

École polytechnique de Louvain

Numerical Study of Natural Convection Driven Turbulence in a Spent Nuclear-Fuel Pool

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1 Introduction

1.1 Context

Since the Fukushima Daiichi nuclear disaster on 11 March 2011, particular attention has been paid to the study of nuclear Spent Fuel Pools (SFP). These pools, located on the power plant site, are designed so that the water cools the spent fuel by absorbing its decay heat and provides shielding from radiation emitted during its decay.

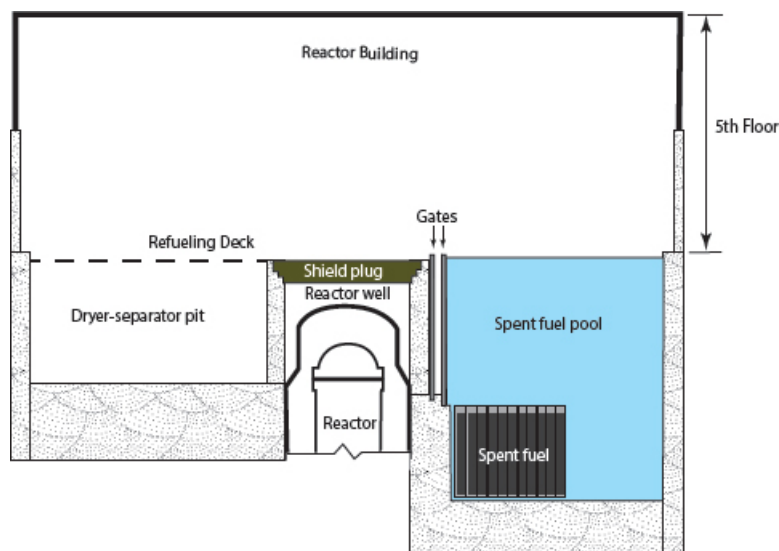


Figure 1: Schematic cross section of the upper portion of a BWR Mark I reactor building showing the configuration of the refueling deck in Units 1-3 of the Fukushima Daiichi plant on March 11, 2011. [1].

On the figure 1, we can observe a schematic cross section of the type of reactor present on the Fukushima Daiichi plant on 11 March 2011. It shows that the pools are located adjacent to the reactor containment building. Dimensions of these pools on Fukushima Daiichi plant are summarized in the table 1.

Table 1: Spent Fuel Storage at the Fukushima Daiichi Plant on March 11, 2011 [1]

Unit number	Decay Heat [MW]	Water Volume [m ³]	Lateral Dimensions [m]	Height [m]
1	0.18	990	12 × 7.2	12
2	0.62	1.390	12.2 × 9.9	12
3	0.54	1.390	12.2 × 9.9	12
4	2.26	1.390	12.2 × 9.9	12

In this accident, the Tōhoku earthquake followed by a tsunami led to the loss of the cooling systems of the nuclear power plant. In addition of the core meltdown of several reactors due to the loss-of-coolant-accident (LOCA), the spent fuel pool of previously shut-down Reactor 4 lost its cooling system and was seen emitting water vapour. During such a prolonged interruption of cooling, there is a risk that the water of the SFP boils off due to the decay heat of the spent fuel rods, potentially leading to an exposure of the fuel and a release of radioactive elements into the atmosphere.

In the absence of forced cooling, the natural evolution of a system like a spent fuel pool will lead to the emergence of complex physical phenomena such as thermally driven turbulence.

In this work, we will focus on this phenomenon by the study of the Rayleigh-Bénard convection. We aim to develop and validate numerical tools that can be used to further study the full problem of nuclear spent fuel pools in the case of cooling system failure.

1.2 Rayleigh-Bénard convection

Thermally driven turbulence is a physical phenomenon occurring in many natural processes and is used in various engineering systems. Such flows can be observed at wide range of scales. For example, it is a subject of study at both larger length scales and timescales in atmospheric convection [2] for climate calculations and smaller scales for weather predictions. This type of convection is also a main driving mechanism in the Earth's outer core [3] or even in ocean circulation [4]. Its technical applications range from miniaturized heat exchangers for the cooling of electronic components to the cooling of fuel assemblies in nuclear Spent-Fuel Pools of large power plants.

The physical mechanisms and equations governing such a thermally driven turbulence are very complex. Unlike in the case of homogeneous and isotropic turbulence (HIT) [5], in the case of thermally driven flows, the temperature cannot generally be considered as a passive scalar and the fluid motion is triggered by buoyancy due to density variations in presence of a gravitational field and specific boundary conditions.

In fluid mechanics, this challenging problem has been studied in the form of the turbulent Rayleigh-Bénard convection (RBC). This idealized system consists in the motion of a fluid layer of height H heated from below and cooled from above. Since the flow and thermal dynamics of such a convection depend on the geometrical setup, the temperature difference between the two horizontal boundaries and the fluid properties, these latter are cast into two dimensionless numbers known as the Rayleigh number Ra and the Prandtl number Pr .

$$Ra \equiv \frac{g\beta\Delta TH^3}{\nu\alpha} \quad \text{and} \quad Pr \equiv \frac{\nu}{\alpha} \quad (1)$$

where g is the acceleration due to gravity, β the thermal expansion coefficient, $\Delta T = (T_h - T_c)$ and H are respectively the temperature difference and the distance between the hot (T_h) and cold (T_c) horizontal plates, ν is the molecular kinematic viscosity and α the thermal diffusivity of the fluid.

The Rayleigh number measures the relative importance between the effects of the buoyancy forces and the product of the thermal and momentum diffusivities. Therefore this dimensionless number characterises the fluid's flow regime and is a good indication as to whether the natural convection flow is laminar or turbulent [6].

The Prandtl is, for its part, a characteristic of the fluid only. It represents the ratio of momentum diffusivity to heat diffusivity in a fluid.

In addition to Ra and Pr , a third important control parameter of Rayleigh-Bénard convection is the aspect ratio of the container

$$\Gamma = \frac{L}{H} \quad (2)$$

where L is either the lateral size of the Rayleigh-Bénard cell in the case of a rectangular cell or the diameter of the cylinder in the case of a cylindrical cell. These two set-ups are the most commonly used in the study of Rayleigh-Bénard convection.

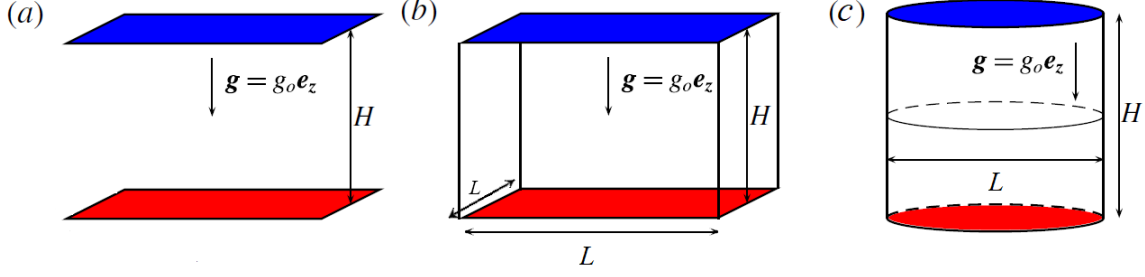


Figure 2: Schematic showing common Rayleigh-Bénard convection set-ups. (a) An infinitely extended fluid layer of height H heated from below and cooled from above. (b) A typical RB convection set-up in a rectangular cell of aspect ratio $\Gamma = \frac{L}{H}$. Cubic cell corresponds to the particular case $\Gamma = 1$. (c) Another typical RB convection set-up in a cylindrical cell of aspect ratio $\Gamma = \frac{L}{H}$. In each case, the red and blue surfaces correspond respectively to the hot and cold boundaries maintained at constant temperatures T_h and T_c . Figure adapted from [7].

A major challenge in the study of the Rayleigh-Bénard convection is the understanding of the turbulent transport mechanisms of heat across the fluid layer. The grasp of the effectiveness of the heat transport as a function of Pr and Ra is fundamental for industrial applications such as design of cooling devices on semiconductor or nuclear power plants. In our case, this heat transport is measured by the upward heat flux through the cell. The corresponding dimensionless number is the Nusselt number

$$Nu = \frac{\dot{q}H}{\alpha\Delta T} \quad (3)$$

defined as the quantity of heat per unit of surface $\dot{q}$ transferred between the hot and cold surfaces, normalized with the conductive heat $(\alpha\Delta T)/H$ which is the heat transferred in absence of convective motion [8].

Another dimensionless number of interest to measure the system response to the imposed control parameters we have just defined is the Reynolds number

$$Re = \frac{UH}{\nu} \quad (4)$$

determining the regime of the flow.

We have just seen that in thermal convection in a given cell, the control parameters are the Rayleigh number Ra and the Prandtl number Pr . The system responds with the Nusselt number Nu and the Reynolds number Re . The key is now to understand the dependences $Nu(Ra, Pr)$ and $Re(Ra, Pr)$. However, despite a thorough investigation in the past, a unifying theory for such dependences is still not fully achieved (see Section 2).

In the simplified case where fluid properties do not change with the temperature, one can obtain that, for a given fluid and for a given aspect ratio, Rayleigh-Bénard convection is only controlled by the Rayleigh number.

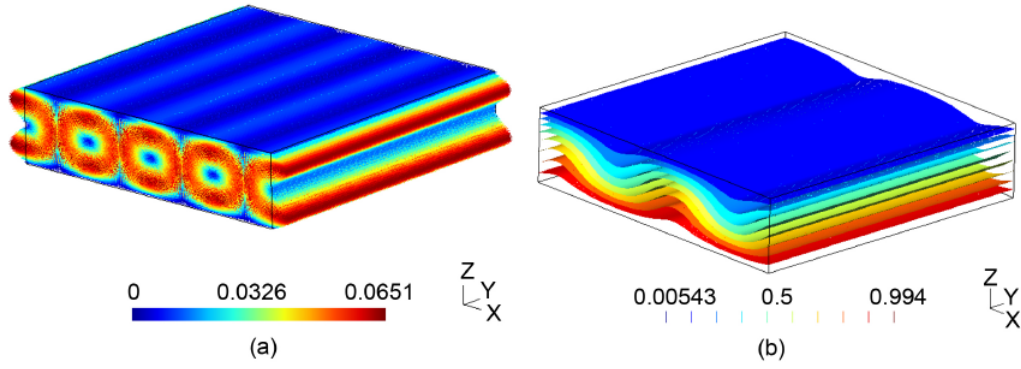


Figure 3: Roll structures at steady state for $Ra = 5000$. (a) Velocity field, $Ra = 5000$. (b) Temperature field, $Ra = 5000$. Figure from [10].

When Ra is smaller than a critical value Ra_c , the driving effect due to buoyancy is not strong enough to overcome the viscosity. In this case, fluid is at rest and the thermal flux is purely due to conduction. This critical value has been found to be dependent on the aspect ratio and being equal to

$$Ra_c(\Gamma = \infty) = 1708$$

for a fluid layer of infinite width and finite height [9]. When the flow enters supercritical regime, i.e. $Ra \geq Ra_c$, flow enters a regime of laminar convection depicting a steady pattern of roll cells. These roll cells are driven by buoyancy forces. Such convection cells is illustrated on figure 3 for the case of infinite plates.

As the Rayleigh number is increased, the pattern becomes more complex allowing more complex stable structures to develop. When Ra becomes greater than a certain value Ra_t , the flow enters a turbulent regime leading to the vanishing of the previous steady structures except for a single roll known as the large scale convection roll. The mechanisms driving the bifurcation from laminar Rayleigh-Bénard convection to turbulent Rayleigh-Bénard convection have been the subject of several studies but is beyond the scope of this work (see [11] and [12]).

Rayleigh-Bénard convection has the benefit to be both mathematically well-defined and relatively straightforwardly achievable experimentally, e.g. using particle image velocimetry (PIV). A comparison can be made with the previously mentioned homogeneous isotropic turbulence whose mathematical description is well known [13]. A significant proportion of theoretical and numerical works on the scaling of structure functions and energy spectra of turbulent flows focused on HIT. However, the laboratory and field measurements are much less abundant due to the difficulty of satisfying the homogeneity and isotropy conditions experimentally.

1.3 From Nuclear Spent Fuel Pool to Rayleigh-Bénard convection

In this Master thesis, we intend to study the flow inside a Spent Fuel Pool (SFP), see figure 4.

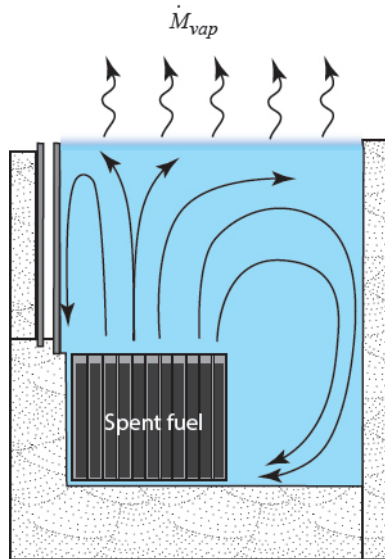


Figure 4: Schematic of spent fuel pool showing the circulation pattern created by the buoyant plume of hot water above the spent fuel [1].

However, as showed on figure 5, this problem is in practice extremely complex since it involves intricate phenomena to model :

- Thermally driven turbulence and natural convection.
- Heat and mass transfer at the top free surface, i.e. the interface air/water with energy removal by vaporisation.
- Decrease of the water level.
- Two-phase flow in the boiling region near the free surface
- Complex geometry of the assembly, may be considered as a porous medium depending on fuel rack occupancy.
- Potential heat losses at concrete walls
- The uneven cooling of fuel assemblies (caused by unstable circulation and flow reversal inside the fuel assemblies) can lead to nucleate boiling at the surface of certain rods. This scenario could create a criticality issue and thus needs to be avoided [16].

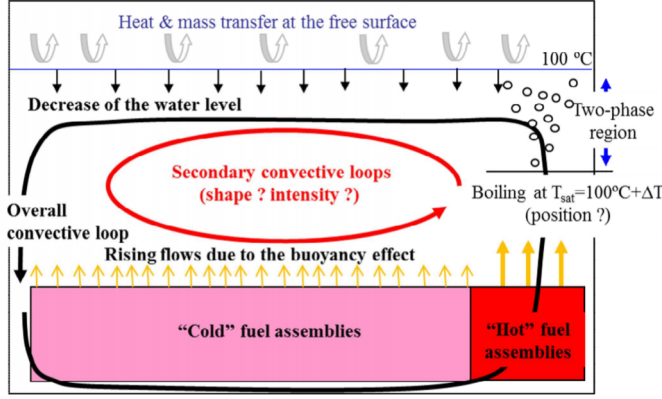


Figure 5: Schematic synthesis of natural convection and boiling phenomena in a spent fuel pool [16].

We thus have to create a simplified model of this problem by making some strong assumptions that will need to be gradually removed in further works.

In this work, we will bring back this problem to the classical Rayleigh-Bénard convection by only considering the upper part of the SFP (allowing us to ignore the geometry of the assembly) and assuming the bottom surface to remain at a constant temperature.

As a second assumption, we will ignore the top free surface and will consider it as a rigid wall maintained at a constant temperature.

These assumptions are summarised on the figure 6 showing the general set-up of our model and its boundary conditions.

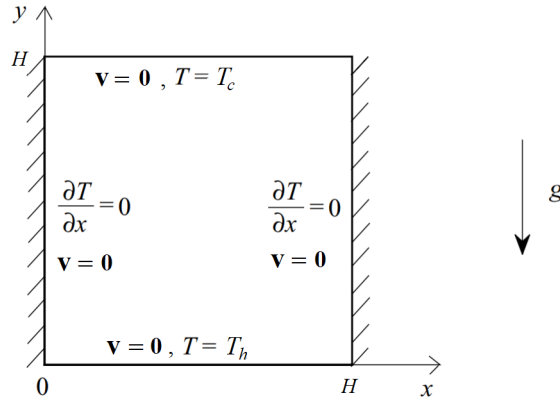


Figure 6: Rayleigh-Bénard convection set-up as a simplified model for SFP used in this work. Boundary conditions are the following : all walls are rigid implying a no-slip condition (i.e. the velocity vector $\mathbf{v}$ is the null vector), top and bottom walls are maintained at constant temperature T_c and T_h and lateral walls are adiabatic.

1.4 Study tools

Numerical study is an essential tool in order to investigate the mechanisms of Rayleigh-Bénard convection and predict the response of such systems existing in nature or in the industry. Even with a mathematically well-defined problem, a purely analytical investigation of fluid mechanics has strong limitations due to the complexity of the set of coupled and nonlinear partial differential equations governing the system known as Navier-Stokes equations. Furthermore, the design and set-up of practical

experiments can be costly. In this context, computational fluid dynamics (CFD) takes an important role in the study of quantities of interest in this type of convection.

Direct Numerical Simulations (DNS) resolves the whole range of spatial and temporal scales of the turbulence, the smallest turbulent scales being known as Kolmogorov microscales. Although this method provides highly accurate results, its computational cost may become a limiting factor when simulating highly turbulent flows represented by large Ra for Rayleigh-Bénard convection.

Therefore, we need to rely on less computationally expensive methods in order to achieve high Ra simulations.

Reynolds-Averaged Navier-Stokes (RANS) only resolves the mean flow and models the fluctuations by solving time-averaged equations and adding a turbulent model to it. This method provides a cheap solution but its accuracy strongly depends on the model reliability.

Large-Eddy Simulations (LES) uses a mathematical model for small turbulent scales so that the mass, momentum and energy equations are space filtered. This implies that the most important scales of the turbulence remain resolved while the smallest ones are unresolved and their effect is taken into account by properly introducing additional terms in the equations. These unresolved terms are known as sub-grid scales (SGS) models and their reliability for a given problem has to be validated against reference results, whether numerical or experimental. The computational cost of this method is greater than for RANS but still much lesser than DNS. Furthermore, the influence of the model is weaker for LES than for RANS, leading to more reliable simulations.

1.5 Objectives of the thesis

The Papalexandris Miltiadis Research Group, as a team of the Thermodynamics and fluid mechanics (TFL) division of the Institute of Mechanics, Materials and Civil Engineering (iMMC) of the Université catholique de Louvain (UCLouvain), conducts research around the study of natural convection and evaporation in wet-storage pools of spent nuclear fuel. The information obtained from this study will complement the other computational results obtained by the research group (these will not be discussed in this study).

In this work, we will carry out both Direct Numerical and wall resolved Large-Eddy Simulations of Rayleigh-Bénard convection problem defined above and compare their predictions with the open-source CFD package OpenFOAM. Particularly, we aim to validate two dynamic sub-grid scales models for our application. The selected SGS models are the following :

- Dynamic- k equation model [14]
- Lagrangian dynamic model [15]

A more in-depth description of these SGS models and of the solver used will be presented further in this work (see Section 3).

More specifically, the control parameters of the simulations carried out in this work are the following :

- *Aspect ratio* : Cubical cavity : $\Gamma = 1$
- *Prandtl number* : Fluid is air at operating mean temperature of 313[K] : $Pr = 0.7$.

- *Rayleigh number* :
 - DNS : Ra ranging from 10^6 to $5 \cdot 10^7$
 - LES : Ra ranging from 10^6 to 10^9
- *Temperature difference between the top and bottom surface* : $\Delta T = 15$ [K].

To sum up, the objective of this work is to validate two SGS models by comparing numerical results obtained with LES against DNS results. LES simulations will be further carried out for larger Rayleigh numbers (i.e. $Ra \geq 10^8$) that are complex performed by DNS with the available resources due to computational cost.

2 State of the art

In this section, we aim to establish the state of the art of some topics that have received a particular attention from the scientific community about Rayleigh-Bénard convection during the last decades. The first topic concerns the scaling properties of the system response, i.e. the dependence of the Nusselt number on Rayleigh and Prandtl numbers.

A second discussed topic will be the scaling of Kolmogorov, Batchelor, Taylor and Bolgiano length scales inside Rayleigh-Bénard convection and their impact on the mesh requirement for Direct Numerical and Large Eddy Simulations.

2.1 Nusselt number scaling with Ra

As presented before, the Nusselt number is a representative measurement of the thermal transport inside the Rayleigh-Bénard convection cell. This system response is of tremendous importance for most technological application of thermally driven convection, including in nuclear spent fuel pool design and analysis.

Therefore a large number of investigation have been led in the past in order to characterise the dependence of Nu on Ra and Pr .

Most theories developed prior to the two last decades predicted power-laws for the scaling of $Nu(Ra, Pr)$ and $Re(Ra, Pr)$ [17]. These power-laws can be written under the general form

$$Nu \sim Ra^{\gamma_{Nu}} Pr^{\alpha_{Nu}}, \quad (5)$$

$$Re \sim Ra^{\gamma_{Re}} Pr^{\alpha_{Re}}, \quad (6)$$

where γ_{Nu} and α_{Nu} are the power law exponent for Nu scaling and γ_{Re} and α_{Re} are the power-law exponent for Re scaling. These exponents have taken different values depending on the theory used and early experiments were only consistent with these dependences over quite restrictive ranges of Ra and Pr . For the sake of simplicity, we will mainly focus our review on γ_{Nu} (i.e. Nu dependence on Ra) since the Prandtl number is kept as $Pr = 0.7$ in all our simulations. We will thus simplify the notation of relation (5) to

$$Nu \sim Ra^{\gamma} \quad (7)$$

Malkus's marginal-stability theory have been established in 1954 and seemed to describe well some of the early experiments conducted at this time. This theory is based on the assumption that the thermal boundary layer thickness grows so as the local Rayleigh number Ra_l (defined with local quantities within the boundary layers) reaches the critical Rayleigh number Ra_c presented in previous section. This theory leads to the power-law exponent $\gamma = \frac{1}{3}$ in such a manner that

$$Nu \sim Ra^{\frac{1}{3}}. \quad (8)$$

However, in the late 1980s, a new theory based on mixing length theory and motivated by ground-breaking experiment [20] led to a new scaling for the Nusselt number :

$$Nu \sim Ra^{\frac{2}{7}}. \quad (9)$$

This theory is based on the following decomposition of Rayleigh-Bénard convection domain. It supposes three layers :

1. A mixed core, with velocity and temperature fluctuations independent of the vertical coordinate.

2. A thermal boundary layer of thickness $\lambda_\theta \sim Nu^{-1}$ along the wall.
3. An intermediate regime dominated by thermal plumes, i.e. thin (thickness of the same magnitude as boundary layers) and hot (temperature close to the wall temperature) sheets detaching from the wall.

The $2/7$ power-law exponent has also been obtained from another theory assuming turbulent boundary layers [21].

However the assumptions made in each theory are very different from each other and the scaling of Nu with Pr predicted by these two theories are not matching.

Furthermore, it has been showed by several experiments (e.g. [22]) that this $\gamma = \frac{2}{7}$ regime does not hold anymore at very large Rayleigh number. At this point, the exact value of this *large* Rayleigh number is not clearly defined and seems to vary with the Prandtl number (a typical range for $0 < Pr \leq 1$, is $Ra \sim 5 \times 10^8 - 10^{11}$) [19].

Considering the previous information, it has been shown that none of the power-laws we defined in this section are sufficiently reliable to predict the behaviour of Rayleigh-Bénard convection for all Rayleigh numbers.

In the last two decades, a unifying theory has been proposed by Grossmann and Lohse [23]. This theory is based on the following set of equations for the kinetic and thermal energy-dissipation rates

$$\langle \epsilon_u \rangle_{t,V} \equiv \nu \sum_i \sum_j \left\langle \left(\frac{\partial u_i(\mathbf{x}, t)}{\partial x_j} \right)^2 \right\rangle_{t,V} = \frac{\nu^3}{H^4} (Nu - 1) Ra Pr^{-2} \quad (10)$$

$$\langle \epsilon_\theta \rangle_{t,V} \equiv \alpha \sum_j \left\langle \left(\frac{\partial \theta(\mathbf{x}, t)}{\partial x_j} \right)^2 \right\rangle_{t,V} = \alpha \frac{\Delta T^2}{H^2} Nu \quad (11)$$

Here, the operator $\langle \cdot \rangle_{t,V}$ denotes the average over time and volume.

Equations 10 and 11 are analytically derived from the Boussinesq equations, as these are widely used for Rayleigh-Bénard convection.

The novel idea is to split the kinetic and thermal energy-dissipation rates into two contributions, bulk contribution and boundary layer contribution. This splitting is motivated by the fact that the physics behind dissipation in these two sub-domains are fundamentally different and thus needs a different model for each.

Figure 7 shows such a boundary-bulk partition. One can observe that the thermal plumes are modelled as a thermal boundary layer by this theory and has the same thickness as these ones, i.e. λ_θ . Other assumptions of this theory are the existence of a large scale wind of typical velocity scale U and that the kinetic boundary layers are modelled with the same thickness λ_u regardless of their position along the walls.

These boundary layers thickness are obtained from the classical Prandtl-Blasius boundary layer theory.

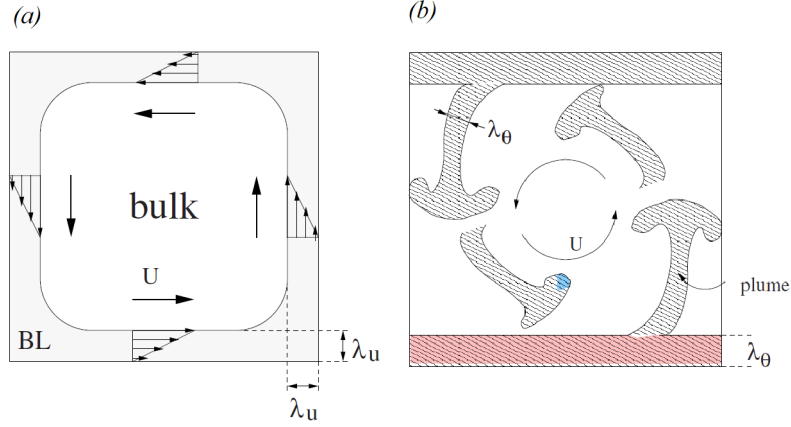


Figure 7: Boundary-bulk partition in a cubical domain. In both figures, (a) kinetic boundary layer and (b) thermal boundary layer, the large scale convection roll with typical velocity amplitude U is sketched. The typical width of the kinetic boundary layer is λ_u , whereas the typical thermal boundary layer thickness and the plume thickness are λ_θ . Figure adapted from [18].

One important outcome of the Grossmann and Lohse theory is the phase diagram represented on the figure 8. This diagram in the $Ra-Pr$ plane shows the different domains, each corresponding to a particular power-law, associated with the couple of parameter (Ra, Pr) . As presented on this diagram, according to this theory, the simulations performed in this work with $Pr = 0.7$ and Ra ranging from 10^6 to 10^9 should cover two specific regimes : II_l and IV_l . According to [24], these regimes correspond to boundary layers such that $\lambda_\theta > \lambda_u$ and the following scalings,

$$II_l \text{ regime : } Nu \sim Ra^{\frac{1}{5}} Pr^{\frac{1}{5}} \quad (12)$$

$$IV_l \text{ regime : } Nu \sim Ra^{\frac{1}{2}} Pr^{\frac{1}{2}} \quad (13)$$

with a transition between these two regimes estimated around $Ra = 10^8$.

Another remarkable result of this theory is the scaling $Re \sim Nu^2$.

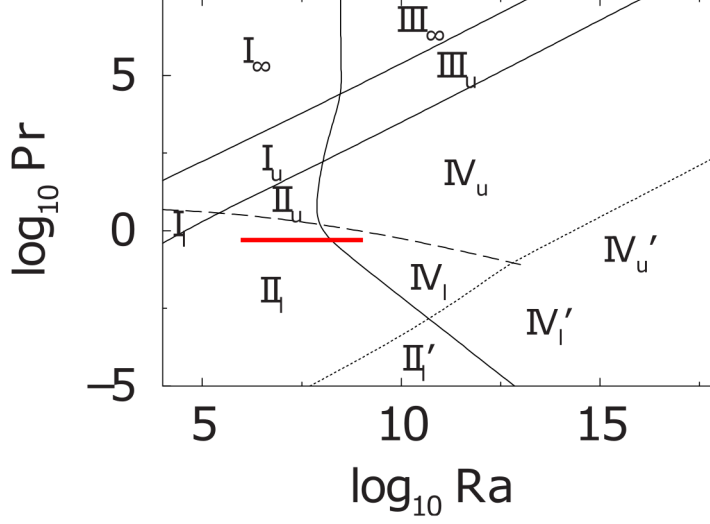


Figure 8: Logarithmic phase diagram in Ra-Pr plane of Rayleigh-Bénard convection regimes identified in Grossmann and Lohse theory. The red line corresponds to the range of numerical simulations performed in this work (i.e. $Pr = 0.7$ and $Ra = 10^6 - 10^9$). The figure is adapted from [18].

Nevertheless, even though this theory is far more robust than the earlier suggested power-laws, this theory has some limitations. As mentioned previously, this theory is built on the Prandtl-Blasius theory, considering temperature as a passive scalar. However, this assumption is obviously not correct in the case of thermally driven turbulence. Therefore, mechanisms such as plume detachment process are probably not properly taken into account in this model and needs further study [18].

2.2 Mesh resolution and length scales

Since we are interested in numerical simulations of Rayleigh-Bénard convection based on DNS and wall-resolved LES methods, it is important to define and quantify the different length scales to be resolved by both methods in order to properly define the grid resolution of our simulations. Indeed, for DNS, every dissipative scales, down to the smallest (i.e. Kolmogorov microscales η), have to be captured by our mesh in order to get accurate results. On the other hand, LES will model these smallest scales using the SGS models. Traditional turbulence theory [25] suggests to truncate the resolved scales in the inertial subrange lying between the integral scale and the Kolmogorov microscale. A more detailed explanation of LES concept and equations will be done later in this work (see Section 3.4).

In this section, we thus intend to define *a priori* rules to properly construct our meshes based on physical analysis of the problem.

Empirical investigation of the mesh resolution requirements in the wall region can turn out to be a harsh task and intensive in computational cost. Indeed, solution accuracy does not only depend on the grid resolution in the boundary layers but also on the mesh resolution in the bulk. Henceforth, purely empirical investigation for the whole mesh resolution requirements needs to be avoided.

As a starting point, we can divide our domain into two sub-domains.

The first one is the bulk of the Rayleigh-Bénard convection cell where we can observe large scale convection. In this region, we aim to use a coarser mesh for the LES than for the DNS in order to reduce computational costs.

In the other hand, we have the wall region, i.e. the boundary layers, of which all scales have to be

resolved by both DNS and wall-resolved LES.

2.2.1 Bulk Resolution Requirements - DNS

As a first step, we can define the resolution requirement in the bulk of the convection cell. In a perfect DNS, the local mesh size should be smaller than the local Kolmogorov scales $\eta_K(\mathbf{x}, t)$ and than the Batchelor scales $\eta_B(\mathbf{x}, t)$ [31].

In order to have a general condition for the global mesh size h^{global} , we introduce global Kolmogorov scale [25] η_K which is defined with the energy dissipation rate of the velocity itself already defined in equation (10), leading to

$$\eta_K = \left(\frac{\nu^3}{\langle \epsilon_u \rangle_{t,V}} \right)^{1/4} = \frac{Pr^{1/2}}{Ra^{1/4}(Nu - 1)^{1/4}} H. \quad (14)$$

In order to capture these scales, the global mesh size h^{global} has to be smaller than η_K . This results in the following requirement on h^{DNS} ,

$$h^{DNS} \leq \frac{Pr^{1/2}}{Ra^{1/4}(Nu - 1)^{1/4}} H. \quad (15)$$

If we focus on the definition of Batchelor microscales, we can draw a relation between these microscales and Kolmogorov ones :

$$\eta_B = \left(\frac{\nu \alpha^2}{\langle \epsilon_u \rangle_{t,V}} \right)^{1/4} = \eta_K Pr^{-1/2} \quad (16)$$

Since our case of interest is at $Pr = 0.7$, we obtain $\eta_B > \eta_K$ and in comparison with grid resolution, the Kolmogorov microscales are the most restrictive ones. We can therefore sum up the resolution criterion to the relation (15) for our DNS.

It is worth noting that specifically for $Pr \leq 1$, a less restrictive criterion is used by [39] and [40], i.e.

$$h^{DNS} \leq \pi \eta \quad (17)$$

allowing mesh cells in the bulk to be larger by a factor π than equation (15). This choice is motivated by the enormous computing cost of the first criterion and the small error induced by the selection of the less restrictive criterion compared to the considerable reduction of computing effort.

2.2.2 Boundary Layers Resolution Requirements - DNS and wall-resolved LES

It now remains to study the boundary layer structure. It has been showed by Zhou *et al.* [26] in the last decade that experimental and numerical boundary layer profiles in Rayleigh-Bénard convection are in really good agreement with the well known Prandtl-Blasius profiles [27] [28]. From the Prandtl-Blasius boundary layer theory, it is possible to derive analytical approximation for the kinetic and thermal boundary layers, respectively λ_u and λ_θ . According to this theory and the developments of Shishkina *et al.* [29], we obtain the following relations for the boundary layers thickness

$$\lambda_\theta = \frac{H}{Nu} \quad (18)$$

$$\lambda_u = \begin{cases} 0.5Nu^{-1}Pr^{1/2}A^{-1}\pi^{-1/2}H, A \approx 0.332 & Pr < 3 \times 10^{-4} \\ 0.5Nu^{-1}Pr^{0.357-0.022 \log Pr}H & 3 \times 10^{-4} \leq Pr \leq 3 \\ 0.5Nu^{-1}Pr^{1/3}E^{-1}H, E \approx 0.982 & Pr > 3 \end{cases} \quad (19)$$

Finally, we found that our case of interest corresponds to a ratio $\frac{\lambda_\theta}{\lambda_u} > 1$ over the whole range of Ra considered, which is in perfect agreement with the Grossmann and Lohse theory presented in the previous section.

We now come to the resolution requirements within these boundary layers. In a perfect DNS, the local mesh size should be smaller than the local Kolmogorov scales $\eta_K(\mathbf{x}, t)$ and than the Batchelor scales $\eta_B(\mathbf{x}, t)$ but also ensure sufficient resolution in the boundary layers. If DNS is underresolved, the measured Nusselt number is overestimated [30].

Shishkina *et al.* [29] derived a theory-based criterion for the grid resolution inside the thermal and kinematic boundary layers based on the Prandtl-Blasius theory. For the case of $Pr \approx 0.7$, they obtained that the minimum numbers of nodes $N_{th,BL}$ and $N_{v,BL}$ placed respectively within the thermal and viscous boundary layers have to satisfy the criterion

$$N_{th,BL} \geq 0.35Ra^{0.15}, \quad 10^6 \leq Ra \leq 10^{10} \quad (20)$$

$$N_{v,BL} \geq 0.311Ra^{0.15}, \quad 10^6 \leq Ra \leq 10^{10} \quad (21)$$

These requirements stand for the boundary layers along the heating and cooling walls. However, as a matter of prudence, we will consider the same mesh resolution in the x , y and z directions even if coarser resolution for lateral directions can be found in the literature. In such a wall-bounded flow, the near wall flow structures are of very small size compared to the large scales flow structures and need to be well resolved. In the absence of robust LES model for these near-wall structures, we want to satisfy this boundary layer criterion in both LES and DNS.

2.2.3 Bulk Resolution - LES

The last step will be to determine a criterion for the mesh refinement in the bulk of the Rayleigh-Bénard convection cell when dealing with Large Eddy Simulations. In order to obtain well-resolved LES, one should ensure that the filtering cutoff done at a wavenumber

$$k_c = \frac{\pi}{h^{LES}}, \quad \text{where } h^{LES} \text{ is the spacing of the mesh in LES,} \quad (22)$$

located within the inertial subrange of the energy spectrum, i.e. where the unfiltered scales become more isotropic such that the sub-grid scale turbulence can be assumed in constant spectral equilibrium. In homogeneous isotropic turbulence, the inertial subrange is characterised by Kolmogorov scaling known as K41 scaling with a particular slope of -5/3 (see figure 9)

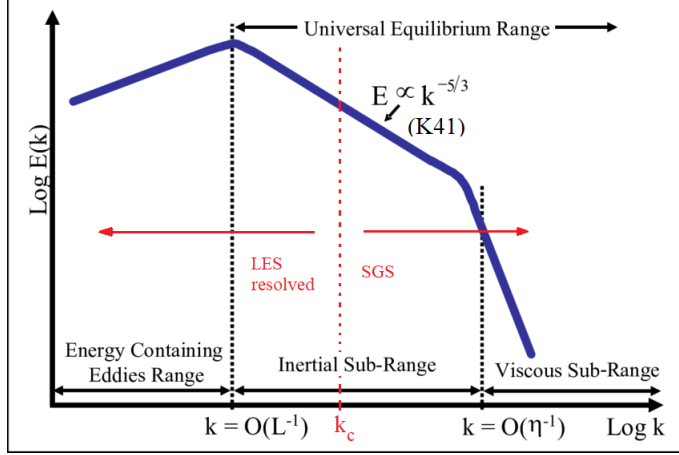


Figure 9: Schematic representation of the energy spectrum of a turbulent flow. E is the kinetic energy and k the wavenumber. The inertial subrange is located between the wavenumbers associated to length scales of order of magnitude of L , the integral length scale, and wavenumbers associated to Kolmogorov length scales, i.e. order of magnitude of η . k_c is an ideal cutoff wavenumber for LES. Figure adapted from [34]

As developed in [35], a cutoff wavenumber located in the inertial range suggests that the modelled rate of energy transfer from large (resolved) to small (unresolved) scales ϵ^{SGS} is of the same order of magnitude that the overall dissipation ϵ . This implies the following relation

$$\epsilon \sim \epsilon_{SGS} = \nu_{SGS} |\bar{S}|^2, \quad (23)$$

where ν_{SGS} is the sub-grid scale kinetic eddy viscosity and $|\bar{S}|^2$ is the magnitude of the resolved strain rate tensor. Under assumption of homogeneous isotropic turbulence, the Kolmogorov theory states

$$|\bar{S}|^2 = 2 \int_0^{k_c} k E(k) dk. \quad (24)$$

Using Kolmogorov constant $C_k \approx 1.6$, one can write the following expression for the kinetic energy $E(k)$,

$$E(k) = C_k \langle \epsilon \rangle^{2/3} k^{-5/3} \quad (25)$$

and insert it in relation (24) to get

$$\langle |\bar{S}|^2 \rangle = \frac{3}{2} C_k \langle \epsilon \rangle^{2/3} \left(\frac{\pi}{h^{LES}} \right)^{4/3}. \quad (26)$$

Finally, assuming that $\langle \epsilon \rangle \approx \langle \nu_{SGS} \rangle \langle |\bar{S}|^2 \rangle$ and using equation (10), we obtain an estimation for h^{LES} ,

$$h^{LES} \approx H \left(\frac{3}{2} C_k \right)^{4/3} \left(\frac{\langle \nu_{SGS} \rangle}{\nu} \right)^{4/3} \frac{\pi \sqrt{Pr}}{((Nu - 1)Ra)^{1/4}} \quad (27)$$

A common choice for the ratio $\langle \nu_{SGS} \rangle / \nu$, i.e. the relative intensity of the unfiltered SGS turbulence, is to ensure that the quantity $\langle \nu_{SGS} \rangle$ stays about the same order of magnitude that ν in order to get well-resolved LES. Therefore a reasonable choice is $\langle \nu_{SGS} \rangle / \nu \leq 10$.

For $\langle \nu_{SGS} \rangle / \nu \leq 1$, we obtain a spatial resolution tending to the resolution required for DNS since the influence of SGS model decreases when this ratio gets smaller.

Another widely used estimation for the spatial resolution in LES is to use the Taylor microscale λ , representative of the inertial range in HIT, as a reference value for our mesh spacing. Still in Kolmogorov theory, this length scale is expressed as

$$\lambda = \sqrt{\frac{15\nu U}{\epsilon}}, \quad (28)$$

where U is a velocity scale for large structures.

Using again equation (10) for the scaling of ϵ with Ra and Pr and estimating U in terms of the resolved turbulence kinetic energy K , [35] obtains for the global Taylor scale (averaged over the whole domain of the Rayleigh-Bénard cell)

$$\frac{\lambda^{global}}{H} = \frac{\sqrt{15}U^*}{((Nu - 1)Ra)^{1/2}}, \quad (29)$$

where we used the dimensionless velocity scale $U^* = \sqrt{KH}/\alpha$.

A scaling relation for U^* has been derived by [36] using DNS analysis. The scaling relation for the dimensionless velocity scale is

$$U^* = \sqrt{0.0027Ra^{1.04} + 0.0312Ra^{0.92}}. \quad (30)$$

Using Nu estimated from power-laws defined previously and the scaling relation for U^* , we are able to compute an estimate for the Taylor microscale and use it as an estimation of the suitable mesh spacing for LES. The reference [35] uses $\lambda^{global}/2$ as a reference value in the estimation of the mesh spacing.

Criteria (27) and (29) have to be used with caution since they are obtained from the Kolmogorov theory assuming HIT which is not exactly the case in thermally driven flows such as Rayleigh Bénard convection.

However, they can be suitable for the bulk region, where turbulence tends to be isotropic [36].

Over the last decade, a new scaling for the inertial range different from K41 has been discussed in many papers (e.g. [32]).

In thermally driven flows such as Rayleigh-Bénard convection, a splitting in the inertial range may be observed with the onset of a new scaling called Bolgiano-Obukhov (BO59) scaling. BO59 scaling should apply above a certain length scale called the Bolgiano length

$$L_B \equiv \epsilon_u^{5/4} \epsilon_\theta^{-3/4} (\alpha g)^{-3/2}. \quad (31)$$

According to [32], such an energy cascade (see figure (10)) is only observable at sufficiently high Rayleigh numbers in Rayleigh-Bénard convection. This is explained by the facts that inertial subrange grows with Ra and the Bolgiano length scale needs to be sufficiently small compared to H in order to fit within this inertial range.

In the context of Large Eddy Simulations, one may wonder if we have to account for Bolgiano length scales in our mesh refinement. In the following development, we will compare these length scales to the Taylor microscales to conclude if, whether or not, a new criterion has to be taken into account for our spatial resolution.

One should be able to insert equations (10) and (11) inside (31) to obtain the ratio for the Bolgiano length scale averaged on the whole volume of the cell L_B^{global} ,

$$\frac{L_B^{global}}{H} = (Nu - 1)^{5/4} Nu^{-3/4} (RaPr)^{-1/4}, \quad (32)$$

which decreases when Ra grows.

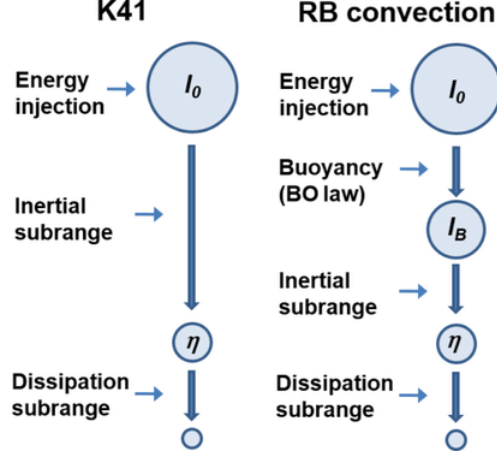


Figure 10: Schematic of the energy cascade. On the left, for Homogeneous Isotropic Turbulence (HIT) with K41 scaling. On the right, BO59 scaling and associated length scales. l_0 is the integral length scale, l_B is the Bolgiano length scale and η is the Kolmogorov length scale. Figure adapted from [37].

Comparing relation (29) with relation (32), we observe that considering an averaging over the whole volume, global Bolgiano length scale is more restrictive than global Taylor scale, i.e. $L_B^{global} < \lambda^{global}$. This suggests that we should use L_B^{global} rather than λ^{global} as an upper bound for our mesh resolution.

However, for Ra computations in our range of interest, i.e. $Ra = 10^8 - 10^9$, performed in [32] and [33], it is agreed that, in the bulk region, local Bolgiano length scale is larger than Taylor microscale, i.e. $L_B^{bulk} > \lambda^{bulk}$, and does not lie into the inertial range. Therefore BO59 scaling is still not observable and it is suggested that such scaling should only be observable at higher Ra and Pr or smaller aspect ratio. This last point needs further study to be confirmed. If we compare this conclusion with the one of the last paragraph about the global scales, we can assume that, on a local view, Bolgiano length scales become very small in the near-wall region and are rapidly growing as we approach the bulk region. Therefore, since we are already wall-resolved in our LES, the application of criterion (32) based on global Bolgiano scale seems less relevant than the use of criterion (29) for the range of Ra and Pr considered. Yet, if one wants to perform LES at higher Ra and Pr , it could be interesting to keep an eye on future studies about Bolgiano length scale.

3 Equations and Models

3.1 Governing Equations

In this section, we will first describe the full set of compressible Navier-Stokes equations governing the the Rayleigh-Bénard convection problem. Secondly, we will motivate the choice of the low-Mach number approximation for our problem and derive the corresponding equations.

3.1.1 Navier-Stokes Equations

The set of Navier-Stokes equations for a compressible Newtonian fluid is composed by the following non-linear partial differential equations :

- Continuity equation :

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (33)$$

where the scalar $\rho \left[\frac{\text{kg}}{\text{m}^3} \right]$ is the fluid density and the vector $\mathbf{u} \left[\frac{\text{m}}{\text{s}} \right]$ is the fluid velocity.

- Momentum equation :

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \tau + \rho \mathbf{g} \quad (34)$$

where the scalar p [Pa] is the fluid pressure, the tensor τ is the viscous stress tensor, and the vector $\mathbf{g} \left[\frac{\text{m}}{\text{s}^2} \right]$ is the gravitational acceleration vector (i.e. $[0 \ -9.81 \ 0]$). Here we assumed that the only body force acting on our system is the buoyancy.

In our problem, we are dealing with a viscous Newtonian fluid. This allows us to write the viscous stress tensor τ under the following form

$$\tau = \mu \left(\left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right), \quad (35)$$

where $\mu \left[\frac{\text{kg}}{\text{m s}} \right]$ is the fluid viscosity and $\mathbf{I}[-]$ stands for the identity matrix.

In a concern of numerical robustness of the solver, it is more convenient to rearrange some terms of the right-hand side. One can group the buoyancy and pressure gradient terms by defining the hydrodynamic pressure as

$$p' = p - \rho \mathbf{g} \cdot \mathbf{h} \quad (36)$$

where $\mathbf{h}$ is the height of the fluid column above the point of action of hydrodynamic pressure.

If we replace the pressure gradient of equation (34) by the hydrodynamic pressure gradient, we can rewrite the momentum equation under the form

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p' + \nabla \cdot \tau + \mathbf{g} \cdot \mathbf{h} \nabla \rho \quad (37)$$

- Energy equation :

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot (\rho \mathbf{u} e) = -\nabla \cdot \mathbf{q} + \sigma : \nabla \mathbf{u} + \rho r \quad (38)$$

where $e \left[\frac{\text{J}}{\text{kg}} \right]$ is the specific internal energy, $\mathbf{q}$ is the heat flux vector, $\sigma = \tau - p \mathbf{I}$ is the stress tensor and r is a heat source term.

In a problem such as Rayleigh-Bénard convection, i.e. a low-Mach number flows, it is reasonable to assume the viscous terms as negligible. A second assumption that can be made is to consider the absence of heat source term within the material volume.

Taking into account these assumptions and defining the specific enthalpy as

$$h \equiv e + \frac{p}{\rho}, \quad (39)$$

and expanding the heat flux divergence using Fourier's law

$$\mathbf{q} = -\kappa \nabla T, \quad (40)$$

where $\kappa \left[\frac{W}{mK} \right]$ is the thermal conductivity and the scalar $T[K]$ is the temperature, we can rewrite the equation (38) in terms of the specific enthalpy h to get

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho \mathbf{u} h) = \nabla \cdot (\kappa \nabla T) + \frac{Dp}{Dt} \quad (41)$$

Where the last term is the material derivative of pressure p .

3.1.2 Equation of State

In all our simulations, the fluid (i.e. air) is assumed to obey the perfect gas relation

$$p = \rho R T = \frac{\rho T}{\gamma M^2} \quad (42)$$

where R is the perfect gas constant, γ is the ratio of specific heats at a reference temperature and M is the Mach number.

3.1.3 Low-Mach Number Approximation

A low-Mach number flow is characterised by small pressure variations but high gradients of temperature and density. This approximation can be applied to our governing equations as soon as the Mach number is low in the entire flow field, which is a reasonable assumption for Rayleigh-Bénard convection.

However, another approximation is widely used when dealing with Rayleigh-Bénard convection. This approximation consists to take the full set of compressible equation defined previously and to assume that the density ρ variations are neglected in the governing equations except in the buoyancy term of the momentum-balance law where a linear relation between density and temperature is assumed. This assumption is known as the Boussinesq approximation and the corresponding equations are the Oberbeck-Boussinesq equations. This set of equations is very popular since it reduces the Rayleigh-Bénard convection problem to an incompressible flow which is extremely convenient on a numerical point of view.

Nonetheless, according to [41], the Boussinesq approximation is only valid for limited temperature gradients in Rayleigh-Bénard convection. These maximal temperature gradients have been estimated to $\Delta T = 2[K]$ for liquids and $\Delta T = 15[K]$ for gaseous flows. Outside of this range, the validity of the Oberbeck-Boussinesq equations is not longer guaranteed and this approximation could lead to inaccurate results.

Since the problem of interest of this work is the natural convection in a spent nuclear-fuel pool, the temperature gradients prone to be observed in case of an accident are outside of this range. This motivates

the development of a low-Mach solver able to ensure accurate results even for large temperature gradients.

In this section, we will present a brief overview of the derivation of the low-Mach number equations (see [42] as reference for a full review). The low-Mach number equations are obtained by expanding the flow variables of the governing equations defined in the previous section, namely ρ , $\mathbf{u}$, T and p , as a power series in $\epsilon = \gamma M^2$:

$$\rho = \rho^{(0)} + \epsilon \rho^{(1)} + O(\epsilon^2) \quad (43)$$

$$\mathbf{u} = \mathbf{u}^{(0)} + \epsilon \mathbf{u}^{(1)} + O(\epsilon^2) \quad (44)$$

$$T = T^{(0)} + \epsilon T^{(1)} + O(\epsilon^2) \quad (45)$$

$$p = \frac{\rho T}{\gamma M^2} = \frac{\rho T}{\epsilon} = \frac{p^{(0)}}{\epsilon} + p^{(1)} + O(\epsilon) \quad (46)$$

Under the approximation of low-Mach number, we have the order of magnitude $\epsilon = \gamma M^2 \ll 1$ allowing us to neglect the high order terms of the power-series equations (43)-(46). In particular, we can observe in equation (46) that the pressure p is the sum of two contributions

- $p^{(0)}$ interpreted as the thermodynamic pressure, spatially uniform
- $p^{(1)}$ interpreted as the dynamic pressure, variable in space

Since $\epsilon \ll 1$, the last term of equation (41), i.e. the material derivative of p , is mostly due to the thermodynamic pressure $p^{(0)}$. However, since the thermodynamic pressure is spatially uniform, it has no contribution to the pressure gradient $\nabla p'$ of the momentum equation (37) which is entirely due to the dynamic pressure $p^{(1)}$.

Taking into account these remarks, we can write the governing equations and the ideal gas law under the form of the low-Mach number approximation equations

$$\frac{\partial \rho^{(0)}}{\partial t} = \nabla \cdot (\rho \mathbf{u}^{(0)}) = 0 \quad (47)$$

$$\frac{\partial \rho^{(0)} \mathbf{u}^{(0)}}{\partial t} + \nabla \cdot (\rho^{(0)} \mathbf{u}^{(0)} \mathbf{u}^{(0)}) = -\nabla p^{(1)} + \nabla \cdot \boldsymbol{\tau}^{(0)} + \mathbf{g} \cdot \mathbf{h} \nabla \rho^{(0)} \quad (48)$$

$$\frac{\partial \rho^{(0)} h^{(0)}}{\partial t} + \nabla \cdot (\rho^{(0)} \mathbf{u}^{(0)} h^{(0)}) = -\nabla \cdot (\kappa \nabla T^{(0)}) + \frac{D p^{(0)}}{D t} \quad (49)$$

$$\rho^{(0)} = \frac{p^{(0)}}{R T^{(0)}} \quad (50)$$

As stated before, in the momentum equation (48), the pressure gradient is solely due to dynamic pressure, i.e. $p^{(1)} = p^{(1)} - \rho^{(0)} \mathbf{g} \cdot \mathbf{h}$.

In our case, the domain is closed. Therefore, the thermodynamic pressure is likely to vary in time while the total mass remains constant and equal to the volume integral of the density

$$M_0 = \int \rho^{(0)} dV. \quad (51)$$

An expression for $p^{(0)}$ may be obtained by integrating equation (50) over the volume V to get

$$p^{(0)} = \frac{M_0}{\int \frac{dV}{RT^{(0)}}} = \frac{M_0}{\int \psi^{(0)} dV} \quad (52)$$

3.2 Finite Volume Method

In order to solve the system of non-linear partial differential equations defined in the previous section, these equations need to be discretised into a system of algebraic equations. Since we will use the open-source CFD package OpenFOAM to perform our simulations, we will discretise our equations following the Finite Volume Method (FVM) on which OpenFoam is based.

In this work, we will go through the main characteristics of this method. For a complete review, a full description of the FVM is presented in [43].

The FVM method presents the following properties

- The space is divided into a finite number of discrete regions called control volumes.
- The method is based on the integral form of governing equations discretised over each control volume. Such an approach ensure that the basic quantities, such as mass and momentum, will therefore be conserved at the discrete level.
- The Cartesian coordinate system in which the governing equations are solved remains constant in time.
- Sets of partial differential equations are solved using a segregated approach, i.e. they are solved one at a time and non-linear equations are linearised before discretisation.

The first step of the FVM is to discretise the domain by subdividing it into non overlapping control volumes (CV), see figure 11. The computational point P is defined as the centroid of each control volume. In a mathematical point of view, this is expressed as

$$\int_{V_P} (\mathbf{x} - \mathbf{x}_P) dV = \mathbf{0} \quad (53)$$

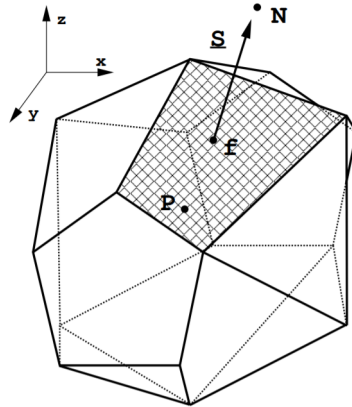


Figure 11: Control volume as presented in [43]. $\mathbf{P}$ is the centroid of the cell, $\mathbf{f}$ is a face of the CV, $\mathbf{S}$ is the face area vector and $\mathbf{N}$ is the centroid of the neighbouring cell.

The boundary of each control volume is a set of flat faces. Each face is shared with at most one neighbouring CV or a boundary of the domain.

The second step of the FVM is to discretise the governing equations. To do so, we can start from the general expression of the transport equation for a scalar variable ϕ

$$\underbrace{\frac{\partial \rho \phi}{\partial t}}_{\text{temporal derivative}} + \underbrace{\nabla \cdot (\rho \mathbf{u} \phi)}_{\text{convection term}} - \underbrace{\nabla \cdot (\rho \Gamma_\phi \nabla \phi)}_{\text{diffusion term}} = \underbrace{S_\phi(\phi)}_{\text{source term}} \quad (54)$$

which has to be rewritten in integral form to be satisfied over the entire control volume V_P

$$\int_t^{t+\Delta t} \left[\frac{\partial}{\partial t} \int_{V_P} \rho \phi dV + \int_{V_P} \nabla \cdot (\rho \mathbf{u} \phi) dV - \int_{V_P} \nabla \cdot (\rho \Gamma_\phi \nabla \phi) dV \right] dt = \int_t^{t+\Delta t} \left(\int_{V_P} S_\phi(\phi) dV \right) dt \quad (55)$$

We can now derive the discretisation for each term of the transport equation. In what follows, we will present the different numerical schemes used in the simulations of this work.

- Gradient scheme :

$$\int_{V_P} \nabla \phi dV = \oint_{\partial V_P} d\mathbf{S} \phi = \sum_f \mathbf{S}_f \phi_f \quad (56)$$

where $\mathbf{S}_f$ is the outward-pointing face area vector of face f .

In this scheme, the gradient is calculated using integrals over faces using Gauss' theorem. ϕ_f is evaluated from cell center values

$$\phi_f = f_x \phi_P + (1 - f_x) \phi_N \quad \text{with} \quad f_x = \overline{fN} / \overline{PN} \quad (57)$$

- Divergence scheme : this scheme is used for the convection terms. One can obtain it from the Gauss' theorem

$$\int_{V_P} \nabla \cdot (\rho \mathbf{u} \phi) dV = \oint_{\partial V_P} d\mathbf{S} \cdot (\rho \mathbf{u} \phi) = \sum_f \mathbf{S}_f \cdot (\rho \mathbf{u} \phi)_f = \sum_f \mathbf{S}_f \cdot (\rho \mathbf{u})_f \phi_f = \sum_f \phi_f F \quad (58)$$

where F represents the mass flux through the face f .

As for the gradient scheme, we use a second-order central differencing scheme popular for LES due to its low numerical dissipation property,

$$\phi_f = f_x \phi_P + (1 - f_x) \phi_N \quad (59)$$

- Laplacian scheme : this scheme is used for the diffusion terms, one more time it is derived from the Gauss' theorem,

$$\int_{V_P} \nabla \cdot (\rho \Gamma_\phi \nabla \phi) dV = \sum_f \mathbf{S}_f \cdot (\rho \Gamma_\phi \nabla \phi)_f = \sum_f (\rho \Gamma_\phi)_f \mathbf{S}_f \cdot (\nabla \phi)_f \quad (60)$$

In the particular case of an orthogonal mesh, which is fortunately our case due to the simple geometry of the problem, we do not have to apply a correction term and the face-normal gradient is evaluated as

$$\mathbf{S}_f \cdot (\nabla \phi)_f = |\mathbf{S}_f| \frac{\phi_N - \phi_P}{\overline{PN}} \quad (61)$$

- Source term discretisation : The first step is to linearise the source term as

$$S_\phi(\phi) = S_u + S_p \phi \quad (62)$$

and the second step is to discretise it as

$$\int_{V_P} S_\phi(\phi) dV = S_u V_P + S_p V_P \phi_P \quad (63)$$

- Time scheme : We use the implicit second-order backward time scheme. This scheme is obtained from a Taylor series expansion of ϕ in time around $\phi(t + \Delta t) = \phi^n$:

$$\phi(t) = \phi^o = \phi^n - \frac{\partial \phi}{\partial t} \Delta t + \frac{1}{2} \frac{\partial^2 \phi}{\partial t^2} \Delta t^2 + O(\Delta t^3). \quad (64)$$

and

$$\phi(t - \Delta t) = \phi^{oo} = \phi^n - 2 \frac{\partial \phi}{\partial t} \Delta t + 2 \frac{\partial^2 \phi}{\partial t^2} \Delta t^2 + O(\Delta t^3). \quad (65)$$

Combining equations (64) and (65), we eliminate the term in the truncation error scaling with Δt and we obtain the second order scheme

$$\frac{\partial \phi}{\partial t} = \frac{\frac{3}{2} \phi^n - 2 \phi^o + \frac{1}{2} \phi^{oo}}{\Delta t} \quad (66)$$

Taking into account the discretisation for each term, the general transport equation can be written in the semi-discretised form

$$\frac{\frac{3}{2} \rho_P^n \phi^n - 2 \rho_P^o \phi^o + \frac{1}{2} \rho_P^{oo} \phi^{oo}}{\Delta t} V_P + \sum_f F \phi_f^n - \sum_f (\rho^n \Gamma_\phi)_f \mathbf{S}_f \cdot (\nabla \phi)_f^n = S_u V_P + S_p V_P \phi_P^n \quad (67)$$

3.3 Numerical Algorithm

In this section, we will describe the discretisation procedure for the low-Mach number approximation equations derived in the section 3.1.3. For the following derivation, we take as reference William A. Hay [44] who has developed and implemented the low-Mach solver used in this work in OpenFOAM. The general idea of this section is to develop a variable density PISO algorithm based on the momentum equations and a pressure Poisson equation. In all further mathematical developments, we will refer to the low-Mach number variables $\rho^{(0)}$, $\mathbf{u}^{(0)}$ and $T^{(0)}$ without the superscript in order to simplify the readability of the equations. Note that the superscripts for the thermodynamic pressure $p^{(0)}$ and the dynamic pressure $p'^{(1)}$ are not dropped.

3.3.1 Pressure Poisson Equation

As a first step, we aim to derive the variable density pressure Poisson equation. Following the discretisation procedure of the Navier-Stokes system for a variable density flow [43], a semi-discretised version of the momentum equation may be formulated as

$$a_p \mathbf{U}_p + \sum_N a_N \mathbf{U}_N - \frac{\mathbf{U}^0}{\Delta t} = -\nabla p'^{(1)} - \mathbf{g} \cdot \mathbf{h} \nabla \rho \quad (68)$$

We introduce a substitution variable $\mathbf{H}$ defined as

$$\mathbf{H}(\mathbf{U}) = - \sum_N a_N \mathbf{U}_N + \frac{\mathbf{U}^o}{\Delta t}, \quad (69)$$

by inserting this new variable in the equation (68), we can obtain the following expression for the velocity at a point P

$$\mathbf{U}_P = \frac{1}{a_P} \mathbf{H}(\mathbf{U}) - \frac{1}{a_P} \nabla p^{(1)} - \frac{1}{a_P} \mathbf{g} \cdot \mathbf{h} \nabla \rho \quad (70)$$

Now, we multiply equation (70) by the density ρ and we take the divergence of each side of this equation to obtain

$$\nabla \cdot (\rho \mathbf{U}_P) = \nabla \cdot \left(\frac{\rho}{a_P} \mathbf{H}(\mathbf{U}) - \frac{\rho}{a_P} \mathbf{g} \cdot \mathbf{h} \nabla \rho \right) - \nabla \cdot \left(\frac{\rho}{a_P} \nabla p^{(1)} \right) \quad (71)$$

Finally, we can combine the momentum equation (71) and the continuity equation (47) to express the following pressure Poisson equation

$$\nabla \cdot \left(\frac{\rho}{a_P} \nabla p^{(1)} \right) = \nabla \cdot \left(\frac{\rho}{a_P} \mathbf{H}(\mathbf{U}) - \frac{\rho}{a_P} \mathbf{g} \cdot \mathbf{h} \nabla \rho \right) + \frac{\partial \rho}{\partial t} \quad (72)$$

Using the state equation, we can replace ρ by $\psi p^{(0)}$, where $\psi = 1/RT$ is the compressibility, in the last term of pressure Poisson equation (72) to get its final discretised form

$$\sum_f \left(\left(\frac{\rho}{a_P} \right)_f (\nabla p^{(1)})_f \right) \cdot \mathbf{S}_f = \sum_f \left(\left(\frac{\rho}{a_P} \mathbf{H}(\mathbf{U}) \right)_f - \left(\frac{\rho}{a_P} \right)_f (\mathbf{g} \cdot \mathbf{h})_f (\nabla \rho)_f \right) \cdot \mathbf{S}_f + \frac{\partial \psi}{\partial t} p^{(0)} \cdot V_P \quad (73)$$

3.3.2 PISO Algorithm

The Pressure-Implicit with Splitting of Operators (PISO) algorithm is a pressure-velocity calculation procedure to solve the Navier-Stokes equations. This predictor-corrector projection scheme is initialised with known ρ , T , $\mathbf{u}$ and p at a time n . The different steps of the PISO algorithm may be written as follows

1. Put ρ^n and $p^{n,(1)}$ in the momentum equation to find the estimate $\mathbf{u}^*$ (predictor step)
2. Put ρ^n and $\mathbf{u}^*$ in the energy equation to find h^* and then T^*
3. Put T^* in the equation of state to find ψ^*
4. Put ψ^* in equation (52) to find $p^{(0)*}$
5. Put $p^{(0)*}$ and T^* in the equation of state to obtain ρ^*
6. Insert $\mathbf{u}^*$ and ρ^* in equation (69) to get the operator $\mathbf{H}(\mathbf{U})^*$
7. Use $\mathbf{H}(\mathbf{U})^*$ and ρ^* to express the pressure Poisson equation (73)
8. Solve the Poisson equation for $p^{(1)*}$
9. Solve equation the momentum equation (70) to obtain the corrected value $\mathbf{u}^{**}$
10. Iterate over step 6 to 9 with $\mathbf{u}^{**}$ instead of $\mathbf{u}^*$ until convergence is attained (under a certain tolerance)

11. Restart the algorithm for the time $n + 1$

3.4 Large Eddy Simulation

As already stated, a major part of this work is based on the validation of Large Eddy simulations and the modelling of the Sub-Grid Scales (SGS) quantities in the problem of Rayleigh-Bénard convection. In this section, we will give an overview of the background of LES modelling and give an insight of the SGS models used in this work.

The main idea behind LES is to decompose every flow variable ϕ into a large scale term $\bar{\phi}$ resolved by the grid, i.e. filtered, and a modelled term ϕ' containing the SGS information. This leads to the following decomposition for a general variable of the flow $\phi(\mathbf{x})$

$$\phi(\mathbf{x}) = \bar{\phi}(\mathbf{x}) + \phi'(\mathbf{x}) \quad (74)$$

In the previous equation, the spatial filtering of $\phi(\mathbf{x})$ is referred as $\bar{\phi}(\mathbf{x})$ and satisfies the following relation on the domain Ω

$$\bar{\phi}(\mathbf{x}) = \int_{\Omega} G_{\Delta}(\mathbf{x} - \mathbf{x}') \phi(\mathbf{x}') d\mathbf{x}' \quad (75)$$

where $G_{\Delta}(\mathbf{x} - \mathbf{x}')$ is the kernel of the filter of which the integral over the domain Ω is equal to 1. Δ is known as the filter width and is a measure of the local grid size.

In OpenFOAM, the filtering function classically used is known as a top-hat or box filter defined as

$$G_{\Delta}(\mathbf{x} - \mathbf{x}') = \begin{cases} \frac{1}{\Delta} & \text{if } |\mathbf{x} - \mathbf{x}'| \leq \frac{\Delta}{2} \\ 0 & \text{otherwise} \end{cases} \quad (76)$$

where we can use the following definition for the filter width $\Delta = (V_c)^{1/3}$ which is the cube root of the cell volume.

3.4.1 Equations filtering

In this section, we will derive the spatially filtered compressible Navier-Stokes equations resolved by Large Eddy Simulations.

Since we are dealing with a compressible flow, we apply a density-weighted filtering known as Favre filtering,

$$\tilde{\phi}(\mathbf{x}) = \frac{\int \rho(\mathbf{x}') \phi(\mathbf{x}') G_{\Delta}(\mathbf{x} - \mathbf{x}') d\mathbf{x}'}{\int \rho(\mathbf{x}') G_{\Delta}(\mathbf{x} - \mathbf{x}') d\mathbf{x}'} = \frac{\overline{\rho(\mathbf{x}) \phi(\mathbf{x})}}{\bar{\rho}(\mathbf{x})} = \frac{\overline{\rho \phi}}{\bar{\rho}} \quad (77)$$

In the following derivation, we will assume the filtering operations and derivatives to be commutative. We can now apply the filtering operation defined in (77) to the set of compressible Navier-Stokes equation presented in the section 3.1.1 to obtain the compressible filtered equations [45]:

$$\frac{\partial \bar{\rho}}{\partial t} - \nabla \cdot \partial \bar{\rho} \tilde{\mathbf{u}} = 0 \quad (78)$$

$$\frac{\partial \bar{\rho} \tilde{\mathbf{u}}}{\partial t} + \nabla \cdot (\partial \bar{\rho} \tilde{\mathbf{u}} \tilde{\mathbf{u}}) = -\nabla \bar{p} + \nabla \cdot \tilde{\tau} - \nabla \cdot \tau_{SGS} + \bar{\rho} \mathbf{g} \quad (79)$$

$$\frac{\partial \bar{\rho} \tilde{h}}{\partial t} + \nabla \cdot (\partial \bar{\rho} \tilde{h} \tilde{\mathbf{u}}) = \frac{\partial \bar{p}}{\partial t} + \tilde{\mathbf{u}} \cdot \nabla \bar{p} - \Pi_{SGS} + \bar{\kappa} \nabla \tilde{T} - \nabla \cdot (C_v q_{SGS}) \quad (80)$$

$$\bar{p} = \bar{\rho} R \tilde{T} \quad (81)$$

where the filtered viscous stress $\tilde{\tau}$ is given by

$$\tilde{\tau} = 2\bar{\mu} \tilde{\mathbf{S}}^* = \bar{\mu} \left(\left(\nabla \tilde{\mathbf{u}} + (\nabla \tilde{\mathbf{u}})^T \right) - \frac{2}{3} (\nabla \cdot \tilde{\mathbf{u}}) \mathbf{I} \right) \quad (82)$$

where $\mathbf{S}^*$ is the traceless strain-rate tensor.

The sub-grid scale stress tensor, sub-grid scale heat flux tensor and the sub-grid scale pressure dilatation are respectively

$$\tau_{SGS} = \bar{\rho} (\widetilde{\mathbf{u}\mathbf{u}} - \tilde{\mathbf{u}}\tilde{\mathbf{u}}) \quad (83)$$

$$q_{SGS} = \bar{\rho} (\widetilde{\mathbf{u}T} - \tilde{\mathbf{u}}\tilde{T}) \quad (84)$$

$$\Pi_{SGS} = \overline{p \nabla \cdot \mathbf{u}} - \bar{p} \nabla \cdot \tilde{\mathbf{u}} \quad (85)$$

The sub-grid scale kinetic energy may be defined, using indicial notation, as

$$\bar{\rho} k_{SGS} = \frac{1}{2} Tr(\tau_{SGS}) = \frac{1}{2} \tau_{SGS, kk} = \frac{1}{2} \bar{\rho} (\widetilde{u_k u_k} - \tilde{u}_k \tilde{u}_k) \quad (86)$$

The sub-grid scale terms that we have derived from the filtered equations cannot be straightforwardly computed from the resolved fields. This motivates the establishment of models in order to compute these terms. Such models are known as sub-grid scales (SGS) models and we will introduce and use two of these models in this work.

3.4.2 Dynamic k -Equation Model

The first SGS model to be discussed in this work is the dynamic k -equation model. The derivation of this model is based on [45] where more information can be found.

The key idea of this model is to solve the compressible SGS kinetic energy transport equation in order to derive k_{SGS} .

One can obtain the SGS kinetic energy equation by following the following steps:

1. Filter the product of the velocity and the momentum equation to obtain

$$\overline{[u_i \times (\text{momentum equation})]} \quad (87)$$

2. Multiply the Favre-filtered velocity and the filtered momentum equation to obtain

$$\tilde{u}_i \times \overline{(\text{momentum equation})} \quad (88)$$

3. Subtract (88) from (87) to obtain the SGS kinetic energy equation as

$$\overline{[u_i \times (\text{momentum equation})]} - \tilde{u}_i \times \overline{(\text{momentum equation})} \quad (89)$$

By applying the described steps and rearrange the terms, one can obtain the following expression for the SGS kinetic equation

$$\begin{aligned} \frac{\partial \bar{\rho}k}{\partial t} = & -\frac{\bar{\rho}k\tilde{u}_j}{\partial x_j} - \tau_{SGS,ij}\tilde{S}_{ij} - 2\bar{\mu} \left[\overline{S_{ij}^*D_{ij}^*} - \overline{S_{ij}^*}\overline{D_{ij}^*} \right] - \frac{\partial}{\partial x_j} \left[\frac{5}{3} \left(\bar{\mu}u_j \left(\overline{u_j \frac{\partial u_k}{\partial x_k}} \right) - \bar{\mu}\tilde{u}_j \frac{\partial \tilde{u}_k}{\partial x_k} \right) \right] \\ & + \frac{\partial}{\partial x_j} \left[\tau_{SGS,ij}u_{ij} + \bar{\mu} \frac{\partial k}{\partial x_j} + \bar{\mu} \frac{\partial}{\partial x_i} \left(\frac{\tau_{SGS,ij}}{\bar{\rho}} \right) + Rq_{SGS,j} \right] - \frac{\partial}{\partial x_j} \left[\frac{1}{2} \bar{\rho} (\overline{u_i u_i u_j} - \overline{u_i} \overline{u_i} \tilde{u}_j) \right] \\ & + \left(\overline{p \frac{\partial u_k}{\partial x_k}} - \bar{p} \frac{\partial \tilde{u}_k}{\partial x_k} \right) \end{aligned} \quad (90)$$

We still need to propose a model for the SGS stress τ_{SGS} and the SGS heat flux q_{SGS} . To do so, we can use eddy viscosity and eddy diffusivity models with $\sqrt{k}$ chosen as the velocity scale. This leads to the following SGS models

$$\tau_{SGS,ij} - \frac{2}{3} \bar{\rho} k \delta_{ij} = -2C_S \Delta \bar{\rho} \sqrt{k} \overline{S_{ij}^*}, \quad (91)$$

$$q_{SGS,j} = -\frac{\mu_t}{Pr_t} \frac{\partial \tilde{T}}{\partial x_j} = -\frac{C_S \Delta \bar{\rho} \sqrt{k}}{Pr_t} \frac{\partial \tilde{T}}{\partial x_j}, \quad (92)$$

where $\mu_t = C_S \Delta \bar{\rho} \sqrt{k}$ is the eddy viscosity and C_S and Pr_t are the model coefficient to be determined dynamically.

3.4.3 Lagrangian Dynamic Model

The second SGS model to be used in this work is the Lagrangian dynamic model. The derivation of the equations behind this model is quite hard to explain succinctly. Therefore we refer the reader to [15] for the mathematical derivation of the equations.

This model can be seen as a Lagrangian version of the popular Smagorinsky SGS model in the sense that the averaging of the flow statistics is done over flow pathlines rather than over directions of statistical homogeneity as done classically by the Smagorinsky SGS model.

In a qualitative point of view, the derivation of the Lagrangian model is obtained by minimizing the error generated by the insertion of the Smagorinsky model in the Germano identity in a Lagrangian frame of reference.

According to [15], such an approach of the SGS modelling produces results equal or superior to those of spatially averaged versions of the dynamic Smagorinsky model.

4 Computational Set-Up

In this section, we will describe the parameters of the numerical simulations performed in this work and set-up the mesh resolutions taking into account the theoretical criterion from literature presented in the section 2.2.

As already stated, the numerical simulation carried out in this work are performed with the CFD package OpenFOAM and the compressible Navier-Stokes equations are solved under the low-Mach approximation by a low-Mach solver implemented in OpenFOAM by [44].

The working fluid is chosen as air at a mean temperature $T_0 = 313[\text{K}]$. These properties correspond to a Prandtl number $Pr = 0.7$. The geometry used to study turbulent Rayleigh-Bénard convection is a cube, i.e. $\Gamma = 1$, bounded by solid walls at each boundary. At each rigid wall, the no-slip and impermeability conditions are applied to the velocity field. The side walls are adiabatic, i.e. $\frac{\partial T}{\partial n} = 0$, and the top and bottom plates are isothermal with temperatures $T_c = 305.5[\text{K}]$ and $T_h = 320.5[\text{K}]$, respectively. Therefore, the temperature difference between the cold and hot plates is fixed at $\Delta T = 15[\text{K}]$. In our simulations, we increase the Rayleigh number of the RBC flow by increasing the size of the box H , every other parameter remaining constant. The height of the domain as a function of the Rayleigh number Ra is thus computed from the relation (1)

$$H(Ra) = \left(\frac{\nu \alpha Ra}{g \beta \Delta T} \right)^{1/3} \quad (93)$$

where the flow properties α , β and ν are determined from correlations for air at $40[\text{K}]$. These values are summarised in the table 2.

Table 2: Air properties

Fluid	Prandtl number $Pr[-]$	Mean Temperature $T_0 [\text{K}]$	Thermal diffusivity $\alpha[\text{m}^2/\text{s}]$	Thermal expansion $\beta[\text{K}^{-1}]$	Kinematic viscosity $\nu[\text{m}^2/\text{s}]$
Air	0.7	40	2.38×10^{-5}	3.2×10^{-3}	1.69×10^{-5}

From the relation (93) and the chosen parameters, we obtain the following set-ups for our simulations

Table 3: Height of the cell as a function of Ra

Rayleigh Number $[-]$	$Ra = 10^6$	$Ra = 10^7$	$Ra = 5 \times 10^7$	$Ra = 10^8$	$Ra = 10^9$
Height $[\text{m}]$	$H = 0.095$	$H = 0.2048$	$H = 0.35$	$H = 0.441$	$H = 0.95$

The thermophysical model used by the solver has the following properties

- Transport model : The dynamic viscosity μ , the thermal conductivity κ and the thermal diffusivity α present in the energy and enthalpy equations are computed using Sutherland's model of OpenFoam. For the dynamic viscosity, Sutherland's law is known as :

$$\mu(T) = \frac{A_s T^{3/2}}{T + T_s} \quad (94)$$

where we have the following parameters for the air : the Sutherland temperature is $T_s = 110.4[\text{K}]$ and the Sutherland coefficient $A_s = 1.458 \times 10^{-6}$.

- Thermodynamic model : c_p is computed as a function of the temperature T from a set of coefficients taken from JANAF tables of thermodynamics.
- Equation of state : perfect gas equation is used, i.e. $\rho = \frac{p}{RT}$

The choice of initial conditions of the problem may have a big impact on the stability of the solver and the time needed to reach statistical stationarity. The most efficient procedure is to set the initial fields for the smallest Rayleigh number, i.e. the one requiring the least computational efforts, with an homogeneous pressure fixed at $p = 10^5$ [Pa] (atmospheric pressure), a zero velocity field and a linear temperature profile between the bottom and the top plates in order to avoid strong local temperature gradients likely to cause instabilities and reduce the convergence time to statistical steady state.

Once the first simulation is performed, we set the initial fields of the next simulations at higher Ra as a mapping of the lower Ra solution on the new computational domain. This procedure allows to save a lot of computation time since we are only interested into statistics of the flow at steady state.

A crucial parameter of the simulations set-up is the design of the mesh. An extremely fine mesh would ensure the accuracy of the solution but would also be extremely expensive on a computational point of view. In order to find the right balance between accuracy and computation time/ressources, we will use the criteria previously defined in the section 2.2.

The quantities of interest will be the following :

- Near-wall region : We need to estimate the viscous and thermal boundary layer thickness $\frac{\lambda_u}{H}$ and $\frac{\lambda_\theta}{H}$ in order to know the number of grid points lying within these boundary layer and verify the criteria (20) and (21).
- DNS Bulk : The quantity of interest is the Kolmogorov length scale η . We want to satisfy the criterion (17),

$$\frac{h^{DNS}}{H} \leq \frac{\pi\eta}{H} \quad (95)$$

- LES Bulk : The quantity of interest is the Taylor length scale λ . We use the expression (29) and obtain an estimate for the grid spacing as the half of Taylor microscale,

$$\frac{h^{LES}}{H} \approx \frac{\lambda}{2H} \quad (96)$$

These estimations require an *a priori* guess of the Nusselt number Nu . In this work, we have employed the scaling relation derived by Kerr [36] from DNS, i.e. $Nu = 0.186Ra^{0.276}$ which is quite close to the $2/7$ scaling discussed in the section 2.1. The estimated length scales and grid resolutions as references at the different Rayleigh numbers are presented in the table 4.

In order to satisfy these conditions while guaranteeing a reasonable computation time, we use a non-uniform spacing. We use a hyperbolic tangent scaling, i.e. the grid spacing becomes finer towards the walls in order to have well-resolved boundary layers. We use the same number of grid points in each direction with the same scaling, $N = N_x = N_y = N_z$. The typical ratio between grid spacing close to the wall and the grid spacing in the bulk in DNS is of the order of 10, i.e. $\frac{h_{bulk}^{DNS}}{h_{BL}^{DNS}} \approx 10$. The smaller number of points chosen to satisfy the mesh resolution criteria for each regime is also indicated in the table 4.

Table 4: Estimated length scales and grid resolutions as references

Ra [-]	10^6	10^7	5×10^7	10^8	10^9
$\frac{\lambda_u}{H}$	0.0519	0.0269	0.0170	0.0139	0.0088
$\frac{\lambda_\theta}{H}$	0.0456	0.0236	0.0149	0.0122	0.0078
$\frac{\pi\eta}{H}$	0.0472	0.0225	0.0134	0.0107	0.0054
$\frac{\lambda}{2H}$	0.0808	0.0541	0.0415	0.0371	0.0286
N^{DNS}	64	96	124	-	-
N^{LES}	24	42	42	64	96

The figure 13 illustrate the grid spacing scaling compared to the global estimates of the Kolmogorov and Taylor length scales at $Ra = 10^7$ and the figure ?? illustrate the mesh used in DNS with 64x64x64 points.

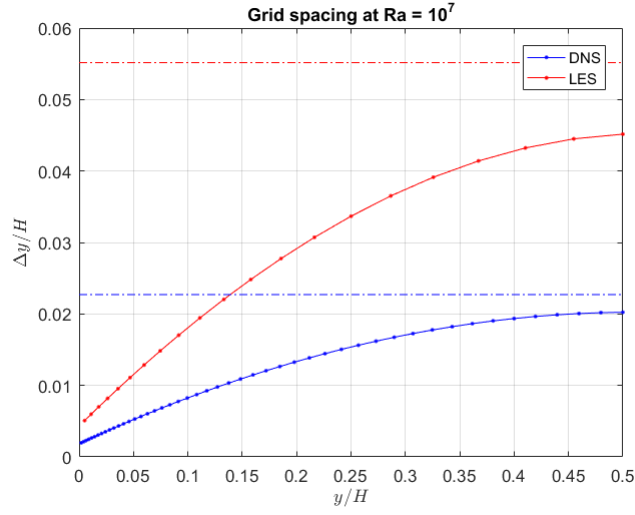


Figure 12: Normalised grid spacing along axis of the cube for DNS (blue curve) and LES (red curve) compared to $\frac{\pi\eta}{H}$ (horizontal line in blue) and $\frac{\lambda}{2H}$ (horizontal line in red) $Ra = 10^7$ on the right.

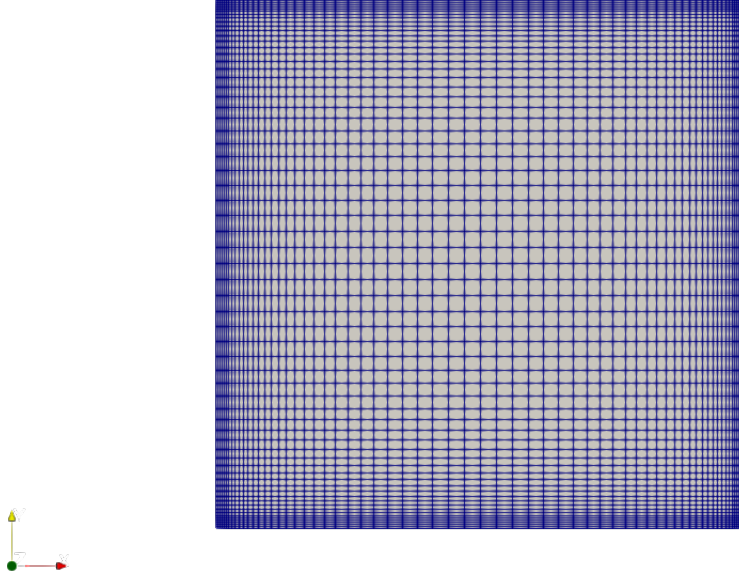


Figure 13: Mesh used for DNS with 64x64x64 points

In the our numerical runs, we want the collection of the flow statistics to begin once the flows becomes fully turbulent and reach the statistical steady state. Therefore, we define a characteristic time scale; the free-fall time

$$t^* = \frac{H}{\sqrt{g\alpha\Delta TH}}$$

where the denominator is also known as the free-fall velocity $U_f = \sqrt{g\alpha\Delta TH}$. This characteristic velocity U_f will be used to non-dimensionalize the velocity field of the flow.

In the following simulations, we consider that a sufficiently long time to be sure to reach the statistically steady state is approximately 500 free-fall time units. Once the steady state is reached, the statistics are collected during at least 300 t^* and preferably during 1000 t^* .

In order to ensure the stability of our calculations, we use an adaptive time step monitor the Courant number

$$C = \frac{u\Delta t}{\Delta x} \leq 0.5. \quad (97)$$

Finally, the Rayleigh-Bénard system response Nu is computed using the following expression

$$\sqrt{RaPr}\langle\rho uT\rangle_{xyzt} + 1, \quad (98)$$

where $\rho = \rho^{dim}/\rho_0$ (with the density reference taken as air at $T_0 = 313[\text{K}]$, i.e. $\rho_0 = 1.1272$), $u = u^{dim}/U_f$ and $T = (T^{dim} - T_0)/\Delta T$ are the non-dimensional flow variables.

In the rest of this work, we will always refer to the non dimensional flow variables.

Taking into account all the previous criteria, we have performed several simulations at each flow regime and using different meshes with the aim to observe the effect of the resolution on the system response.

The simulations parameters and the mean heat flux Nu are summarised in the table 5.

Table 5: Simulation parameters and corresponding Nusselt number. The type of simulation is named "DNS" for Direct Numerical Simulation, "DK" for LES using the dynamic k -equation SGS model and "DL" for LES using the dynamic Lagrangian SGS model. The actual number of grid points within the boundary layers is compared to the minimum number of point to resolve the thermal and viscous boundary layer from equation (20) and (21). The averaging time in free-fall time units is t_{avg}^*

Ra	Type	N	$N_{th.BL}$	$N_{v.BL}$	$\frac{h^{max}}{H}$	$\frac{h^{max}}{h^{min}}$	Nu	$Nu_{ref[32]}$	t_{avg}^*
10^6	DNS	96	17/2.8	16/2.5	0.02	10.2	8.34	8.32	1500
10^6	DNS	64	11/2.8	11/2.5	0.03	10	8.342	8.32	3000
10^6	LES without model	24	4/2.8	3/2.5	0.07	5	8.42	8.32	3000
10^6	DL	24	4/2.8	3/2.5	0.07	5	8.42	8.32	3000
10^6	DK	24	4/2.8	3/2.5	0.07	5	8.39	8.32	3000
10^6	DK	42	9/2.8	9/2.5	0.05	18	8.31	8.32	1500
10^7	DNS	96	11/3.9	10/3.5	0.02	10	16.37	16.3	1000
10^7	LES without model	42	5/3.9	5/3.5	0.04	8.9	17.2	16.3	1000
10^7	DL	64	9/3.9	8/3.5	0.032	13	16.5	16.3	2000
10^7	DL	42	5/3.9	5/3.5	0.04	8.9	16.8	16.3	1000
10^7	DK	64	9/3.9	8/3.5	0.032	13	16.6	16.3	1000
10^7	DK	42	5/3.9	5/3.5	0.04	8.9	16.7	16.3	1000
5×10^7	DNS	124	8/5	8/4.4	0.014	6.5	26	25.6	800
5×10^7	LES without model	64	8/5	9/4.4	0.038	28	29.2	25.6	1600
5×10^7	DK	64	8/5	9/4.4	0.038	28	27.6	25.6	1600
5×10^7	DK	42	6/5	6/4.4	0.06	33	28.3	25.6	800
5×10^7	DL	42	6/5	6/4.4	0.06	13	28.25	25.6	800
10^8	DK	96	15/5.5	14/5	0.029	64	33.8	31.3	600
10^8	DK	64	8/5.5	7/5	0.038	28	35	31.3	600
10^8	DL	64	8/5.5	7/5	0.038	28	35.2	31.3	600
10^9	DK	96	10/7.8	9/7	0.028	52	71.3	63.4	300
10^9	DL	96	10/7.8	9/7	0.028	52	72	63.4	300

5 Numerical results

In this section, we will further develop the results obtained from the simulations of the table 5. The final objective of this work is to validate or not the accuracy of the SGS models used against the DNS data. To do so, we will compare the DNS and LES results obtained for the time averaged Nusselt number Nu and the flow statistic at $Ra = 10^6$, $Ra = 10^7$ and $Ra = 5 \times 10^7$.

For $Ra = 10^8$ and $Ra = 10^9$, the actual computational resources are not sufficient to perform an accurate DNS satisfying the mesh requirement defined previously. Therefore, for this range of Ra , only LES is performed and discussed.

As a last study, we will make a brief overview of the non Oberbeck-Boussinesq effects occurring when we increase the temperature gradient between the hot and the cold plates at small Rayleigh number.

Before comparing LES results to DNS results, one should ensure the validity of the latter. In this work, we check the validity of our DNS results by two means :

1. Grid convergence analysis
2. Comparison with DNS results from the literature, i.e. [32] and [46].

The grid convergence analysis is only performed for the low- Ra in order to determine if the criteria used for the design of the DNS mesh resolution is sufficient to guarantee the quality of results. As presented in the table 5, we performed 3 DNS simulation at $Ra = 10^6$ with 3 different mesh resolution : 24, 64 and 96 points.

On purpose, the $N = 24$ simulation has a very coarse mesh that fits LES resolution requirements but does not fit DNS resolution requirements. In other word, this case corresponds to a LES simulation without SGS model. Still, the obtained Nu is in relatively good agreement with the reference value with an error of the order of 1.2%. When refining the resolution with the $N = 64$ and $N = 96$, which are both satisfying the DNS requirements, we observe that the resulting Nusselt number Nu does not longer vary as we increase the grid resolution. Therefore, we can assume that the DNS criteria defined previously should be sufficient to guarantee the validity of our DNS. In addition, the Nu obtained is in extremely good agreement with the chosen reference with an error well smaller than 1%.

For the next flow regimes, we also obtain really good agreement between Nu obtained from our DNS and the values of the reference. In each regime, error remains lower than 2% which allow us to validate our DNS solutions.

5.1 $Ra = 10^6$ Regime - DNS and LES

In these sections, we intend to validate the SGS models used for our LES with our DNS solution.

Even with the coarse mesh $N = 24$, the Nu is in very good agreement with our DNS solution with an error lower than 1% for both SGS models.

The flow statistics for the $Ra = 10^6$ regime with the LES mesh $N = 24$ and the DNS mesh $N = 64$ are presented on the figure 14 to 16. These statistics are obtained from time-averaging the flow data for each time step and these mean flow quantities are spatially averaged along the homogeneous horizontal directions x and z .

The statistics of interest are the time-average temperature $\langle T \rangle$, its fluctuation $T_{rms} = \langle T'^2 \rangle^{1/2}$, the

fluctuations of the horizontal velocity u and the vertical velocity v , i.e. $u_{rms} = \langle u'^2 \rangle^{1/2}$ and $v_{rms} = \langle v'^2 \rangle^{1/2}$, the turbulent kinetic energy

$$K = \frac{1}{2}(\langle u'^2 \rangle + \langle v'^2 \rangle + \langle w'^2 \rangle)$$

and the resolved turbulent heat flux $\langle v'T' \rangle$. These statistics are defined using the non-dimensional flow variables T , u , v and w .

The benefits of a SGS model are more evident when we compare their statistics to the statistics obtained by running a simulation on the same mesh without the application of the SGS model. This procedure will be done in the further analysis. However, for the particular regime $Ra = 10^6$, the behaviour of the solution with the dynamic Lagrangian model is the same as the behaviour without any model. Therefore, exceptionally, we do not superimpose the case "LES no model" to the other statistics for the sake of clarity.

Since we are at low Rayleigh number, the benefits of the dynamic k -equation model are not fully visible when only comparing the Nu (only less than 1% of accuracy is gained compared to the "LES no model" case, already extremely close to the DNS value). However the effect of the DK SGS model is much more visible on the flow statistics where it can correct the temperature and velocities fluctuations by a value of 10% compared to the case without model. The same remark is applicable for the kinetic turbulent energy.

As already mentioned, the dynamic Lagrangian model does not provide satisfying results at this regime since it does not have any effect on the flow statistics and under estimates the kinetic energy and the turbulent heat flux.

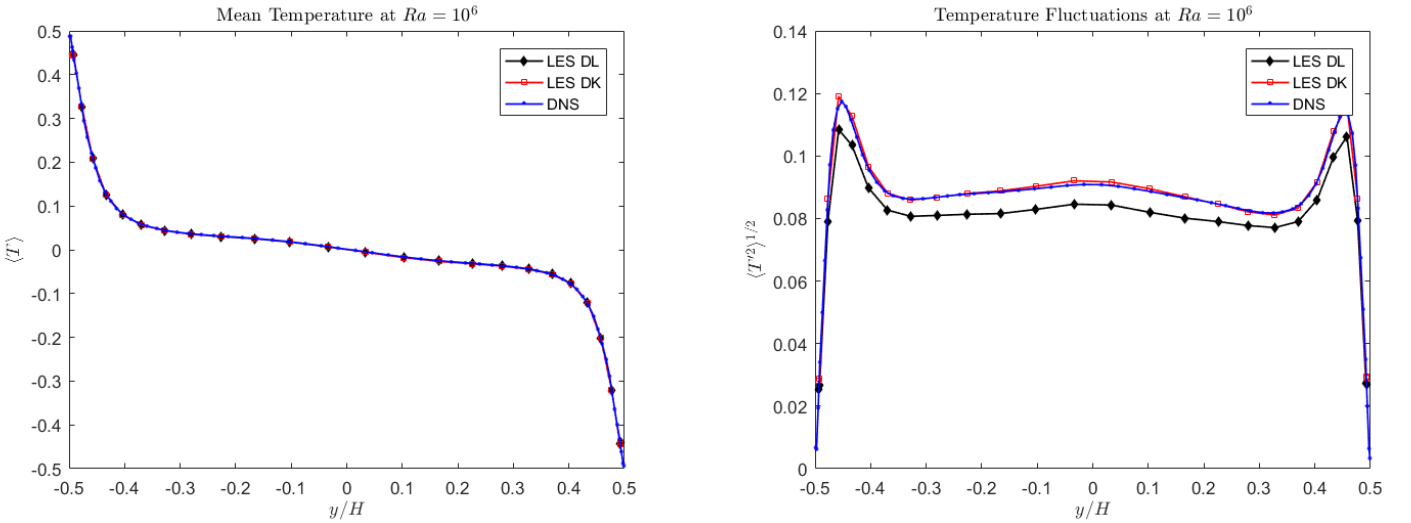


Figure 14: Time-average resolved temperature $\langle T \rangle$ and resolved temperature fluctuation $T_{rms} = \langle T'^2 \rangle^{1/2}$ at flow regime $Ra = 10^6$. The results obtained from the dynamic Lagrangian SGS model (DL) are presented in black, from the dynamic k -equation SGS model (DK) are presented in black and from DNS in blue.

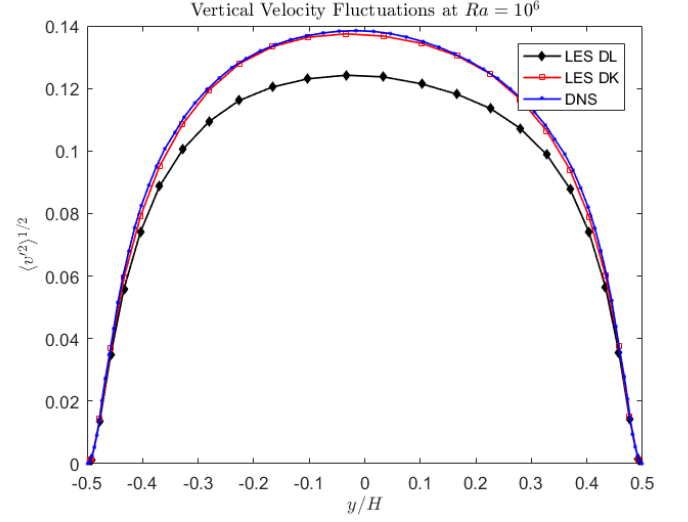
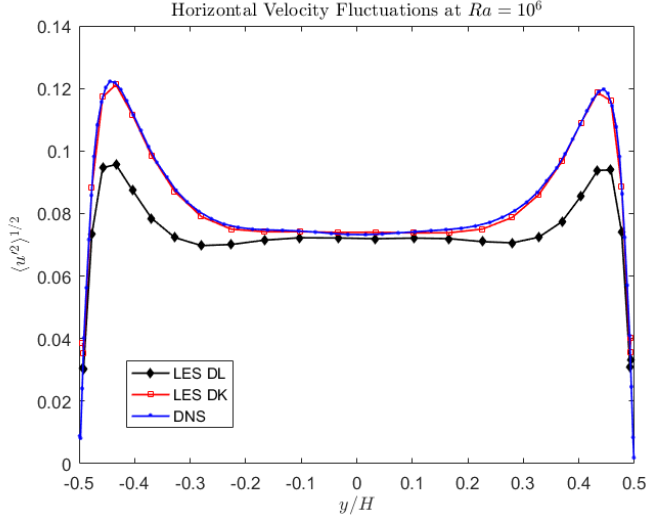


Figure 15: Resolved horizontal and vertical velocity fluctuations $u_{rms} = \langle u'^2 \rangle^{1/2}$ and $v_{rms} = \langle v'^2 \rangle^{1/2}$ at flow regime $Ra = 10^6$. The results obtained from the dynamic Lagrangian SGS model (DL) are presented in black, from the dynamic k -equation SGS model (DK) are presented in black and from DNS in blue.

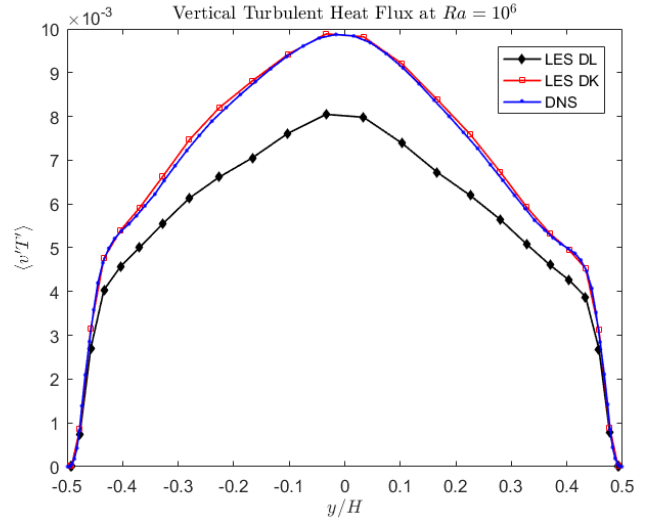
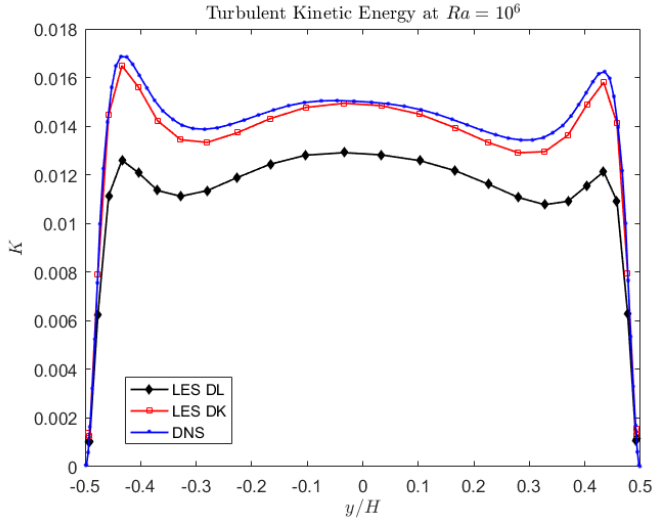


Figure 16: Resolved turbulent kinetic energy K and resolved turbulent heat flux $\langle v'T' \rangle$ at flow regime $Ra = 10^6$. The results obtained from the dynamic Lagrangian SGS model (DL) are presented in black, from the dynamic k -equation SGS model (DK) are presented in black and from DNS in blue.

5.2 $Ra = 10^7$ Regime - DNS and LES

With the coarser mesh defined for this regime, i.e. $N = 42$, the Nu obtained is still in good agreement with our DNS solution with an error estimated at 2% for the dynamic Lagrangian model and at 2.5% for the dynamic Lagrangian model compared to an error of more than 5% for the same mesh without SGS model.

The flow statistics for the $Ra = 10^7$ regime with the LES mesh $N = 42$ and the DNS mesh $N = 96$ are presented on the figure 14 to 16.

We observe that the DK SGS model provides again a really good approximation of the SGS quantities since its statistics profiles are really close to the DNS.

The DL SGS model is giving slightly more satisfying results at this regime than at the previous since it shows the same behaviour that the DK model with a much lesser effect. However it provides much better results than the case without model which is over-estimating the vertical velocity fluctuations and the turbulent kinematic energy K by 30% and the resolved heat flux by 40%. The statistics obtained with the two SGS models are closer to the DNS statistics but they are still over-estimated due to insufficient resolution of the mesh. With a refined mesh with $N = 64$ for these LES, the error on the Nusselt number compared to DNS decreases to 1.4% with the dynamic k -equation model.

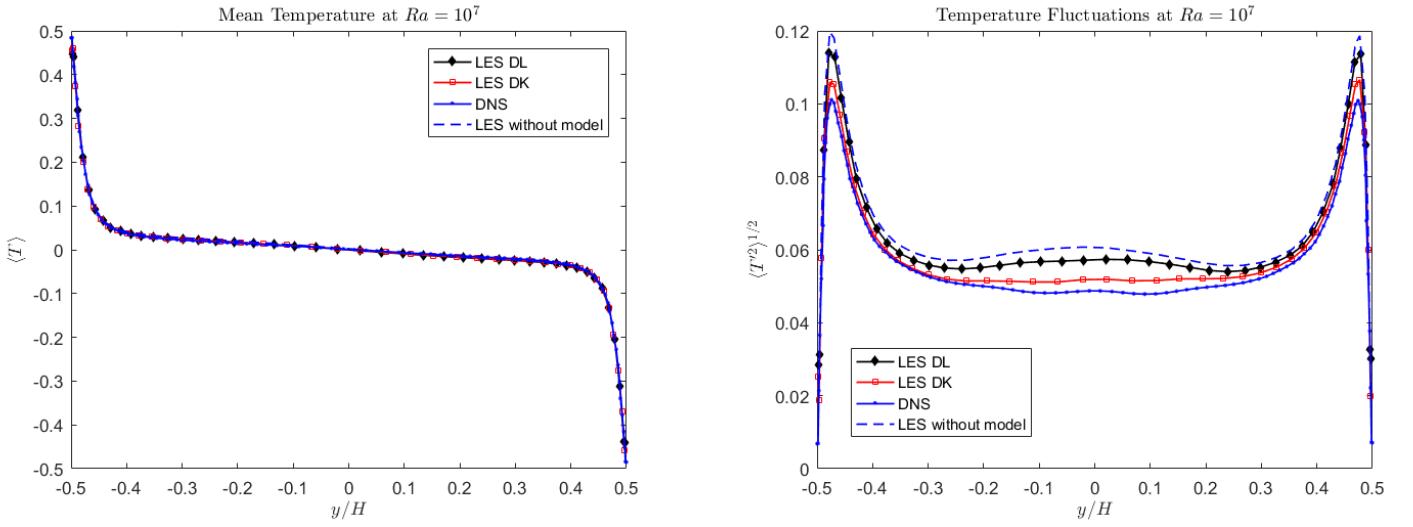


Figure 17: Time-average resolved temperature $\langle T \rangle$ and resolved temperature fluctuation $T_{rms} = \langle T'^2 \rangle^{1/2}$ at flow regime $Ra = 10^7$. The results obtained from the dynamic Lagrangian SGS model (DL) are presented in black, from the dynamic k -equation SGS model (DK) are presented in black and from DNS in blue.

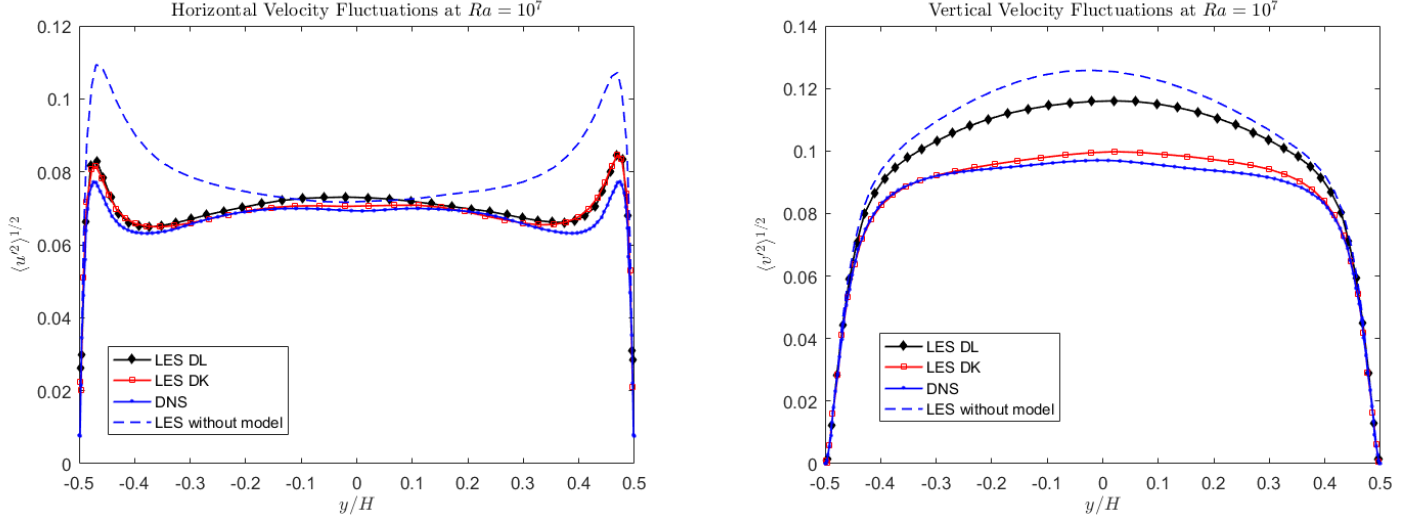


Figure 18: Resolved horizontal and vertical velocity fluctuations $u_{rms} = \langle u'^2 \rangle^{1/2}$ and $v_{rms} = \langle v'^2 \rangle^{1/2}$ at flow regime $Ra = 10^7$. The results obtained from the dynamic Lagrangian SGS model (DL) are presented in black, from the dynamic k -equation SGS model (DK) are presented in black and from DNS in blue.

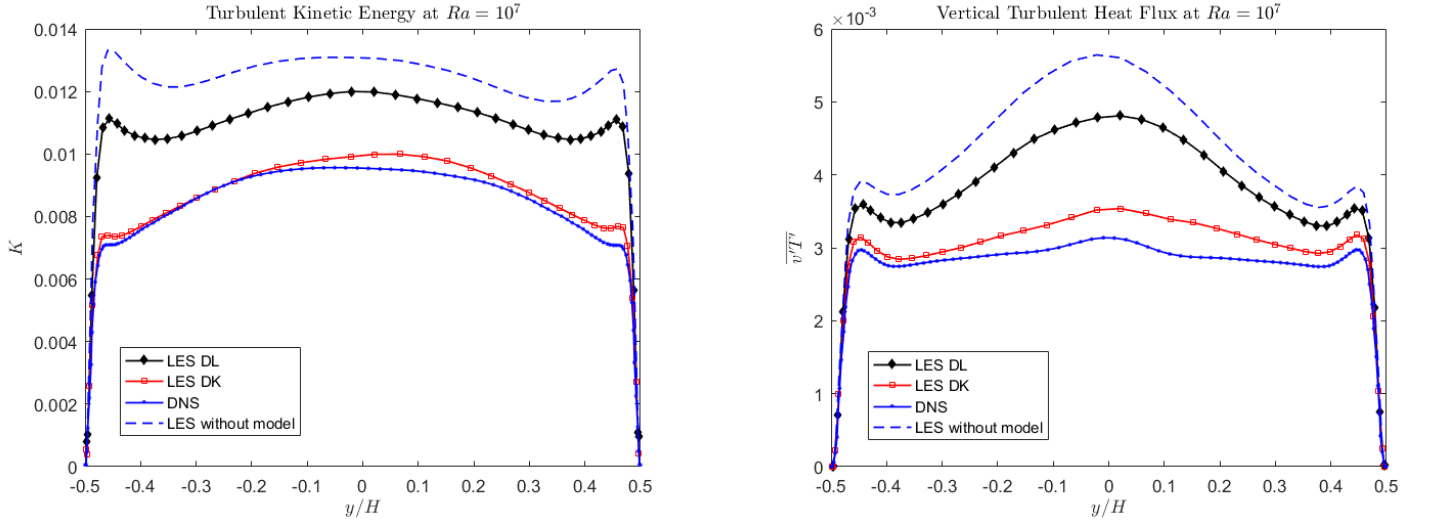


Figure 19: Resolved turbulent kinetic energy K and resolved turbulent heat flux $\langle v'T' \rangle$ at flow regime $Ra = 10^7$. The results obtained from the dynamic Lagrangian SGS model (DL) are presented in black, from the dynamic k -equation SGS model (DK) are presented in black and from DNS in blue.

5.3 $Ra = 5 \times 10^7$ Regime - DNS and LES

This regime is the higher we have reached with DNS due to computational costs.

With the coarser mesh defined for this regime, i.e. $N = 42$, the Nu error obtained between the Nu calculated from the LES fields and the Nu obtained in DNS is growing and reaches 8% for both models compared to an error greater than 12% without SGS model. Since this error seems too high to be a satisfying approximation of the system response, we decided to run an LES with a finer grid, i.e.

$N = 64$. With the refined grid, the error obtained on the Nu calculation decreases to 6% which is still a bigger error than for the previous regimes but remains reasonable for an approximation.

The flow statistics for the $Ra = 5 \times 10^7$ regime with the LES mesh $N = 42$ and the DNS mesh $N = 124$ are presented on the figure 20 to 22.

We can make the same observations that in the regime $Ra = 1 \times 10^7$ for the dynamic k -equation model which is providing a non negligible enhancement to the flow statistics compared to the case without model which is again over-estimating the kinetic energy and the heat transfer. The gain in accuracy may be estimated to an error reduced by more than 60% compared to the case without SGS model for all the flow statistics with a mesh two times coarser than for DNS.

The results obtained with the dynamic Lagrangian model at this regime are not satisfying and present a behaviour quite different from the DK SGS model since the DL model under estimates the turbulent kinetic energy and the turbulent heat flux while the DK model is over estimating these flow properties. Various test on the mesh resolution in the boundary layer and in the bulk have been performed in order to propose an explanation for this phenomena but the results remain inconclusive.

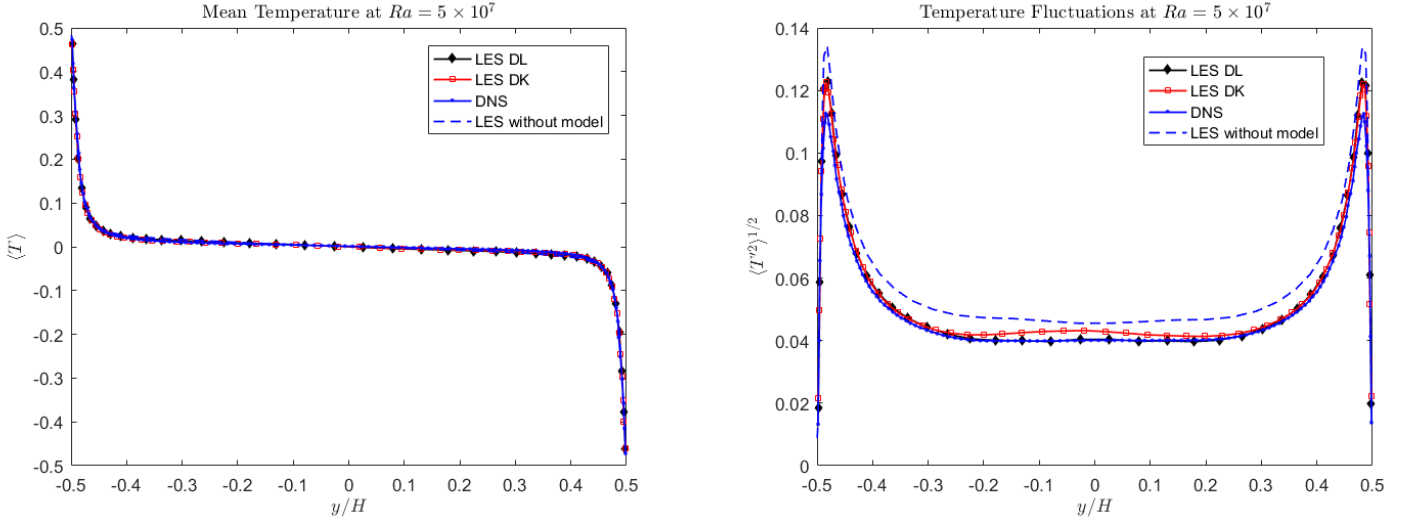


Figure 20: Time-average resolved temperature $\langle T \rangle$ and resolved temperature fluctuation $T_{rms} = \langle T'^2 \rangle^{1/2}$ at flow regime $Ra = 5 \times 10^7$. The results obtained from the dynamic Lagrangian SGS model (DL) are presented in black, from the dynamic k -equation SGS model (DK) are presented in black and from DNS in blue.

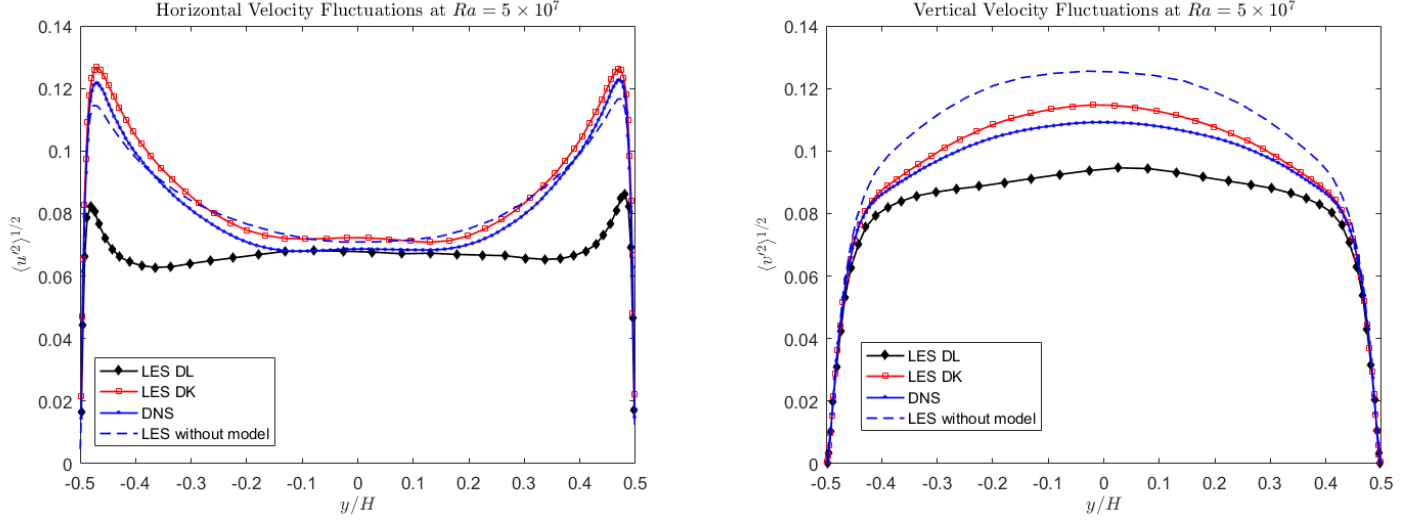


Figure 21: Resolved horizontal and vertical velocity fluctuations $u_{rms} = \langle u'^2 \rangle^{1/2}$ and $v_{rms} = \langle v'^2 \rangle^{1/2}$ at flow regime $Ra = 5 \times 10^7$. The results obtained from the dynamic Lagrangian SGS model (DL) are presented in black, from the dynamic k -equation SGS model (DK) are presented in black and from DNS in blue.

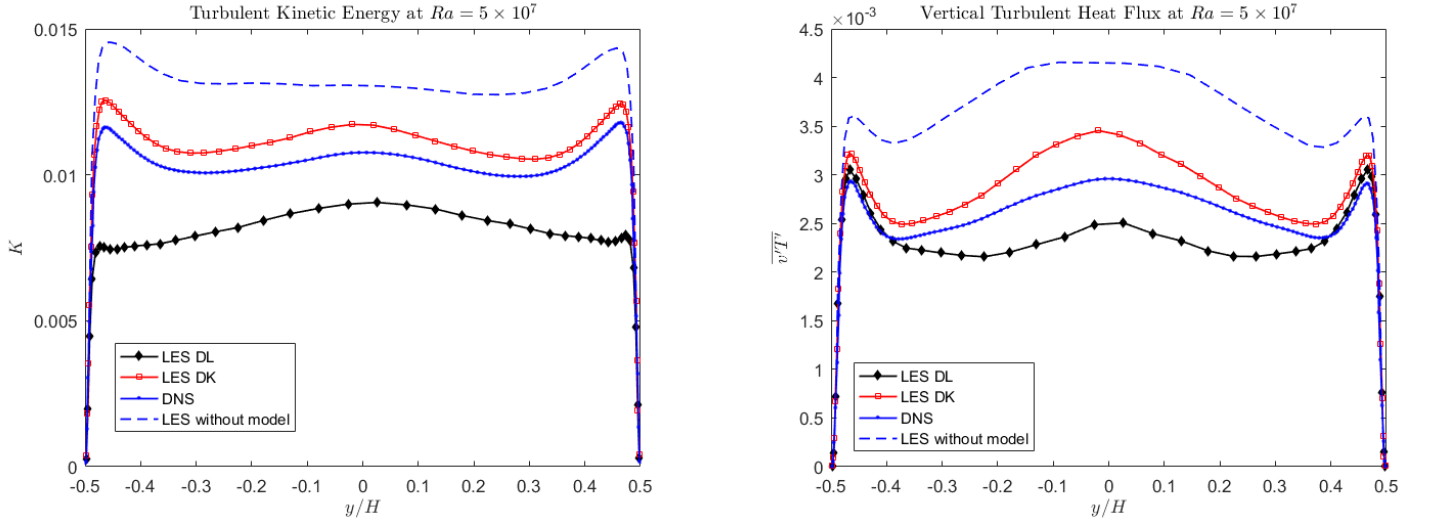


Figure 22: Resolved turbulent kinetic energy K and resolved turbulent heat flux $\langle v'T' \rangle$ at flow regime $Ra = 5 \times 10^7$. The results obtained from the dynamic Lagrangian SGS model (DL) are presented in black, from the dynamic k -equation SGS model (DK) are presented in black and from DNS in blue.

Taking into account the results obtained at the different regimes, it is reasonable to conclude that the mesh requirements defined in the previous sections are sufficient to guarantee a relatively well-resolved LES with the dynamic k -equation SGS model compared to DNS up to $Ra = 5 \times 10^7$.

In the other hand, the results obtained with the dynamic Lagrangian are quite inconsistent and do not allow us to validate the accuracy of its prediction with the actual mesh resolutions. More work may be needed in order to define different mesh requirement criteria for this SGS model leading to potentially better results.

5.4 Scaling of the statistics with Ra

In this section, we aim to foresee the scaling of the flow statistics with the Ra number ranging from 10^6 to 10^9 using LES and the dynamic k -equation sub-grid scale model.

Since the results obtained with the dynamic Lagrangian model does not allow to validate its results and ensure the quality of the results for $Ra \geq 5 \times 10^7$, we do not present its scaling here.

The grid spacing is still determined *a priori* from the criteria defined in the previous section. The flow statistics at the different regime are presented on the figure 23 to 27.

On the figure 23, we observe the scaling of the total heat transfer across the fluid layer, i.e. the Nusselt number average over time and the horizontal directions. The fact that this heat transfer remains constant in the whole domain ensure that we have reached a statistically steady state of turbulence when. However the difference between the Nusselt number obtained for the two large Ra , i.e. $Ra = 10^8 - 10^9$, and the reference Nusselt number is non negligible, indicating that the mesh used in this work is probably not fine enough to give a well resolved LES. Our computational resources being limited, we are not able to perform a more accurate simulation in this work. However, it could be interesting to observe the grid dependence of the solution in order to define better criteria for the mesh requirement of LES simulations at high Rayleigh number.

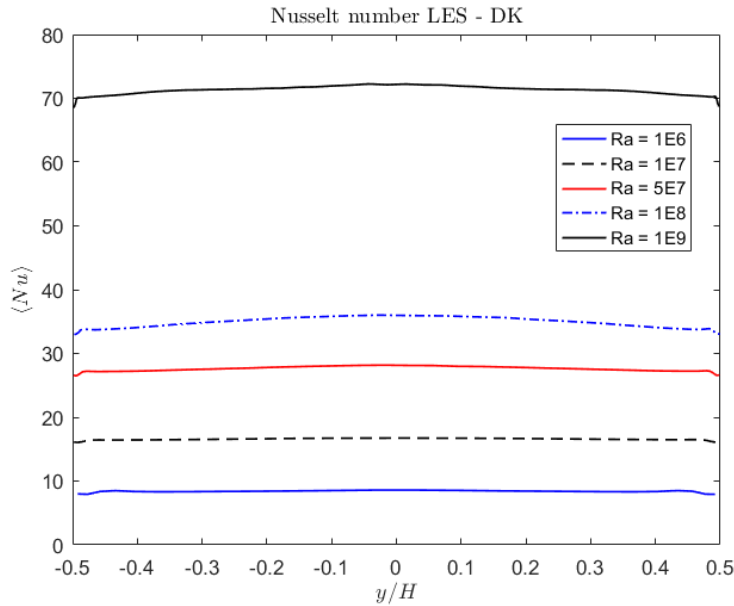


Figure 23: Time-averaged Nusselt number across the domain computed with the dynamic k -equation model at flow regime ranging from $Ra = 10^6 - 10^9$.

In figure 24, we observe that the ratio of boundary layer thickness of the thermal boundary layer to the height of the cell is decreasing as Ra increases. The thermal boundary layer thickness is characterise by the high temperature gradient in the near wall region. In the same way, the maximum value of the temperature fluctuation is shifted toward the wall when the Ra becomes larger while the intensity of the fluctuations in the center of the cell decreases.

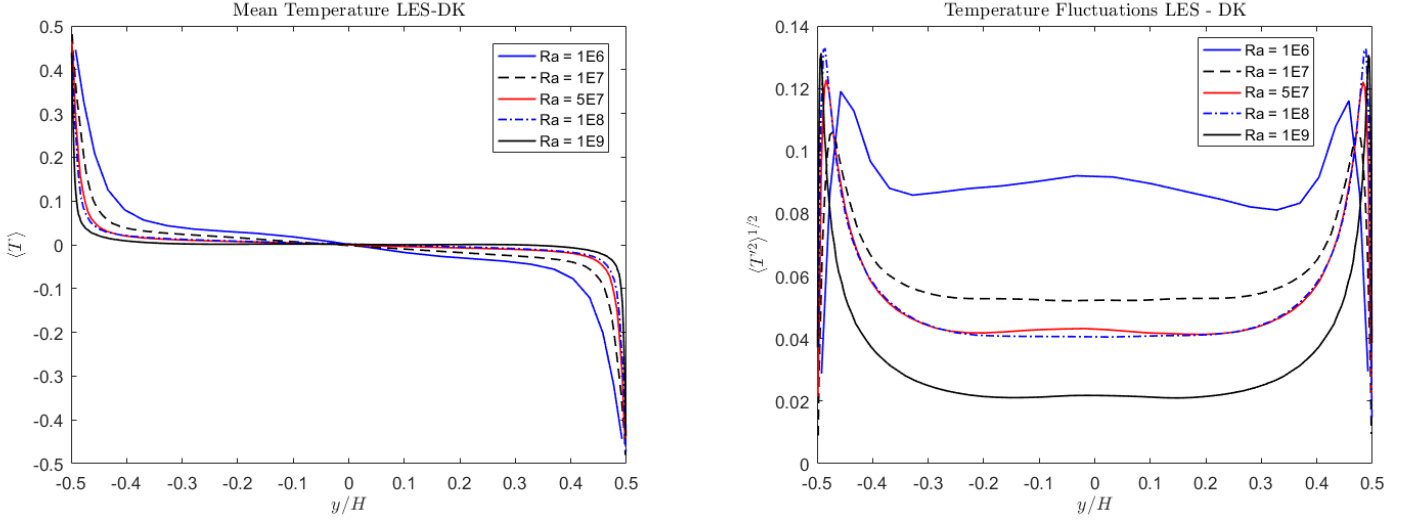


Figure 24: Time-average resolved temperature $\langle T \rangle$ and resolved temperature fluctuation $T_{rms} = \langle T'^2 \rangle^{1/2}$ computed with the dynamic k -equation model at flow regime ranging from $Ra = 10^6 - 10^9$.

In figure 25, we observe the presence of a peak of the horizontal velocity fluctuations in the near wall region that is also shifted towards the wall when the Rayleigh increases. This peak indicates the effect of the shear stress caused by the no-slip condition at the wall. The maximum vertical velocity fluctuation is attained in the center of the domain.

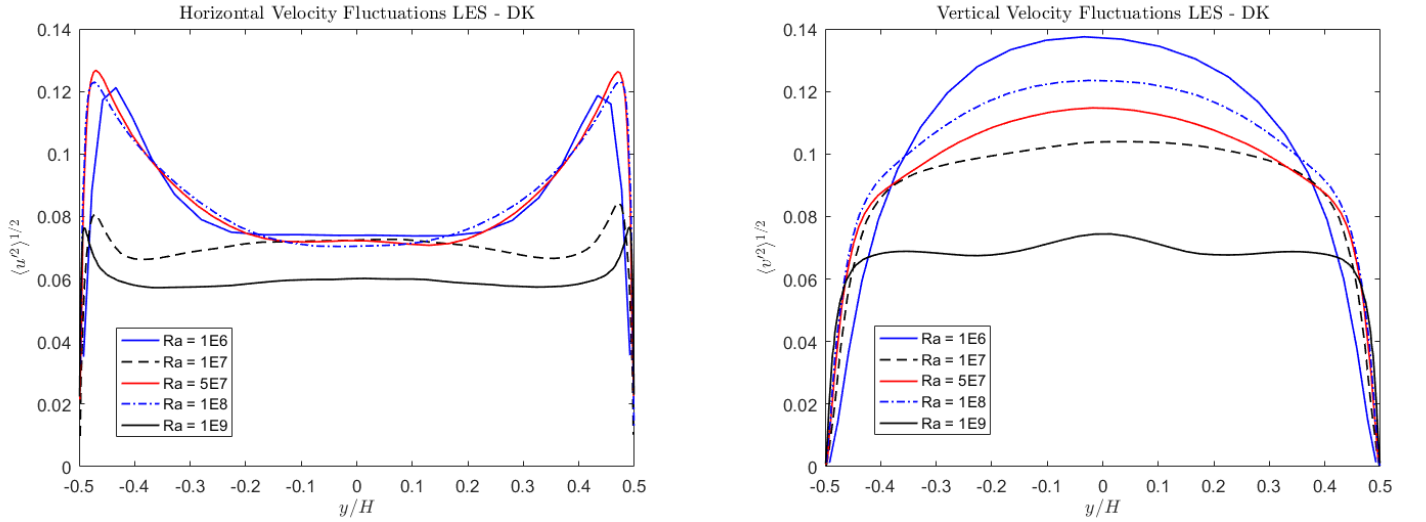


Figure 25: Resolved horizontal and vertical velocity fluctuations $u_{rms} = \langle u'^2 \rangle^{1/2}$ and $v_{rms} = \langle v'^2 \rangle^{1/2}$ computed with the dynamic k -equation model at flow regime ranging from $Ra = 10^6 - 10^9$.

In figure 26, the resolved kinetic turbulent energy K exhibits a rapid increase the the walls, probably due to the turbulence energy transported by the thermal plumes, and attain its peak value near the end of the boundary layer. This peak value seems to decrease when the Ra increases and the profile tends to become more flat in the center when the Rayleigh number is increasing.

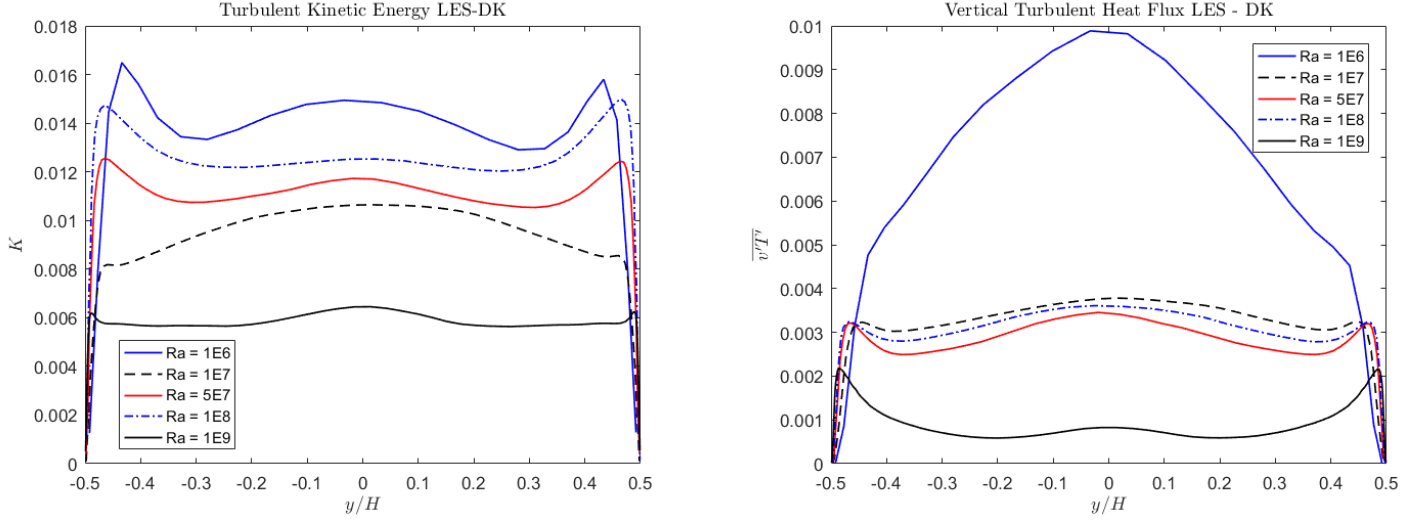


Figure 26: Resolved turbulent kinetic energy K and resolved turbulent heat flux $\langle v'T' \rangle$ computed with the dynamic k -equation model at flow regime ranging from $Ra = 10^6 - 10^9$.

The figure 27 represent the sub-grid scale quantities k_{SGS} , the SGS kinetic energy and ν_{SGS} the SGS eddy viscosity. As expected, the values increase as Ra increases because of the increase of the grid spacing in the bulk region. The contribution of the SGS model becomes greater when we increase width of the mesh.

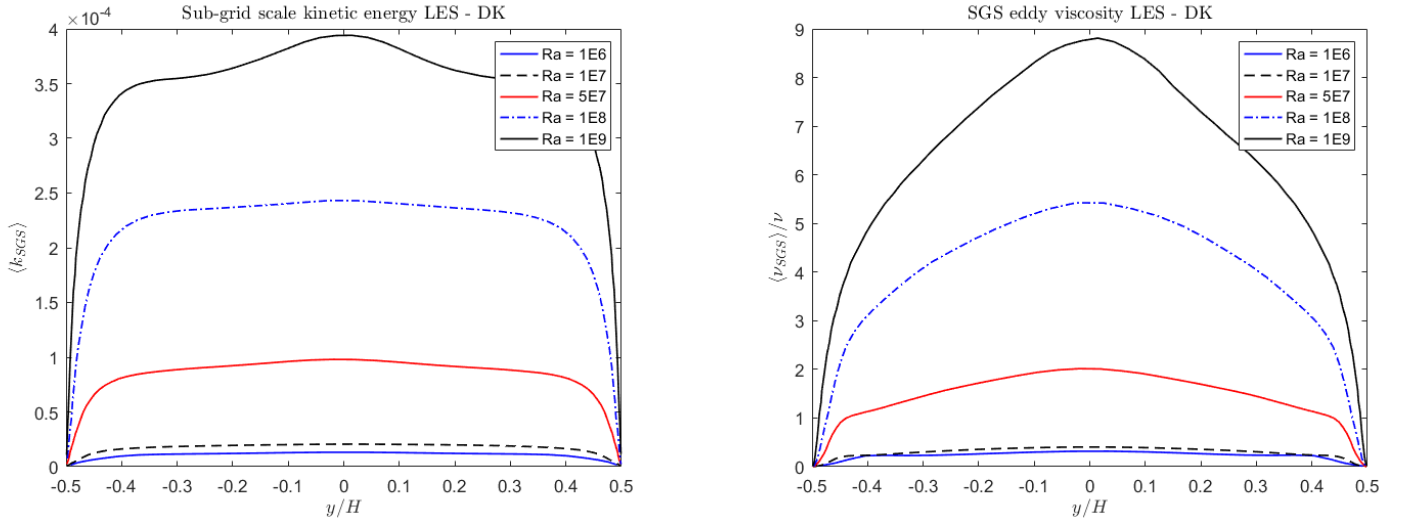


Figure 27: Time-averaged sub-grid scale kinetic energy k_{SGS} and time-averaged SGS eddy viscosity ν_{SGS} compared to global viscosity ν computed with the dynamic k -equation model at flow regime ranging from $Ra = 10^6 - 10^9$.

An important remark concerns the ratio ν_{SGS}/ν discussed in the section 2.2.3. In that section, we mentioned that the ratio ν_{SGS}/ν should not exceed the value of 10 in order to have a well resolved LES. However, it have been stated by [35] that in order to have accurate simulation a better practice is to design meshes corresponding to lower values of ν_{SGS}/ν . In their work, they obtained $\nu_{SGS}/\nu \approx 2.7$ as an upper bound for their simulations at $Ra = 10^9$. According to this paper, it is likely that the results

presented here for the regimes $Ra = 10^8$ and $Ra = 10^9$ are using a too coarse mesh. However these too coarse meshes are the best we can do with the computational resources available for this work.

Finally, as an illustration of the simulation performed by LES with the dynamic k -equation model, we present here some of the 3D flow characteristics representative of the Rayleigh-Bénard convection problem.

The figure 28 represents the time-averaged streamlines. We can observe the mean wind governing the convection along one of the diagonal of the cube and small recirculation regions in some of the corners. We can identify two counter rotating flow structures converging at the mean plane. Such flow structures have been described in other simulations [46], suggesting that our simulation has a correct description of the global mean flow structures from a qualitative point of view.

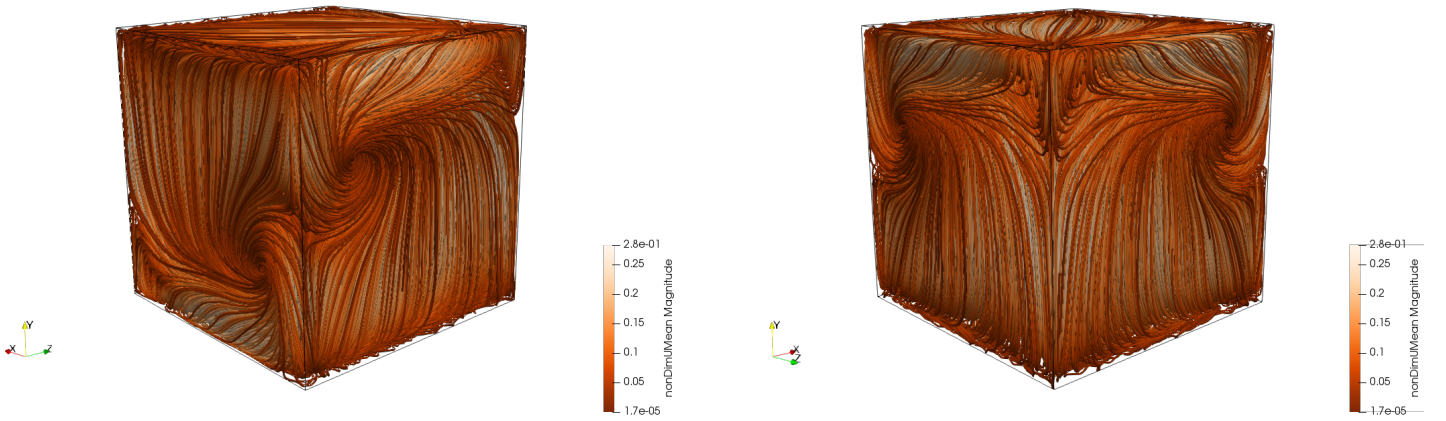


Figure 28: Streamlines of the mean flow in the cubical cell at $Ra = 10^9$. The velocity scale represent the magnitude of the non-dimensional velocity defined with the free-fall velocity.

The heat flux at the wall $Nu_w(x, y) = \left(\frac{\partial \langle T(x, z) \rangle_t}{\partial y} \right)_w$ is represented on the left of the figure 29 where we can see the influence off the mean wind circulation on the local heat flux at the wall.

On the right, we find a representation of the instantaneous temperature field were the thermal plumes are clearly visible.

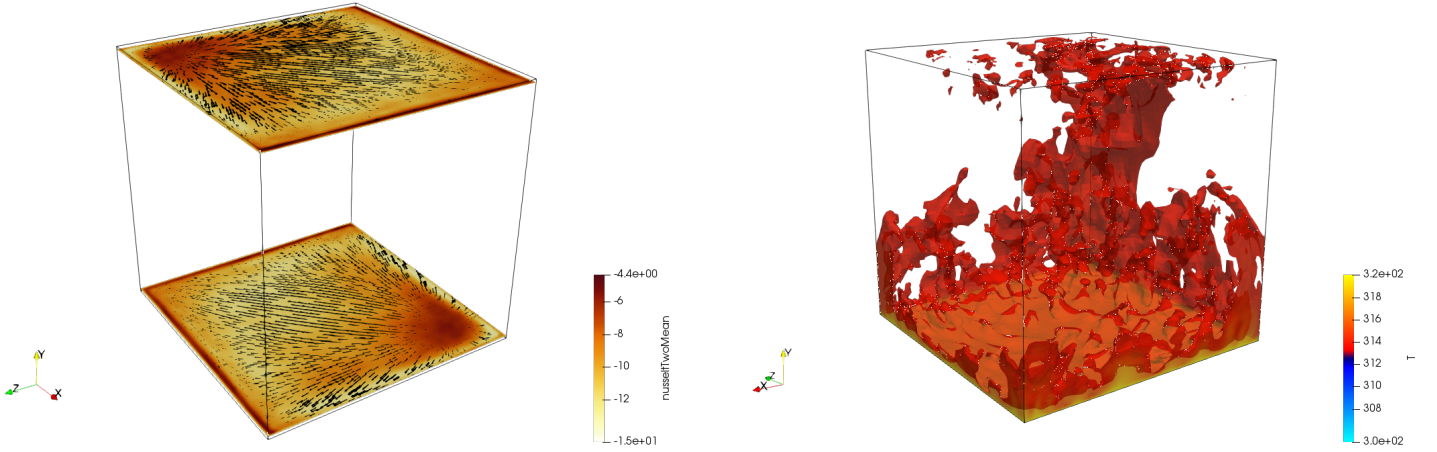


Figure 29: On the left : Contour color plot of the time averaged vertical heat flux at the bottom and top plates and the velocity vectors representing the large scale convection. On the right : Isosurface of the non dimensional instantaneous temperature field at $t = 1000$.

As a conclusion, the dynamic k -equation SGS model produces qualitatively and quantitatively good solutions for the problem of Rayleigh-Bénard convection over the range of Ra considered provided that the mesh is sufficiently fine in the bulk at large Ra .

It seems that the mesh resolution required in order to ensure the accuracy of the results at high Rayleigh number has not been fully satisfied in this work but the solution obtained is still satisfying on a qualitative perspective. If the computational resources are available, the next milestone would be to further study the grid dependence of the LES solution in order to derive appropriate mesh resolution requirements for large Rayleigh numbers. LES is an essential tool to investigate Rayleigh-Bénard problem at high Ra since accurate DNS requires tremendous computational resources. In the case $Ra = 10^9$, DNS would have required at least a $300 \times 300 \times 300$ mesh to be performed while we initially identified the LES requirements to be around $100 \times 100 \times 100$. Even if we have to refine the mesh for LES, it would significantly improve the computational time and resources needed to solve this problem.

5.5 High Temperature Gradient

In this last part, we will focus on the flow statistics at the regime $Ra = 10^6$ when the temperature gradient is increased from $\Delta T = 15[\text{K}]$ to $\Delta T = 60[\text{K}]$. This temperature gradient is more likely to be representative of the real conditions under which the cooling of the nuclear spent fuel pool occurs. In such conditions, since we use a low-Mach solver instead of a solver using the Boussinesq approximation, we should be able to observe non-Oberbeck-Boussinesq (NOB) effects [47]. The aim of this part is to determine if whether or not such effects are observed in our simulations. We do not ensure the accuracy of these results on a quantitative point of view since the mesh requirements are likely to change.

When large temperature gradients appear, one may observe strong variations of the kinematic viscosity and of the thermal expansion coefficient leading to an asymmetry with respect to the mid plane of the cell. As illustrated on the figure 30, this asymmetry results in a different temperature T_c in the centre of the cell which normally is equal to the mean temperature in the Oberbeck-Boussinesq (OB) case.

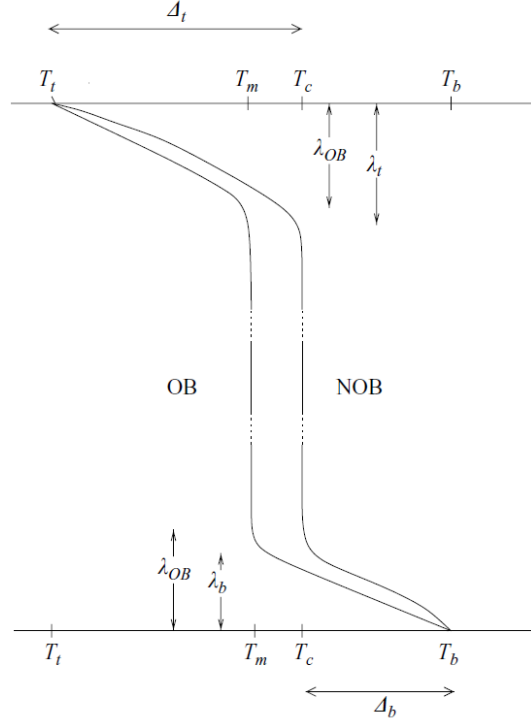


Figure 30: Time-averaged temperature vs. height y in the Oberbeck-Boussinesq (OB) and non-Oberbeck-Boussinesq (NOB) cases, respectively. The indices t and b refer respectively to the top and bottom plates. Figure from [47].

The figure also shows that the boundary layer thickness is also affected by the NOB effects because we are no longer ensured to be in the classical case of the Blasius BL theory. This might have an impact on the mesh resolution of our simulation and a refinement may be needed in order to have accurate results. However, this problem will not be taken into account in this work and may need to be the object of further study.

The parameters used in these simulations are summarised in the table 6.

Table 6: Simulation parameters and corresponding Nusselt number for the case $\Delta T = 60[\text{K}]$.

Ra	Type	N	$N_{\text{th.BL}}$	$N_{\text{v.BL}}$	$\frac{h^{\text{max}}}{H}$	$\frac{h^{\text{max}}}{h^{\text{min}}}$	Nu	$Nu_{\text{ref}[32]}$	t_{avg}^*
10^6	DNS	64	11/2.8	11/2.5	0.03	10	8.33	8.32	1600
10^6	DK	24	4/2.8	3/2.5	0.07	5	8.46	8.32	1600
10^6	DL	24	4/2.8	3/2.5	0.07	5	8.46	8.32	1600

As we can see, the Nusselt number obtained by DNS is really close to the one from the reference, which means that the mesh is likely to be sufficiently fine for our problem. However, the Nu obtained with LES are in less good agreement with the reference, probably due to an insufficient resolution of the boundary layers.

The figures 31 to 33 illustrate the flow statistics of the Rayleigh-Bénard convection with a large gradient of temperature. As expected, we observe a flow asymmetry with a greater kinetic energy and heat flux found in the bottom side, near the heating plate. However, we do not observe a difference between the temperature in the center of the Rayleigh-Bénard convection cell and the mean temperature of the flow.

This effect may be revealed at higher Ra , when the center region is larger.

Overall, the flow statistics are well captured by our LES simulations and correspond to the DNS, despite an inaccuracy in the estimation of the Nusselt number.

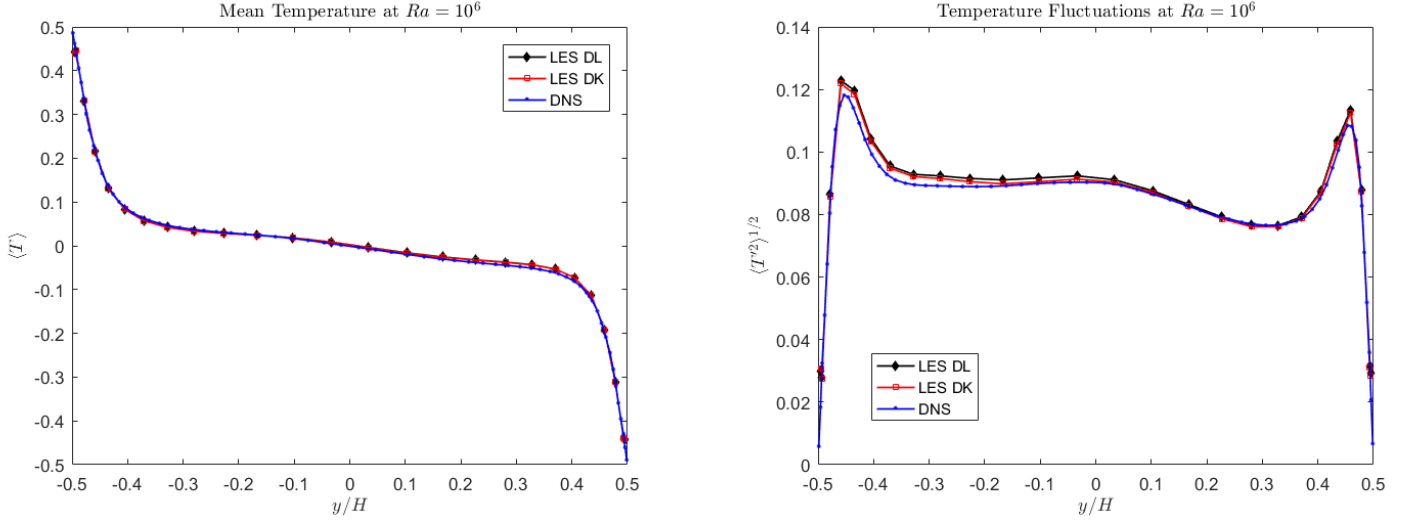


Figure 31: Time-average resolved temperature $\langle T \rangle$ and resolved temperature fluctuation $T_{rms} = \langle T'^2 \rangle^{1/2}$ at flow regime $Ra = 10^6$ with high temperature gradient $\Delta T = 60[\text{K}]$. The results obtained from the dynamic Lagrangian SGS model (DL) are presented in black, from the dynamic k -equation SGS model (DK) are presented in black and from DNS in blue.

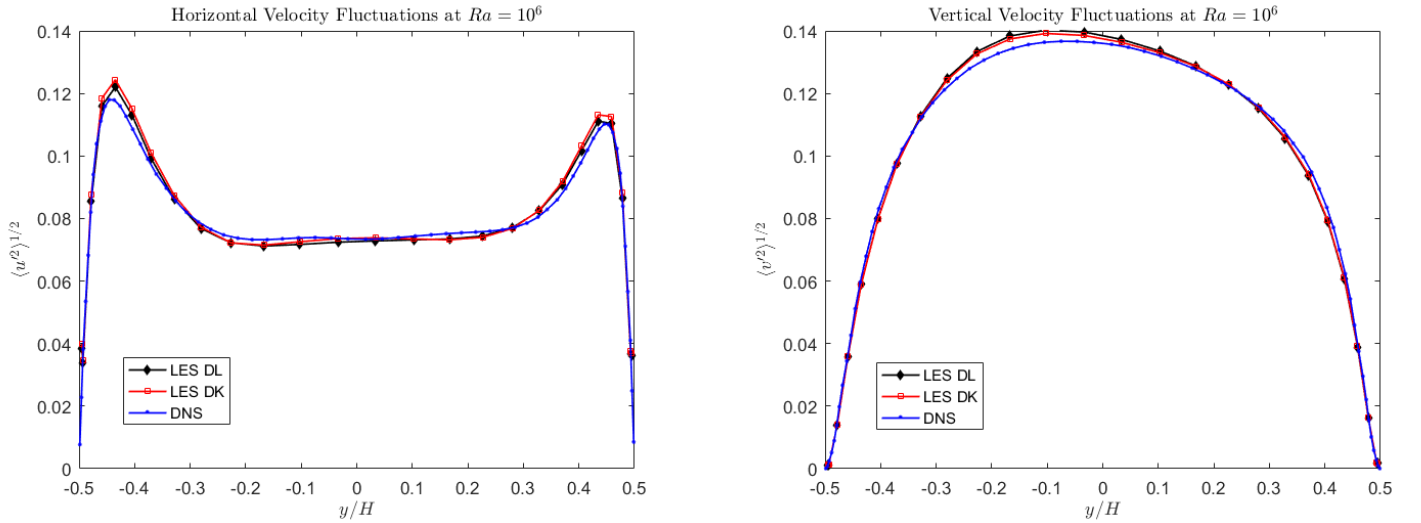


Figure 32: Resolved horizontal and vertical velocity fluctuations $u_{rms} = \langle u'^2 \rangle^{1/2}$ and $v_{rms} = \langle v'^2 \rangle^{1/2}$ at flow regime $Ra = 10^6$ with high temperature gradient $\Delta T = 60[\text{K}]$. The results obtained from the dynamic Lagrangian SGS model (DL) are presented in black, from the dynamic k -equation SGS model (DK) are presented in black and from DNS in blue.

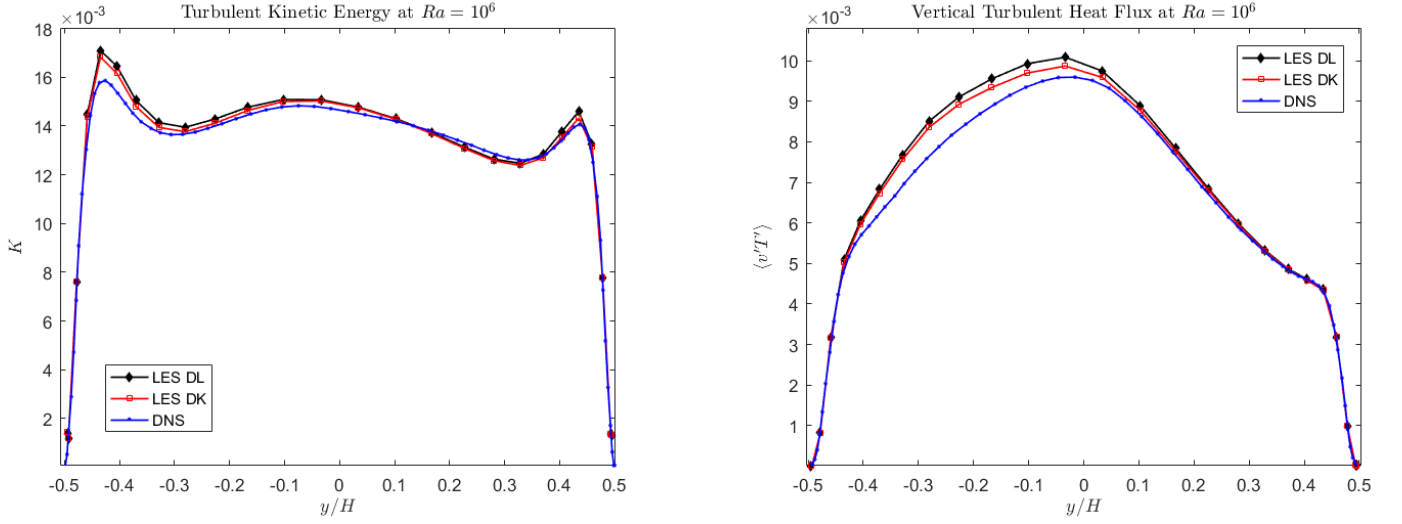


Figure 33: Resolved turbulent kinetic energy K and resolved turbulent heat flux $\langle v'T' \rangle$ at flow regime $Ra = 10^6$ with high temperature gradient $\Delta T = 60[\text{K}]$. The results obtained from the dynamic Lagrangian SGS model (DL) are presented in black, from the dynamic k -equation SGS model (DK) are presented in red and from DNS in blue.

This section is only a short overview of the presence of non-Oberbeck-Boussinesq effect and more work has to be done in order to determine the appropriate resolution requirements and quantify the flow statistics over a wide range of Rayleigh numbers.

6 Conclusion

In this thesis, we intended to validate the numerical performance of two sub-grid scales models, the dynamic k -equation model and the dynamic Lagrangian model, for an application representative of the flow inside a Spent Fuel Pool of nuclear power plants.

The validation of these models has been performed by comparing the results of Large Eddy Simulations using the chosen SGS models to those of Direct Numerical Simulations for the classical problem of Rayleigh-Bénard convection in a cubic cell. These simulations have been performed considering the working fluid as air at 313[K] characterised by the Prandtl number $Pr = 0.7$. The results between LES and DNS have been compared over a range of Rayleigh number $Ra = 10^6, 10^7, 5 \times 10^7$ and further simulations have been performed up to $Ra = 10^8, 10^9$ using LES. In addition, we made an extensive review of the mesh requirement in order to perform accurate DNS and well resolved LES.

The dynamic k -equation sub-grid scale model has yielded to solutions in really good agreement with the DNS solutions over the range of Rayleigh number considered. However it seems that a mesh finer than the requirements defined is needed to obtain a well-resolved LES from $Ra \approx 10^8$. Overall, this SGS model seems to have a good potential in modelling the sub-grid scales for Rayleigh-Bénard convection. The dynamic Lagrangian sub-grid scale model have shown inconsistent behaviours over the comparison range with DNS. Despite the meeting of the *a priori* grid resolution criteria, the results obtained using this SGS model does not allow us to validate the dynamic Lagrangian model as a suitable sub-grid scale model for Rayleigh-Bénard convection.

We solved the Rayleigh-Bénard problem using the low-Mach approximation rather than the classical Boussinesq approximation in order to be able to compute accurately large temperature gradient flows. The non-Oberbeck-Boussinesq effects have been highlighted when the temperature difference between the two plates is increased to $\Delta T = 60[\text{K}]$. Further study about this particular case is needed in order to fully determine the performances of the SGS models in this configuration.

To conclude, the identification of the dynamic k -equation sub-grid scale model as a reliable SGS model for LES in Rayleigh-Bénard convection allows us to further study the natural convection driven turbulence in a spent nuclear-fuel pool at large Rayleigh numbers while saving considerable computation time and resources compared to DNS. Therefore, this work makes way to further studies. Especially about the non-Oberbeck-Boussinesq effects and the introduction of more complex boundary conditions taking into account the physical phenomena occurring in a spent nuclear-fuel pool, e.g. modelisation of the free surface at the interface air/water and of the corresponding heat and mass transfers.

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