC state therefore also has a negligible influence on the evaporation rate at the interface. These results are in fact in accordance with experimental observations [36], where the geometry of the tanks, that is surface shape and crucially aspect ratio, had no determinable influence on evaporation rates when experimental error was taken into account.

Case	Γ	Ra	T_{low} (K)	$\frac{\partial\tilde{T}}{\partial y}$ ($\frac{\text{K}}{\text{m}}$)	T_{int} (K)	$\dot{m}''$ (g/s/m ²)
LES5	1	1.3×10^8	365.65	-13700	352.95	3.77
LES6	1/2	1.1×10^9	365.65	-13600	352.65	3.73
LES7	1/4	8.8×10^9	365.65	-13250	352.35	3.63

Table 5.7: Thermal boundary conditions for the study of the aspect ratio. In this table, T_{low} is the fixed lower wall temperature, and $\partial\tilde{T}/\partial y$, T_{int} and $\dot{m}''$ are respectively the time- and area-averaged temperature gradient, temperature and evaporative mass flux at the upper boundary taken from the statistically stationary solution. For all cases the time- and area-averaged normalised interface temperature, $\langle\hat{\theta}_{\text{int}}\rangle_{xz} = -0.5$.

With respect to any eventual influence of the aspect ratio on the mean flow properties we assess the dimensionless heat transfer. We start by presenting figure 5.13, where we plot the profiles of the different contributions of Nu_y . The statistically stationary nature of the simulations at aspect ratios $\Gamma = 1$ and $1/2$ is again inferred from the flat profile of $Nu_{\text{conv}} - Nu_{\text{turb}}$ across the domain in figure 5.13a. However, we note that ideally we would have taken more statistics for the aspect ratio $\Gamma = 1/4$ simulation. We monitored the statistics throughout and confirm that the profile flattens with time. This suggests that if the simulations were carried out over many hundreds more free-fall

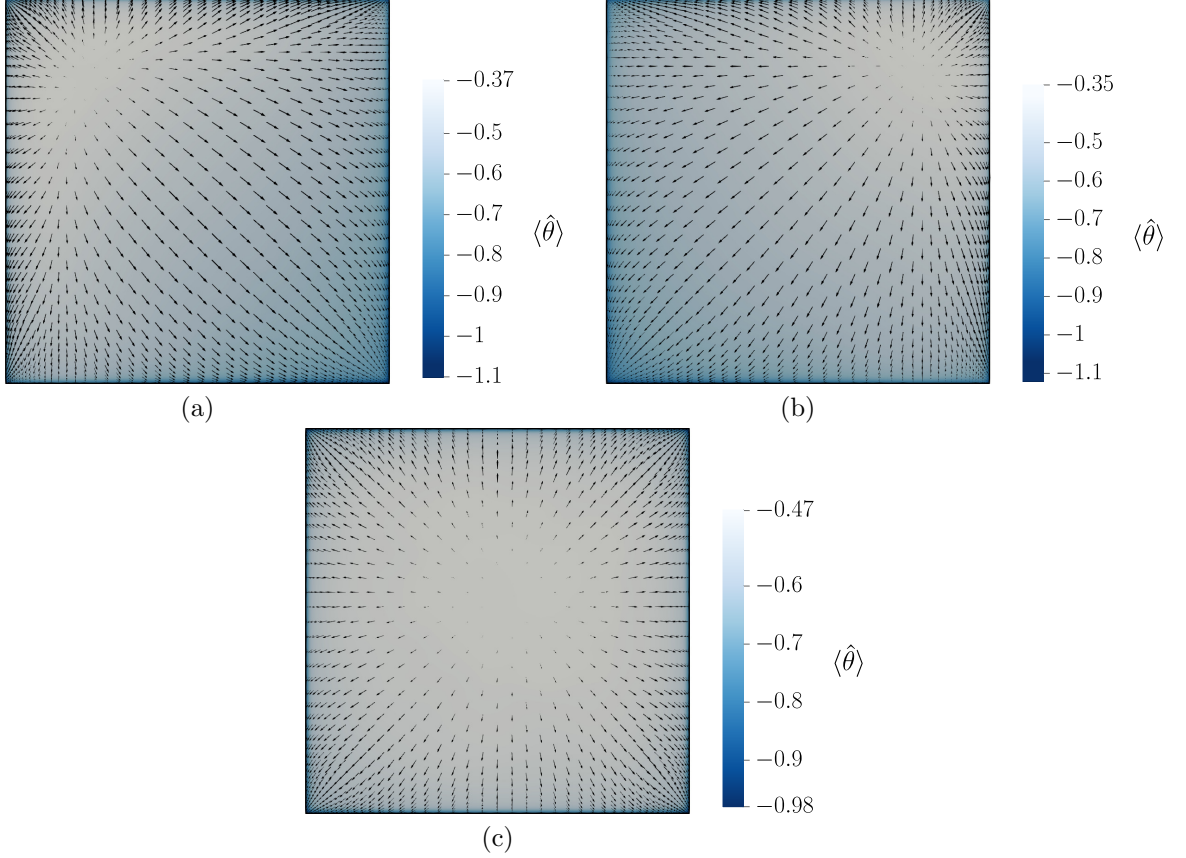


Figure 5.12: Time-averaged normalised interface temperatures, $\langle \hat{\theta} \rangle$, with superimposed time-averaged velocity vectors scaled by magnitude. (a) Aspect ratio $\Gamma = 1$ at $Ra = 1.2 \times 10^8$, (b) aspect ratio $\Gamma = 1/2$ at $Ra = 1.1 \times 10^9$ and (c) aspect ratio $\Gamma = 1/4$ at $Ra = 8.8 \times 10^9$.

times the simulation would be fully statistically stationary. Table 5.5 shows that we ran this simulation for $800 t_{\text{ff}}$ which is already longer than the vast majority of earlier studies, with the notable exception of Foroozani *et al.* [66, 94] who specifically looked at LSC dynamics over long time periods. The global Nusselt, however, varies only by 1.5% if half the averaging time, that is $400 t_{\text{ff}}$, is used. This result suggests that Nu is representative of a statistically stationary value.

We now present a Ra – Nu scaling analysis covering a parameter space of nearly 3 decades of Ra . This analysis is based on all seven LES, it therefore includes simulations of variable T_{ref} and Γ which is only permitted as the Nu dependency on Pr and Γ is essentially absent [113]. This is certainly true for water at $Pr = 2$, where the thermal boundary layer is sheltered within the hydrodynamic one. Any eventual impact on thermal boundary layer thicknesses as a result of a transition in LSC flow state is then buffered [119]. We obtain the following power-law fit,

$$Nu = 0.170 Ra^{0.302}, \quad (5.27)$$

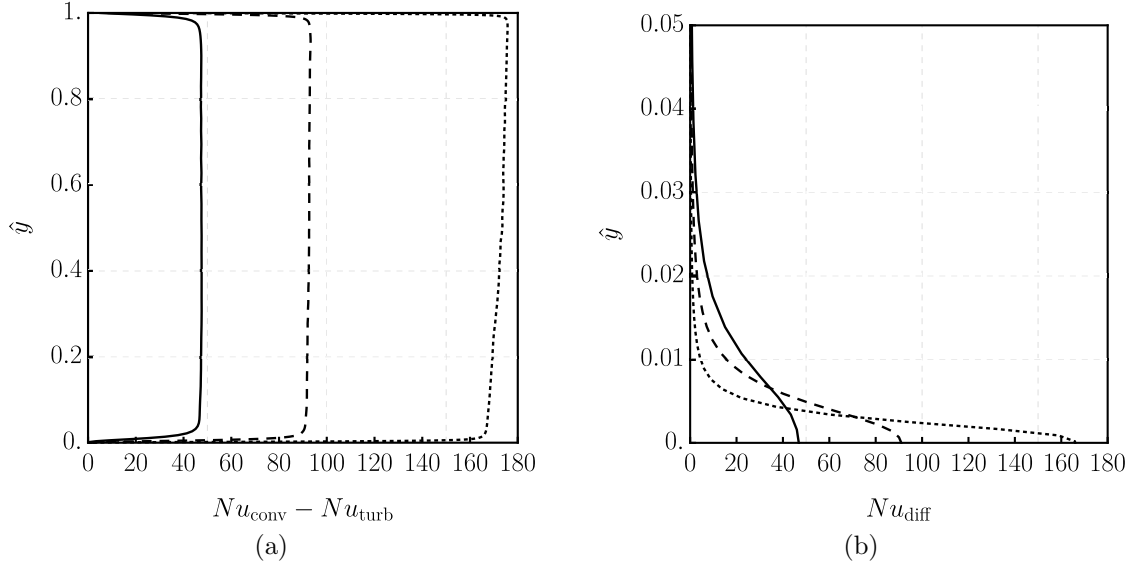


Figure 5.13: Plots of the time- and area-averaged components of Nu_y as Ra is increased (Γ is decreased). (a) $Nu_{\text{conv}} - Nu_{\text{turb}}$ across the vertical direction and (b) Nu_{diff} zoom on lower boundary. The legend is as follows: aspect ratio $\Gamma = 1$ at $Ra = 1.3 \times 10^8$ (—), aspect ratio $\Gamma = 1/2$ at $Ra = 1.1 \times 10^9$ (---) and aspect ratio $\Gamma = 1/4$ at $Ra = 8.8 \times 10^9$ (.....).

which is remarkably close to the scaling obtained from previous DNS studies in the similar thermal convection configuration of the previous chapter (see also [91]), which gave $Nu = 0.178Ra^{0.301}$ over a smaller parameter space. The reduced prefactor here corresponds to the slight underestimation of the LES discussed earlier and the exponent in (5.27) is in good agreement with experimental turbulent RBC studies [82] which give $Nu \propto Ra^{0.309}$.

We also provide the relevant global Re in table 5.8. For the study of the effect of the aspect ratio, we update Ra via the height of the domain and, as discussed, the thermal boundary conditions remained almost constant. A power-law fit over the aspect ratio range gives $Re \propto (\frac{1}{\Gamma})^{1.07}$; suggesting that the turbulence intensity increases almost linearly with aspect ratio.

We now assess the influence of the aspect ratio on the flow statistics and start by presenting the rms of vertical and in-plane velocity fluctuations in figure 5.14. We first concentrate on the rms of vertical velocity fluctuations, $\hat{v}_{\text{rms}}$, where figure 5.14a shows that the near-parabolic profile observed in figure 5.3a persists in all simulations. In figure 5.14b, we again observe approximately the same trend over all Ra investigated; a peak by the lower wall represents a hydrodynamic boundary layer, the bulk $\bar{u}_{\text{rms}}$ profile shows a bump owing to the contained nature of the flow and a maximum is found at the upper boundary. Overall, we conclude that the influence of the aspect ratio is limited, as we see the same global trends that would otherwise be observed if the standard manner of increasing Ra had been used. That is, the rms of velocity fluctuations are positively correlated with Ra , table 5.8 shows thinning of the hydrodynamic boundary

Case	Γ	Ra	Nu	$\hat{\delta}_{\theta_{\text{int}}}$	$\hat{\delta}_{\theta_{\text{low}}}$	$\hat{\delta}_{\mathbf{u}}$	Re
LES5	1	1.3×10^8	47.4	0.0074	0.010	0.022	1150
LES6	1/2	1.1×10^9	92.4	0.0036	0.0059	0.012	2555
LES7	1/4	8.8×10^9	172.5	0.0022	0.0026	0.008	5265

Table 5.8: Time-averaged results for the study of the aspect ratio. In this table, Nu is the global Nusselt number, $\hat{\delta}_{\theta_{\text{int}}}$ and $\hat{\delta}_{\theta_{\text{low}}}$ are the thermal boundary layer heights at the interface and the lower wall respectively, whereas $\hat{\delta}_{\mathbf{u}}$ is the hydrodynamic boundary layer height at the lower wall. Finally, we provide the global Reynolds number, Re , defined in the text.

layer with Ra and the same global profiles are maintained in $\hat{v}_{\text{rms}}$ and $\bar{u}_{\text{rms}}$.

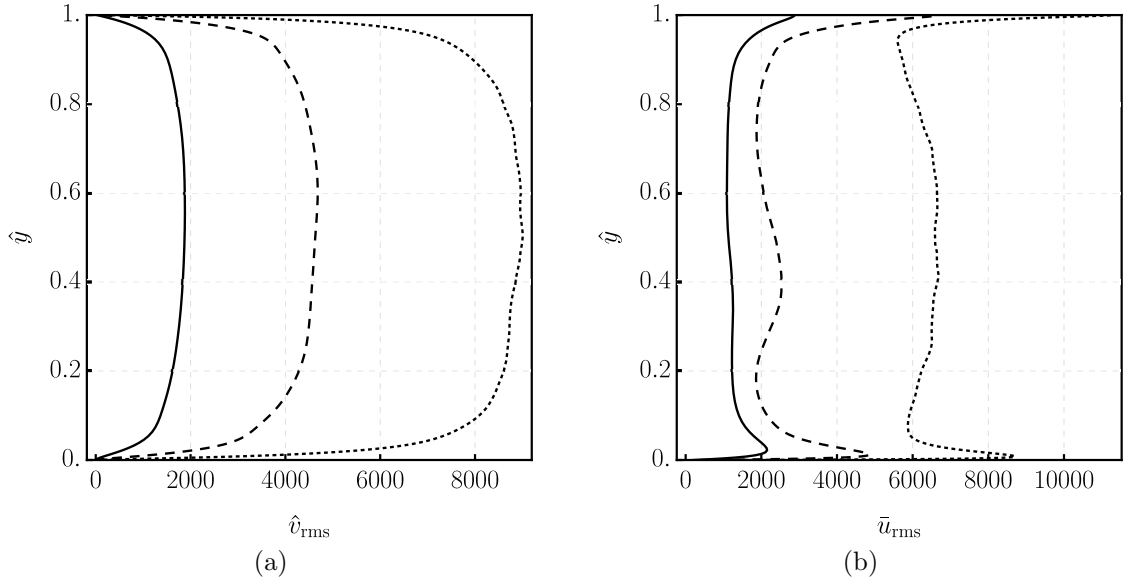


Figure 5.14: Plots of the rms of velocity fluctuations as Ra is increased (Γ is decreased). (a) $\hat{v}_{\text{rms}}$ and (b) dimensionless $\bar{u}_{\text{rms}}$. The velocities have been made dimensionless by κ_{ref}/H and The legend is as follows: aspect ratio $\Gamma = 1$ at $Ra = 1.3 \times 10^8$ (—), aspect ratio $\Gamma = 1/2$ at $Ra = 1.1 \times 10^9$ (- - -) and aspect ratio $\Gamma = 1/4$ at $Ra = 8.8 \times 10^9$ (.....).

We next discuss the time- and area-averaged normalised temperature distribution in the domain as the aspect ratio is decreased. Figure 5.15a suggests a subtle difference between the cases at aspect ratios $\Gamma = 1$ and $\Gamma = 1/2$ where the single-roll state is present and the case at aspect ratio $\Gamma = 1/4$, where a non-single-roll state dominates. In the current thermal configuration, the temperature in the bulk is expected to be constant and equal to a value shifted towards the cold upper boundary temperature [67, 91]. This is indeed the case for aspect ratios $\Gamma = 1$ and $\Gamma = 1/2$. However, for the case at aspect ratio $\Gamma = 1/4$, figure 5.15a clearly shows that outside of the boundary layers, the bulk temperature is not constant but in fact increases linearly. Consequently,

the bulk temperature is, in general, warmer than for the larger aspect ratio cases. We note that the trend is unchanged if we take only the first half of the averaging time, $400 t_{\text{ff}}$, and consequently we do not put this feature of the flow down to lack of statistics. Indeed, a peak in bulk fluid temperature as a result of a transition to the dual-roll state has been reported before [16]. Therein, the flow feature was described as being caused by the bringing into contact of the fluid transported from the hot and cold plates in the cell centre, albeit for a fluid at $Pr < 1$ and in a cylindrical domain of aspect ratio $\Gamma = 1/2$. On the basis of our findings, we therefore conclude that the observed bulk temperature gradient is the same effect played out in the cuboidal domain of aspect ratio $\Gamma = 1/4$.

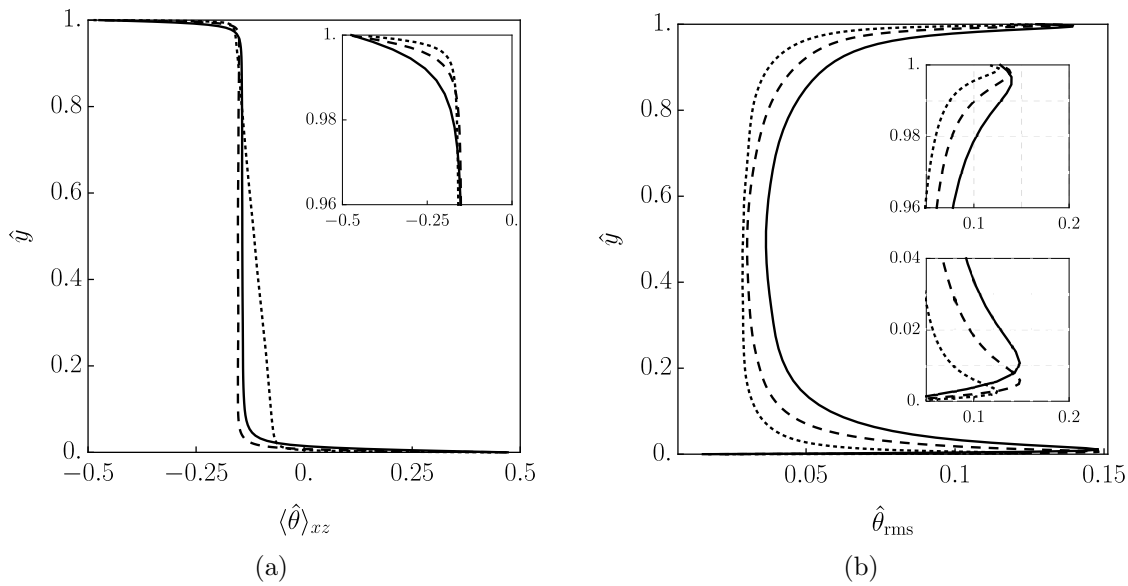


Figure 5.15: Temperature plots as Ra is increased (Γ is decreased). (a) Time- and area-averaged temperature, $\langle \hat{\theta} \rangle_{xz}$ and (b) rms of the temperature fluctuations, $\hat{\theta}_{\text{rms}}$. The legend is as follows: aspect ratio $\Gamma = 1$ at $Ra = 1.3 \times 10^8$ (—), aspect ratio $\Gamma = 1/2$ at $Ra = 1.1 \times 10^9$ (---) and aspect ratio $\Gamma = 1/4$ at $Ra = 8.8 \times 10^9$ (.....).

Concentrating next on figure 5.15b, we observe the same general trends as seen in figure 5.4b. That is, a peak at the lower boundary which defines the lower thermal boundary layer height, a dip in the centre of the domain and a maximum at the upper boundary. As Ra is increased the dimensionless thermal boundary layer heights are decreased as seen in table 5.8. The dip in the bulk is reduced, albeit less than one might expect for the largest Ra (smallest Γ), and the maximum at the surface is nearly constant.

Bower and Saylor [30] considered whether water-side natural convection can affect evaporation rates. Therein, it was argued that two different tanks of different depths, and hence Ra , could have different water-side turbulence intensities, and for example, different interface $\hat{\theta}_{\text{rms}}$ values. In turn, this could have an impact on the mass flux

at the free surface. Indeed, according to the experiments in [30], progressively deeper tanks lead to an increased free surface temperature and hence evaporative mass flux. In other words, Sh was positively correlated with water-side Ra . This experimental study, however, was inconclusive, and it was hypothesised that the results could be due to an experimental artifact. In particular, in [30] the experimental procedure led to the surface temperatures of shallower tanks being cooler than those of deeper tanks at the beginning of the experiments. Further, the flow feature of an increased $\hat{\theta}_{\text{rms}}$ at the interface at higher Ra is not observed in our study; this can be verified in figure 5.15b which shows a constant interface value as Ra is increased.

Table 5.8 provides values for $\hat{\delta}_{\theta_{\text{int}}}$ where there is visible upper thermal boundary layer thinning as a result of increasing Ra . This is further observed in the inset of figure 5.15a. However, it is of interest here to analyse the *dimensional* upper thermal boundary layer height as Ra is increased. With the interface (see table 5.7) and bulk (see figure 5.15a) temperatures approximately constant, all quantities on the rhs of (5.26) remain unchanged with Ra , and hence $\delta_{\theta_{\text{int}}}$ is also. If the thermal boundary layer on the water-side of the air-water interface remains the same thickness, then heat and mass transfer at the interface should indeed be controlled by the air-side conditions as is the case here. As such, we can now conclude that water-side natural convection does not play a role on evaporation rates at the free-surface, if the surface is assumed stationary as is the case here.

5.7 Conclusions

In this chapter, we have presented and validated an algorithm for dynamically predicting evaporation rates at an air-water interface in thermal convection. The simulation strategy builds on the work carried out in the previous chapter by eliminating the requirement for iterative simulations and calculating the evaporation rates locally and at each time-step. Over a series of LES in a cubic domain, the algorithm and simulation strategy were shown to accurately reproduce experimental measurements of evaporative mass flux and interface temperatures. The validation of the updated free-surface evaporation algorithm is therefore considered a success.

We then fixed the thermal boundary condition at the lower wall to be representative of the highest evaporation rate investigated, approaching the high-mass transfer conditions seen in the SFP. Following this, we carried out simulations where the aspect ratio was reduced from $\Gamma = 1$ (cubic), to $\Gamma = 1/2$ and $\Gamma = 1/4$. Using the results from all the LES over the Pr and Γ ranges, we extended the parameter space of the Ra - Nu scaling of the previous chapter and found the same exponent, $\sim Nu \propto Ra^{0.3}$. This represents a significant contribution to the literature on thermal convection.

The aspect ratio was shown to have an influence on the structure the LSC. For

the smallest aspect ratio investigated, the LSC changes from a steady single-roll to a non-single-roll state. As a result, the temperature field on the upper boundary was affected due to the location of the LSC impingement point. However, the time- and area-averaged free surface temperature and evaporation rate remained unchanged. We therefore conclude that the water-side turbulence and LSC state play no measurable role on the evaporation rate above, which remained steady as Ra was increased over two orders of magnitude (and Γ reduced to $1/4$).

Many of the observations on the influence of the aspect ratio on the state of the LSC, originally made in cylindrical containers, have been shown to be equally applicable in cuboidal domains. For instance, the likelihood of the single-roll state diminishes greatly in the lowest aspect ratio domain investigated here, and is dominant in domains of aspect ratio $\Gamma = 1$ and $1/2$. However, we observe that the eventual transition to a dual-roll state at low aspect ratio had no determinable impact on the heat transfer within the domain, at least within the accuracy of the LES carried out.

Chapter 6

Conclusions and future perspectives

In this final chapter, we provide our concluding remarks of the thesis followed by some perspectives on future research.

6.1 Concluding remarks

This thesis has focused on improving our understanding of thermal convection in water pools driven by free-surface evaporation above and a heated wall below. At each step, we have included further physics, in an attempt to understand the relative importance of the modelling assumptions.

First, we provided the governing equations and developed a low-Mach number solver to solve them, using the open-source CFD code, OpenFOAM® v1806. We subsequently used this code in the following three chapters, which represent three stand-alone numerical studies.

Secondly, we simulated a novel modified “turbulent RBC” set-up, whereby the classical configuration was updated with a shear-free upper boundary condition. This set-up was a first attempt to understand the impact of a free surface on turbulent RBC. Further, instead of modelling the evaporation directly, we assumed a fixed temperature drop across a cuboid domain. This temperature drop represented a larger value than that seen in reality, however, the aim was to assess the combined roles of the non-Oberbeck–Boussinesq conditions and the free-slip upper boundary.

Direct numerical and wall-resolved Large-Eddy Simulations of a thermal convective flow were presented over a range of $Ra = 10^7$ – 10^9 . The free-slip upper boundary condition was shown to increase convective heat transfer as a result of the fewer hydrodynamic boundary layers. Further, the first- and second-order statistics were also seen to be impacted, most noticeably in the removal of the homogeneity in the thermal boundary layer heights at the lower and upper boundaries. This was the first time such an observation had been made for a thermal convection configuration with a free surface. Moreover, we observed for the first time that the presence of the free-slip

shifts the mean temperature profile towards the temperature at the cold upper boundary. This latter observation has interesting consequences for nuclear safety studies and should be investigated further in any future experimental work.

We then carried out a turbulent kinetic energy budget at two locations for the DNS at $Ra = 10^7$; at mid-height and at mid-width. Both profiles showed that, in the bulk, the dominant term was the work of the mean pressure, which was balanced by the work of the fluctuating pressure and the turbulent kinetic energy dissipation. Interestingly, we also showed that the work of the mean pressure is dominant due to the hydrostatic component of the mean-pressure gradient but also depends on the density fluctuations which were small but critically, non-zero. In other words, even though the deviation from the Oberbeck–Boussinesq conditions were small with regard to the fluid density, the effect of this deviation can be significant.

Thirdly, a significant improvement to the numerical set-up was then made by prescribing a constant heat flux boundary condition above, representative of the evaporation occurring at an air-water interface. Over a series of direct-numerical simulations we were then able to analyse, for the first time, the effect of increasing evaporation rates on the water-side convection below the interface. Overall, five cases were investigated, with the heat flux applied at the upper boundary increased between each case. For the cubic domain of interest, a sixteenfold increase in evaporation rates was investigated, covering a range of Ra from 7.5×10^6 up to 1.3×10^8 for the convective flow beneath the interface.

In each case, the time-averaged temperature at the upper boundary showed significant spatial variation, but the time- and area-averaged value matched well with the predicted mean temperatures corresponding to the prescribed heat fluxes. In this chapter, we also provided for the first time, a power-law fit for the prediction of the dimensionless heat transfer in this particular thermal convection configuration, $Nu = 0.178Ra^{0.301}$. The observed exponent is similar to that seen in turbulent RBC between two rigid boundaries, and also to that seen between two free boundaries; in each case the exponent is unchanged ($\sim Ra^{0.3}$). A discrepancy is observed, however, in the prefactor accounting for the presence of the shear-free surface. Developing this power law for the novel configuration investigated has filled an important gap in, and is a valuable contribution to, the thermal convection literature.

Another observed consequence of the shear-free upper boundary, was the asymmetric large-scale circulation that formed. The LSC impinged the shear-free surface near one corner, whereupon it was accelerated, suggesting the presence of strong surface currents, before falling back down in the opposite corner. This acceleration led to inhomogeneous recirculation zones in the cubic geometry, which became taller and thinner with increasing Ra . As a result, we were able to conclude for the first time, that the free surface does indeed have an impact on the structure of the large-scale

circulation.

The shear-free upper boundary, with its spatially-variable temperature, again introduced inhomogeneities in the heights of thermal boundary layers between the lower wall and upper boundary. As a result, the mean temperature profile was again shifted in the bulk towards the cooler upper boundary temperature. This suggests that the shear-free boundary effect is more important than the non-Oberbeck–Boussinesq conditions which tend to have the opposite effect for water as the convecting fluid.

Lastly, a novel algorithm for dynamically predicting evaporation rates at an air-water interface was developed, implemented and validated. The simulation strategy built on the work carried out in the previous chapter by eliminating the requirement for iterative simulations and calculating the evaporation rates locally and at each time-step. Over a series of Large-Eddy Simulations in a cubic domain, the algorithm and simulation strategy were shown to accurately reproduce experimental measurements of evaporative mass flux and interface temperatures. To the best of our knowledge, this is the first time such an evaporation model has been implemented and validated in a CFD code.

Further studies at the highest evaporation rate were then carried out, investigating the aspect ratios of $\Gamma = 1/2$ and $\Gamma = 1/4$ for the first time. The aspect ratio was shown to have an influence on the structure, or state, of the LSC. For the smallest aspect ratio investigated, the LSC changed from a steady single-roll to a dual-roll state. As a result, the temperature field on the upper boundary was affected due to the location of the LSC impingement point. However, the time- and area-averaged free surface temperature and evaporation rate remained unchanged, at least within the accuracy of the LES carried out. We therefore conclude that the water-side turbulence and LSC structure play no measurable role on the evaporation rate above, which remained steady across two orders of magnitude of Ra and across all investigated Γ .

Finally, additional originality of this work lies in the finding that, many of the observations on aspect ratio influence on LSC states made in cylindrical containers, remain valid also in cuboidal domains. Specifically, the likelihood of the single-roll state diminished significantly in the lowest aspect ratio domain, and was dominant in domains of aspect ratio $\Gamma = 1$ and $1/2$. Finally, as Nu has been shown to be insensitive to the aspect ratio and Pr , it was permitted to use the predictions of all seven simulations carried out in the chapter to extend the parameter space of the Ra – Nu scaling developed in the previous chapter. We found the relation $Nu \propto Ra^{0.302}$, which is essentially the same exponent as that predicted in the DNS of the previous chapter.

The results of the thesis have been published in three separate scientific publications [67, 91, 107]. More practically, the results are industrially significant and useful for the nuclear industry with respect to the modelling of the early stages of an SFP-

LOCA with system codes. For example, the evaporation algorithm provided as figure 5.1 has been validated against experimental results and can be integrated into such system codes. Furthermore, these latter codes often require models and correlations. The Ra – Nu relation developed in chapter 4 is specific to the case of evaporation at a free surface when the bottom of the container is a uniformly heated wall. Such a relation is useful to the nuclear industry in its current state, however, improvements to the representativeness of the computational set-up would be required before such a correlation could be integrated into a system code.

6.2 Future perspectives

We now conclude the thesis by proposing potential future research avenues. Throughout this thesis, we have modelled thermal convection driven by the heat evacuated at a free surface of a water pool. However, the associated mass loss was not taken into account, and the inclusion of this aspect would represent an immediate improvement to the modelling approach. Furthermore, due to computational resource restrictions, we have not been able to simulate the Rayleigh numbers seen in industrial flows of this type. Moreover, the free-surface evaporation relevant to many industrial applications, often exists concurrently with other boiling phenomena. Finally, a uniformly heated lower wall below can be improved by modelling the geometry of any internal heat source more precisely. With these thoughts in mind, the paragraphs that follow are propositions for future research.

First, and as already mentioned, the maximum Ra investigated herein is limited by computational resources. We have carried out DNS up to a maximum of $Ra \approx 10^8$ and LES up to $Ra \approx 10^{10}$, whereas in one industrial example a realistically attainable Ra was shown to be the region of 10^{14} . In the literature, the highest Ra attained in a DNS of turbulent RBC is also $\approx 10^{14}$. These simulations required vast computational resources and even these were later shown to be under-resolved [120]. It is therefore interesting to consider the idea of how to attain higher Ra turbulent convection with LES.

In this thesis, we used the guidelines provided by Shishkina *et al.* [77] to calculate the required resolution of the (upper and lower) thermal and hydrodynamic boundary layers. Therein, the adopted Prandtl–Blasius theory assumes laminar boundary layers. The boundary layers in thermal convection are, however, expected to reach a turbulent state, at least intermittently, when Ra approaches 10^{14} . In chapter 5, we showed that it is difficult to obtain high Ra in LES when the cell size must expand significantly to ensure resolved boundary layers and a realistic total number of cells. One solution to this problem is to borrow from the turbulence literature in channel flows. Wherein, wall-models have been proposed to capture the physics of the boundary layers without

requiring their full resolution. To the authors knowledge, the same approach has not yet been adopted in thermal convection and could create valuable contributions to highly turbulent thermal convection literature.

Secondly, the role played by bubbles on the heat and momentum transfer in thermal convection is not well known and DNS could be used to further our understanding. A two-phase approach where nucleation, that is boiling, is simulated, is possible within a Volume-of-Fluid or level-set method; similar to the proposed numerical treatment in the Appendix. However, a simpler alternative would be to develop the single-phase code from this thesis into a Eulerian-Lagrangian approach so that bubbles can be *injected* and their effect measured.

There exists already experimental and numerical publications that have realised the role of bubbles in increasing heat transfer in classical natural convection configurations [121]. The presence of the rising bubbles was shown to slightly enhance heat flux in the domain and was attributed to droplet induced mixing. On the other hand, the temperature profile in the bulk was unaffected for the geometry investigated. The impact on the turbulent statistics was more significant where the rms of vertical velocity fluctuations in the bulk was increased by an order of magnitude. All of these conclusions were Ra -dependent; playing a less important role as Ra was increased. Such a method could be updated via the boundary conditions outlined in this thesis, and further, by incorporating a porous media approach to modelling the heat source. The conclusions of such a study would have both academic and industrial interest.

Lastly, depending on the application, a heated lower wall may not be appropriate to represent an internal heat source of complex geometry. An alternative is to model the exact geometry, which can be computationally expensive. Another option, which is relevant to the case of the SFP, is to consider the fuel racks as a heated porous medium, which would represent both a pressure drop and an internal heat source. If this avenue was pursued, the most obvious areas to research would be the mean flow properties.

One could examine how the porous media affects the Ra - Nu scaling in the domain, compared to the relations found in the literature and those developed herein. The roughness of the fuel assemblies, represented as the interface between the porous media and the upper volume, would have a significant role to play [110, 122–124]. Any disturbances to the lower thermal boundary layer would have an impact on the overall heat transfer scaling and could, according to some research, trigger the ultimate regime where $Nu \propto Ra^{0.5}$. The combined effect of the presence of bubbles and porous media on bulk temperature profile, and turbulent statistics should also be investigated. This work would feed in well to the development of closure models for both system and two-phase CFD codes.

Appendix A

A two-phase approach for simulating an evaporating free surface

In this Appendix, for completion purposes, we propose a mathematical formulation and a possible numerical treatment for capturing the full range of physics across an evaporating free surface. More specifically, in what follows, we propose a method that takes into account both the gas-side and the liquid-side flow.

The basic principle in the formulation presented below is that the liquid and fluid phase are not miscible. Accordingly, thermodynamic properties can be assigned values at any point in the fluid domain by introducing an indicator function, $f(\mathbf{x}, t)$, field which takes a value of 1 for the gaseous and 0 for the liquid phase. The density, or any other fluid property, is then calculated based on the local value,

$$\rho = \rho_l + (\rho_g - \rho_l) f, \quad (\text{A.1})$$

where the subscripts g and l stand for gas and liquid, respectively. The indicator function field is then advected via an equation similar to the following,

$$\frac{\partial f}{\partial t} + \mathbf{u}_\Gamma \cdot \nabla f = 0, \quad (\text{A.2})$$

where $\mathbf{u}_\Gamma$ is the interface velocity.

A set of governing equations can then be written, which is valid for both the liquid and gaseous phases. Such a single-field formulation necessitates the introduction of source terms to account for the role of the interface [125]. The continuity equation remains the same as in the single-phase governing equations, whereas, source terms appear on the rhs of both the momentum and the energy equations, related to surface tension and evaporation phenomenon, respectively. Further, a species conservation

equation is required for the water-vapour which is produced from the evaporation, so that the system of governing equations gives,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (\text{A.3})$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \nabla \cdot \boldsymbol{\tau} - \nabla p + \rho \mathbf{g} + \int_{\Gamma(t)} \gamma \kappa_{\Gamma} \mathbf{n}_{\Gamma} \delta(\mathbf{x} - \mathbf{x}_{\Gamma}) \, ds, \quad (\text{A.4})$$

$$\frac{\partial (\rho c_p T)}{\partial t} + \nabla \cdot (\rho c_p \mathbf{u} T) = \nabla \cdot (\lambda \nabla T) + \frac{dp_0(t)}{dt} - \int_{\Gamma(t)} \dot{m}'' h_{lv} \delta(\mathbf{x} - \mathbf{x}_{\Gamma}) \, ds, \quad (\text{A.5})$$

$$\frac{\partial (\rho Y_v)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_v) = \nabla \cdot (\rho D \nabla Y_v), \quad (\text{A.6})$$

where γ is the surface tension coefficient, κ_{Γ} is the interface curvature, $\mathbf{n}_{\Gamma}$ is the unit normal at the interface, δ is a Dirac delta function, which is non-zero at an interface (that is at $\mathbf{x}_{\Gamma}$) only, $\dot{m}''$ is the evaporative mass flux and h_{lv} is the latent heat of vapourisation. Also, in (A.6), Y_v is the vapour concentration and D is the mass diffusivity of water vapour in air.

The surface tension force term is included in (A.4) for completion purposes above. However, from hereon its contribution is ignored, as it is negligible for the case of thermal convection driven by an evaporating free surface with no boiling. Further, due to the open domain, the term $\frac{dp_0(t)}{dt}$ in (A.5) is zero for the applications of interest here.

We next consider any control volume containing a gaseous phase on top of a liquid. The transition zone between the two phases is very thin and, as such, the interface is considered as a discontinuity, dividing two separate control volumes. Integrating (A.3)–(A.6) over these two control volumes and adding the results, provides the jump relations that hold across the interface [126]. First, we have the jump relation for the continuity equation, (A.3), which states that the mass is conserved across the interface,

$$\dot{m}'' = \rho_l (\mathbf{u}_l - \mathbf{u}_{\Gamma}) \cdot \mathbf{n}_{\Gamma} = \rho_g (\mathbf{u}_g - \mathbf{u}_{\Gamma}) \cdot \mathbf{n}_{\Gamma}, \quad (\text{A.7})$$

which can be manipulated to give a relation for the interface velocity, $\mathbf{u}_{\Gamma}$

$$\mathbf{u}_{\Gamma} \cdot \mathbf{n}_{\Gamma} = \frac{1}{2} (\mathbf{u}_l + \mathbf{u}_g) \cdot \mathbf{n}_{\Gamma} - \frac{\dot{m}''}{2} \left(\frac{1}{\rho_l} + \frac{1}{\rho_g} \right), \quad (\text{A.8})$$

Or, equally, (A.7) can be manipulated to give the following relation for the difference between the gas and liquid velocities,

$$(\mathbf{u}_g - \mathbf{u}_l) \cdot \mathbf{n}_{\Gamma} = \dot{m}'' \left(\frac{1}{\rho_g} - \frac{1}{\rho_l} \right). \quad (\text{A.9})$$

The momentum equation, (A.4), jump relation gives,

$$\dot{m}'' (\mathbf{u}_g - \mathbf{u}_l) = (\boldsymbol{\tau}_g - \boldsymbol{\tau}_l) \cdot \mathbf{n}_\Gamma - (p_g - p_l) \mathbf{I} \cdot \mathbf{n}_\Gamma. \quad (\text{A.10})$$

Taking the inner product of (A.10) with $\mathbf{n}_\Gamma$ and combining with (A.9), we get the following relation,

$$\dot{m}''^2 \left(\frac{1}{\rho_g} - \frac{1}{\rho_l} \right) = ((\boldsymbol{\tau}_g - \boldsymbol{\tau}_l) \cdot \mathbf{n}_\Gamma) \cdot \mathbf{n}_\Gamma - (p_g - p_l). \quad (\text{A.11})$$

Then, the energy equation, (A.5), gives,

$$\dot{m}'' (h_{lv} + (c_{p_g} - c_{p_l}) T_\Gamma) = \lambda_g (\mathbf{n}_\Gamma \cdot \boldsymbol{\nabla} T)_g - \lambda_l (\mathbf{n}_\Gamma \cdot \boldsymbol{\nabla} T)_l, \quad (\text{A.12})$$

whereas, the jump relation for the water vapour species equation, (A.6), jump relation gives,

$$\dot{m}'' (1 - Y_v) = \rho_g D (\mathbf{n}_\Gamma \cdot \boldsymbol{\nabla} Y_v), \quad (\text{A.13})$$

where ρ_g and Y_v are evaluated at the interface. First, the gaseous density for the bi-component mixture of air and water vapour is determined from,

$$\rho_g = \frac{M_w p_v}{RT} + \frac{M_a (p_0 - p_v)}{RT}. \quad (\text{A.14})$$

Then, the vapour concentration at the interface is found from,

$$Y_{v,\Gamma} = \frac{p_{v,\Gamma} M_w}{p_{v,\Gamma} M_w + (p_0 - p_v) M_a}. \quad (\text{A.15})$$

The vapour pressure at the interface, $p_{v,\Gamma}$, is assumed to be at saturation. As in the earlier chapters, we find $p_{v,\Gamma}$ from a Wagner equation [97] of the following form,

$$p_{v,\Gamma} = p_c \exp((a\tau + b\tau^{1.5} + c\tau^3 + d\tau^6)/T_r), \quad (\text{A.16})$$

where p_c and T_c are respectively the critical pressure and temperature, $T_r = T_\Gamma/T_c$ is the reduced temperature and $\tau = 1 - T_r$, with the constants available in the literature [115].

A possible solution procedure can then be formulated as follows,

1. Estimate $\dot{m}''$ from (A.13)
2. Estimate $\mathbf{u}_\Gamma \cdot \mathbf{n}_\Gamma$ from (A.8)
3. Apply numerical method to solve (A.2) and hence compute new interface location
4. Integrate the energy equation, (A.5), ensuring that (A.12) is satisfied

5. Calculate $p_{v,\Gamma}$ from (A.16)
6. Calculate $Y_{v,\Gamma}$ from (A.15)
7. Integrate vapour species equation, (A.6), using $Y_{v,\Gamma}$ as boundary condition
8. Integrate momentum equation, (A.4), ensuring that (A.11) is satisfied to find $\mathbf{u}$ and p .

The above system of equations can be treated numerically via a front-tracking [127], Volume-of-Fluid [128] or immersed boundary [129] method. All of these methods solve a single set of governing equations for the whole domain and treat the different phases as one fluid with variable thermodynamic properties. The difference is in how the interface is advected, that is step 3 of the above proposed algorithm.

Finally, it is worth mentioning that enforcing jumps across the interface is a far from trivial task and all the numerical treatments proposed above are computationally demanding due to interfacial resolution requirements.

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