

École polytechnique de Louvain

Numerical study of natural convection of water in a nuclear spent fuel pool

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1 Introduction

Today, nuclear energy provides about 10 % of the world electricity [1] throughout 442 operational reactors located in 30 countries [2]. Another 53 reactors are under construction and 187 have already been shut down. Table 1 summarizes the top 5 countries having the more operational reactors and the top 5 countries having the biggest nuclear share in their electricity production, while also pointing out Belgium’s position in these rankings.

	Country	Number of operational reactors		Country	Nuclear share of electricity generation
1	USA	96	1	France	71,7 %
2	France	57	2	Slovakia	55 %
3	China	48	3	Ukraine	53%
4	Russia	38	4	Hungary	50,6 %
5	Japan	33	5	Sweden	40,3%
11	Belgium	7	6	Belgium	39 %

Table 1: Countries having the most operational reactors or the highest nuclear share [2].

Because nuclear energy continues to be used all around the world, spent fuel continues to be created and must be dealt with. As spent fuel emits radiations and gives off heat during years, it is usually stored at the bottom of spent nuclear fuel pools. Indeed, the water of those pools act as a shield against radiations and as a coolant to remove heat. Spent nuclear fuel pools, nevertheless, can become hazardous if the amount of water contained in the pool decreases, due to evaporation, leaks, etc. It is thus interesting to model the water flows and the heat transfer happening inside it to gain insight and prevent any catastrophe.

Since the spent fuel is placed at the bottom of the pool, the heat is evacuated by means of Rayleigh-Bénard convection. Rayleigh-Bénard convection is a type of natural convection that occurs when a fluid is heated from below and cooled down from above. Due to the temperature gradient, the hot fluid rises while the cold one sinks, forming a flow. Furthermore, in such an application the flow is considered to be turbulent and forms a Large Scale Circulation (LSC). Inside a cubical container, the Large Scale Circulation aligns itself to one of the diagonal. It has previously been observed, for other fluids than water, that the LSC however does not stay indefinitely in the same diagonal with the same direction but reorients itself randomly in time.

This project aims at modelling the natural convection that takes place inside a spent nuclear fuel pool. To do so, OpenFOAM, an open source CFD (Computational Fluid Dynamics) software will be used to simulate the flow and the heat transfer inside it. The code will rely on the Low Mach Number Equations to which turbulence is added throughout Large Eddy Simulation, LES. This will allow us to resolve the water flow in a cubical container representing the spent nuclear fuel pool.

Two different cases will be analysed and compared against each other. The difference between the two cases lies in the boundary conditions used to modelize the water-air interaction at the surface of the pool. The first case will consider the upper surface as a

fixed wall which involves a zero velocity at the surface. This case will be referred to as classical Rayleigh-Bénard convection (RBC) since it is the classical way of analyzing such a convection. The other one will consider the surface of the pool as a free-surface. This will allow to draw near the real spent nuclear fuel pools conditions where evaporation takes place at the free-surface of the pool. To gain insight on the flow characteristics without increasing the complexity of the model too much, we will here settle for a free-surface boundary condition at the surface of the pool.

As a first step, we will compare the two cases, for a Rayleigh number of $Ra = 2 * 10^7$. We will first take interest in the formation of a Large Scale Circulation and then analyze the flow statistics. Plots of the mean and root mean square (rms) temperature and velocity profiles as well as the turbulent heat flux will be presented (either along the center-line of the cube or by using area-averages). This will enable us to observe that the free-slip case has smaller thermal boundary layers, a colder mean temperature, a higher Nusselt number and turbulent heat flux. We will also see that the statistical profiles are usually symmetric for classical Rayleigh-Bénard convection as opposed to the ones obtained for the free-slip cases. In a second step, we will focus on the influence of higher Rayleigh number ($Ra = 2 * 10^7, 5 * 10^7$ and 10^8), for both boundary condition, on the statistics. Thinner boundary layers as well as higher rms values will be observed with increasing Rayleigh number. Finally, we will examine the influence of the upper boundary conditions on the existence, frequency and properties of the re-orientations at $Ra = 2 * 10^7$.

This report will first introduce the reader to Nuclear Spent Fuel Pools, their role in nuclear power plants, the challenges and links with Rayleigh-Bénard convection. Then, the model used by the OpenFOAM solver which relies on the Low Mach Number equations will be discussed. Once the basic functioning of the solver has been outlined, one will talk about the case set-up, involving the mesh, the initial and boundary conditions, the turbulence models as well as all the other information necessary for the case to run properly. At this point, all the necessary theoretical information concerning the simulation will have been presented and we will go on with the results. First, an analysis of various fields and properties composing the flows will be presented before studying re-orientations of the flow. Finally, a conclusion will complete this report, highlighting the differences that this project has been able to identify between classical Rayleigh-Bénard convection and our free-slip case which better approximates the reality of spent nuclear fuel pools.

2 Context

2.1 Nuclear Spent Fuel Pools

To understand the motives of this project, namely a better understanding of natural convection inside a spent fuel nuclear pool, one should first be familiar with spent nuclear fuel pools, their functions, designs and challenges. This section aims at introducing nuclear fuel pools, their role inside a power plant and their future evolution.

The following subsections will briefly introduce the reader to the basics of the nuclear cycle, the composition of a nuclear power plant, the management of the spent nuclear fuel and the role of the spent nuclear fuel pool in it. Finally, a more specific description of the nuclear fuel pool will be given before ending by a discussion about the future challenges that await nuclear spent fuel pools.

2.1.1 Nuclear cycle

Nuclear electricity is created from the fission of fissile atoms such as uranium or plutonium: this reaction creates heat which is used to form steam, which then drives a turbine. The turbine itself powers an alternator generating electricity [3, 4].

The main component of a plant is thus the reactor, in which the nuclear reaction takes place. The nuclear fuel is placed inside the reactor. Once a uranium nucleus absorbs a neutron, it splits up (fission), generating a huge amount of heat and liberating other neutrons that will produce more fission. The fission reaction is thus a chain reaction that must be controlled to stay at a constant rate [4].

Since the reaction creates heat, water, from what is called the primary circuit, flows around the reactor to recover the heat, see Figure 1. The water from this primary circuit is pressurized to avoid it from boiling, and is radioactive. The heat is passed on to the secondary circuit inside a steam generator. The water of the secondary circuit thus becomes steam that drives the turbine. After the water has gone through the turbine, it must be condensed before reaching the steam generator again. The condensation is made possible by a third circuit, the cooling circuit. While the primary and secondary circuits are closed, the third one is open: water can be released and/or pumped in a river, lake... after being cooled by air in a cooling tower (which is not present in all plants) [3, 5].

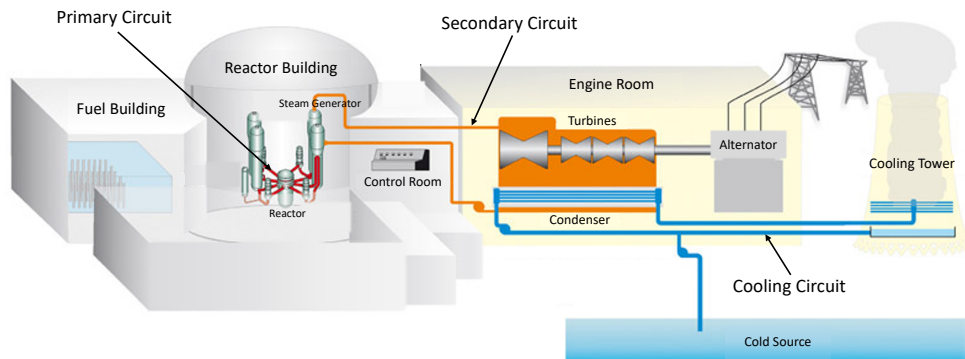


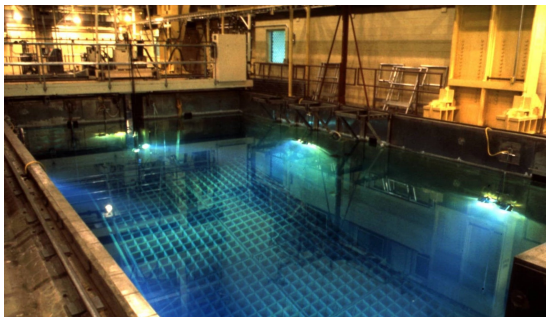
Figure 1: Nuclear Power Plant Infrastructure [6].

2.1.2 Nuclear Power Plants

As a nuclear power plant consists of many different elements, such as water circuits, turbine, alternator, fuel storage facilities, pumps and so on, it requires a specific infrastructure. A nuclear power plant can be decomposed into 5 specific facilities: the control room, the reactor building, the fuel building, the engine room and the cooling tower. The first one, the control room, controls the chain reaction happening in the reactor and centralizes data coming from all over the plant. The control room can be seen as the "brain" of the power plant. The reactor is located in the reactor building with the primary circuit and its pumps and pressurizer (to avoid water from boiling). The vapor generator with part of the secondary circuit is also present in the reactor building. Next to this reactor building, one can find the fuel building. It stores new, unused fuel as well as spent fuel in what is called a spent fuel nuclear pool. The water of the pool dissipates the heat still generated by the spent fuel and creates a shield against radiations still emerging from the spent fuel. The engine room, on the other hand, contains part of the secondary circuit as well as the turbine and the alternator. The condenser with a part of the cooling circuit and its pump is also installed in the engine room. Finally a cooling tower is present to reduce the cooling water temperature before reusing it or rejecting it in the river. Figure 1 illustrates the power plant infrastructure containing these five premises [4].

2.1.3 Nuclear Fuel Management

One of the principal challenges of nuclear power is the fuel management. The fuel, usually uranium, must undergo several steps before being used: mining, milling, conversion, and enrichment. After this, the fuel is fabricated as pellets gathered inside rods. These rods are put inside the reactor where they will undergo the fission chain reaction for about 4 to 5 years [7, 8].



(a) Spent Nuclear Fuel Pool [9].



(b) Dry Cask [10].

Figure 2

Afterwards, the spent fuel is taken out of the reactor and placed in a spent nuclear fuel pool located inside the nuclear power plant, for at least 1 year, see Figure 2a. The fuel is moved from the nuclear reactor to the pool underwater to avoid to release any radiation in the atmosphere surrounding it. The pool allows the fuel to be covered by at least 6 meters of water, which provides radiation shielding as well as cooling. After a certain period, the spent fuel is either kept in the pool or moved to underwater storage (other pools) or to

dry casks. Dry casks, see Figure 2b, are steel cylinders filled with inert gas that are made to contain spent fuel rods. The steel cylinders are additionally surrounded by concrete or steel to provide radiation shielding. The fuel inside the casks is cooled by air [11, 12]. The spent fuel pool as well as the dry cask are means of interim storage until the radiation level released by the spent fuel decreases sufficiently.

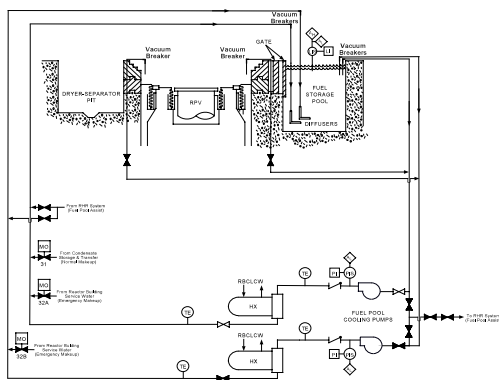
After several years, the nuclear fuel can be reprocessed. This enables to recover some of the unused plutonium and uranium that can be reused later on. The other components (that cannot be reused) are called final waste and are poured into molten glass before being disposed of. The reprocessing step allows to reuse part of the fuel and to reduce the volume of waste that must be disposed of. However, reprocessing is not always performed [7, 13]. Finally, the nuclear waste must be disposed of by burying it underground [8].

2.1.4 Spent nuclear fuel pool

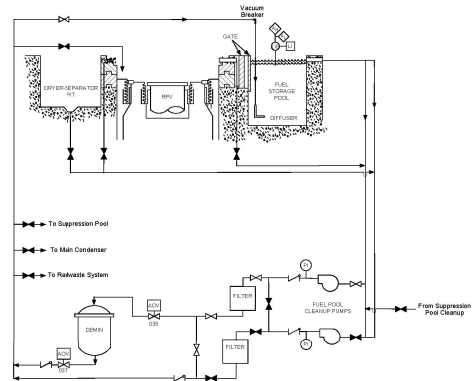
As the previous sections have presented the basic principles of nuclear energy as well as the infrastructure that it requires, the role of the Spent Fuel Pool, sometimes referred to as SFP, appears to be crucial in the waste management part. Since the fuel rods are still very radioactive and still give off a huge amount of heat, every single fuel rod must be placed in a pool for a certain time in order to guarantee safety. Nuclear spent fuel pools are thus a key component in the nuclear technology and its waste management.

The pool is located in the fuel building, right next to the reactor. Indeed, the reactor and the pool are only separated by a gate, that can be opened when the spent fuel needs to be transferred underwater from the reactor to the spent fuel pool. The transfer is done by flooding the reactor tank, opening the gate, and moving the fuel underwater to the pool [14].

Spent fuel pools are made of reinforced concrete with stainless steel liners. As the fuel releases heat, it must be fitted with a Fuel Pool Cooling and Cleanup system, FPCC, that aims at keeping the water at a specific temperature despite the heat released by the spent fuel. It also ensures a good water quality in terms of minerality [15]. Both the cooling and cleaning systems function in closed loop. They are respectively represented in Figures 3a and 3b. On these figures, one can also see the gate separating the reactor from the spent fuel pool.



(a) SFP Cooling System [15].



(b) SFP Cleaning System [15].

Figure 3

The cooling system removes water from the pool throughout suction lines and cools that water in some heat exchanger before re-injecting it at the bottom of the pool throughout diffusers. The cleaning system, on the other hand, captures water via overflow and pushes it across filters and demineralizers before reinjecting it in a way similar to the one of the cooling system [15]. Both systems are duplicated in parallel to decrease the probability of failure. If the pool was to lose water, either due to a leak or due to a failure of the cooling system, leading to water evaporation and the uncovering of the fuel, the consequences can be dramatic. What would happen in such a situation is zirconium rod oxidation, ignition of fuel elements, radioactivity release, and even hydrogen explosion [16].

2.1.5 Previous issues involving Spent Nuclear Fuel Pools

The Fukushima disaster of 2011 has raised awareness concerning the design of nuclear spent fuel pools. Indeed, on March 11 2011, on the east-coast of Japan, an earthquake erupted. As the Fukushima Daichii nuclear power plant was located on the coast, the plant was shut down automatically: control rods were inserted in between the fuel rods to stop the nuclear fission chain reaction from happening. Even though the reactor shutdown was successful, the tsunami that occurred shortly after disabled the electricity generator as well as the diesel-fuel emergency generator, creating a complete black-out at the plant. No more electricity at the plant meant no more cooling systems, neither for the reactors nor for the spent fuel pools [17, 18]. Due to the loss of cooling, problems started to emerge, especially in units 1 to 4 (Fukushima Daichii has 6 units in total). At first, the focus was put on units 1, 2 and 3. Unit 4 reactor was in maintenance when the events occurred and was thus empty. Fuel melting happened in all 3 reactors due to a drop of cooling water level and was followed by hydrogen explosions in units 1 and 3. The water levels of the pools also decreased due to the combination of sloshing during the earthquake and explosions but also due to evaporation since the pools cooling and cleanup system relied on a power source that was no longer present. The loss of power also led to a failure of the monitoring devices, cutting off any instant information. Hopefully, water addition has been made possible by using pump trucks and fire hose, and nowadays alternate cooling systems are in place. To everyone's complete surprise, a hydrogen explosion occurred in Unit 4 on March 15 even though its reactor did not contain any fuel since it was under maintenance. It might have been due to a hydrogen leak coming from unit 3 through the ventilation system. However, this event raised awareness concerning the spent fuel pool of unit 4. Since all the fuel from the reactor had been moved to the pool for maintenance, the pool was heavily loaded in fuel and consequently its water level decreased due to evaporation. Water was thus added to avoid further damages. Even though nothing bad happened, it seems that a bit of luck came in: since the reactor was under maintenance, everything was flooded. Experts believe that a leak from the reactor well to the spent fuel (across the gate) helped prevent the water level from dropping too low [17, 19, 20, 21] The Prime Minister in charge at the time even said that it felt like they escaped the worst "by the grace of Gods" [17].

Even though Fukushima's tragedy has become very famous worldwide, it is not the only nuclear accident involving spent fuel pools to ever happen. To cite only one other, the Haddam Neck plant in Connecticut has seen, on August 21st 1984, its reactor well loose 200 000 gallons (equivalent to 757 m^3) of water in about 20 minutes due to a bad seal design during a refueling operation. Hopefully, the gate to the pool was closed and

the spent fuel remained safe [21, 22]. In the U.S. exclusively, reference [21] states that their would have been more than 60 accidents in between 1981 and 2011 involving a loss of pool water.

2.1.6 Conclusion

The Fukushima accident has advertised the fact that spent fuel nuclear pools may not have a sufficient safety level: they do not have the same containment structure as the reactor, they do not always have a backup power supply nor sturdy enough instrumentation and, in more and more places, they are used longer than designed to with a higher amount of spent fuel stored [21]. This has brought out the fact that more attention should be given to the pool, its design, safety requirements and understanding of flow and heat transfer inside it as well as the evaporation of water at its surface.

2.2 Rayleigh-Bénard Convection

As explained in the previous section, spent nuclear fuel pools can become very hazardous when the water contained in it decreases. This water drop is typically caused by the heat released by the spent fuel rods placed at the bottom of the pool and leading to evaporation at the surface. To better understand this phenomenon, this Master thesis focuses on gaining insight on the heat and mass fluxes taking place inside the pool (while neglecting any evaporation). This section will therefore present the Rayleigh-Bénard convection as it governs the heat transfer inside the pool.

Rayleigh-Bénard convection is a specific case of natural convection, also referred to as free convection. Natural convection is due to buoyancy forces created by the combination of a body force and a density gradient. In the case of Rayleigh-Bénard convection, the body force is the gravity while the density gradient is caused thermally: the fluid is heated from below and cooled from above. This results in a buoyancy-driven flow that makes the denser fluid from the top sink and the lighter fluid from the bottom rise, creating a circulation pattern as one can see on Figure 4 [23, 24]. This phenomenon takes place in various natural flows (e.g. oceans, atmosphere, etc.) as well as in engineering creations such as spent nuclear fuel pools, which is the main focus of this report [25, 26].

Rayleigh-Bénard convection can be characterized by several parameters. First of all is the dimensionless Prandtl number, defined as the ratio between momentum diffusivity and thermal diffusivity [23, 24, 25, 26, 27, 28]:

$$Pr = \frac{\nu}{\alpha} [-] \quad (1)$$

where ν [m^2/s] is the kinematic viscosity of the fluid and α [m^2/s] is its thermal diffusivity. The Prandtl number depends only on the fluid itself and gives an indication about its behaviour: if the fluid is more likely to transfer heat by convection (high momentum diffusivity), it bears a high Prandtl number, and displays a low one if it transfers heat mainly by conduction (high thermal diffusivity).

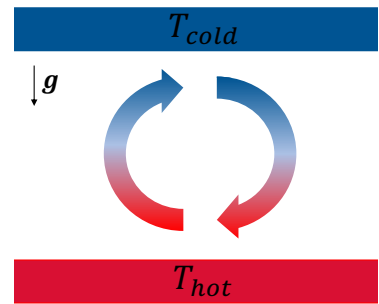


Figure 4: Convection circulation pattern.

Since natural convection is driven by buoyancy forces that must overcome the viscous forces of the fluid in order to create the convection motion, an interesting number is the Grashof number. The Grashof number is defined as the ratio between buoyancy forces and viscous forces [23, 24]:

$$Gr = \frac{g \beta \Delta T h^3}{\nu^2} = \frac{\text{buoyancy forces}}{\text{viscous forces}} [-] \quad (2)$$

where $g [m/s^2]$ is the gravitational acceleration, $\beta [1/K]$ is the thermal expansion coefficient, $\Delta T [K]$ the temperature difference between the hot (bottom) and the cold (top) horizontal plates, $h [m]$ the height of the domain (distance between the two plates) and $\nu [m^2/s]$ the kinematic viscosity.

However, in practice, the Grashof number is only used through its inclusion into the Rayleigh number. The Rayleigh number is defined as the product of the Grashof number with the Prandtl number [23, 24, 25, 26, 27, 28]:

$$Ra = Gr Pr = \frac{g \beta \Delta T L^3}{\nu \alpha} [-] \quad (3)$$

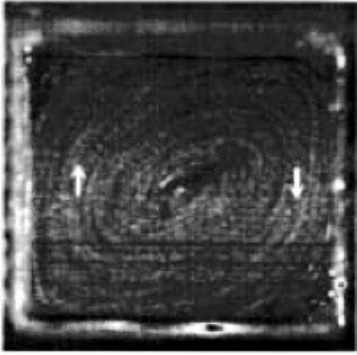


Figure 5: Single roll convection cell [29].

The Rayleigh number measures the turbulence intensity of the fluid [28]. Indeed, flow instabilities are amplified when the Rayleigh number increases and this will strongly affect the heat transfer. Three different ways of transferring heat exist for different values of the Rayleigh number. At low Rayleigh number, i.e. under a critical Rayleigh number Ra_c whose value depends mainly on the top and bottom boundary conditions, the buoyancy forces do not exceed the viscous forces present inside the fluid: the fluid does not exhibit a bulk motion, it is stable. The heat transfer occurs by conduction only [30, 31]. When the Rayleigh number exceeds the critical value Ra_c , convection starts to take place in a laminar form.

In this flow regime, the flow organises itself in convection cells, first discovered by Henri Bénard, that can take various shapes. Figure 5 introduces the flow topology of a single roll convection cell. One can see that the fluid rises on the left side and sinks on the right, the whole flow following a circular pattern. Convection cells can also take other forms, such as toroidal roll, four roll structures or hexagonal cells [30, 29, 32]. If the Rayleigh number continues to increase, the flow disturbances will intensify and the flow will become turbulent. This occurs for values of the Rayleigh number higher than Ra_t [23]. As from this value, thermal plumes are emitted from the hot and cold plates and allows for the formation of a specific structure called Large Scale Circulation (LSC) or mean wind [25] whose configuration will depend on the geometry of the container.

The geometry and aspect ratio, $\Gamma = \frac{L}{H}$ also plays an important role in describing Rayleigh-Bénard convection. The most common geometry encountered is the cylinder. Two other possible geometries are a cube or two parallel infinite plates. The aspect ratio is defined as the ratio between the horizontal, L , and the vertical, H , lengths of the geometry [25]. Figure 6 presents these three common geometries and their respective aspect ratio.

In most cases, only the Prandtl number, the Rayleigh number and the aspect ratio are used to define a system or case study [27, 33]. The system will answer these imposed parameters with a heat flux. The dimensionless heat flux is defined by the Nusselt number [23, 24, 26]:

$$Nu = \frac{h_c h}{\kappa} \quad (4)$$

where h_c [$W/m^2 K$] is the heat transfer coefficient, h [m] the height of the system and κ [$W/m K$] the thermal conductivity. A lot of correlations for $Nu(Ra, Pr)$ are proposed in [23, 24]. They depend on the range of values of both Ra and Pr as well as on the geometry of the container. Convection allows to generate heat fluxes much higher than what could be obtained with conduction.

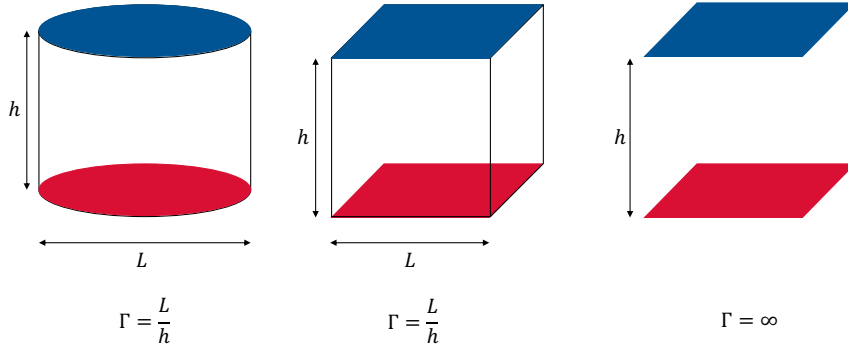


Figure 6: Common geometries to study Rayleigh-Bénard Convection, and their aspect ratio.

2.3 Rayleigh-Bénard convection inside a spent nuclear fuel pool

As the previous sections have just explained, nuclear spent fuel pools have become an area of concern mainly due to safety issues. The main concern is that the water level must not decrease to avoid the spent fuel to heat too importantly or, worse, to enter in contact with air as this would lead to damages to the fuel, ignition of the fuel, radiation release or even hydrogen explosions. This report thus aims at investigating the thermal convection happening inside a spent fuel nuclear pool. To do so, the spent fuel pool must be considerably simplified to achieve the simple Rayleigh-Bénard convection configuration described before. The simplifications are described hereafter and illustrated on Figure 7

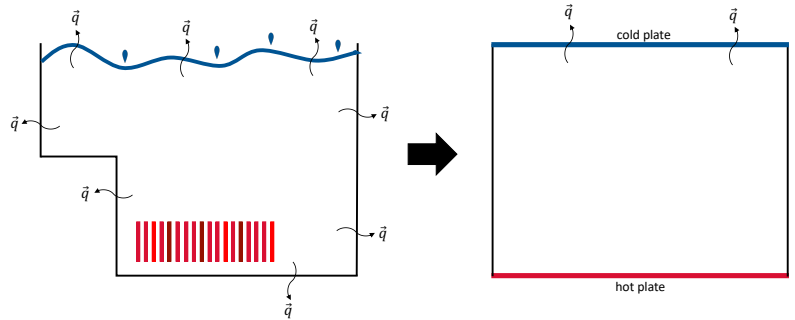


Figure 7: From Spent Fuel Pool to Model.

The evaporation (mass transfer) happening at the upper-surface in contact with the air will be neglected. The fuel rods will be modeled by a flat hot plate at the bottom of the pool, neglecting the flow of water in-between them as well as beneath them and the

difference of heat released by these (which depends on the time they have already stayed in the pool). The assumption that the lateral walls are perfectly insulated is also made and the geometry is highly simplified to become a perfect cube.

Now that the basic assumptions have been made, the following section will focus on creating a model for the natural convection happening inside this simplified pool.

3 Model

As this project aims at analysing numerically the natural convection inside a nuclear spent fuel pool, this section will present the equations that model the phenomenon. Then, the assumptions that can be made to simplify these equations, known as the Low Mach number approximation, will be introduced. Finally, we will introduce how the OpenFOAM solver deals with the low Mach number equations to obtain a solution.

3.1 Governing equations

Rayleigh-Bénard convection and, more generally, natural convection draws on the Navier-Stokes equations as its governing equations. The Navier-Stokes equations for a compressible fluid undergoing Rayleigh-Bénard convection, see equations 5, are composed of a continuity equation, a momentum equation and an energy equation. Several assumptions are made to obtain the set of equations 5. Concerning the conservation of momentum, since in natural convection the buoyancy force is the only force acting inside the fluid, the only body force taken into account is the one caused by gravity [23]. Furthermore, the energy equation relies on Fourier's law of thermal conduction. This law expresses the heat flux as $\mathbf{q} = -k \nabla T$. The energy equation also neglects any radiative heat flux as well as the dissipation of energy due to viscous effects.

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 \\ \frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= -\nabla p + \nabla \cdot \tau + \rho \mathbf{g} \\ \frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho \mathbf{u} h) &= \nabla \cdot (k \nabla T) + \frac{\partial p}{\partial t} \end{aligned} \tag{5}$$

with

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

Table 2 summarises the different variables used in equations 5.

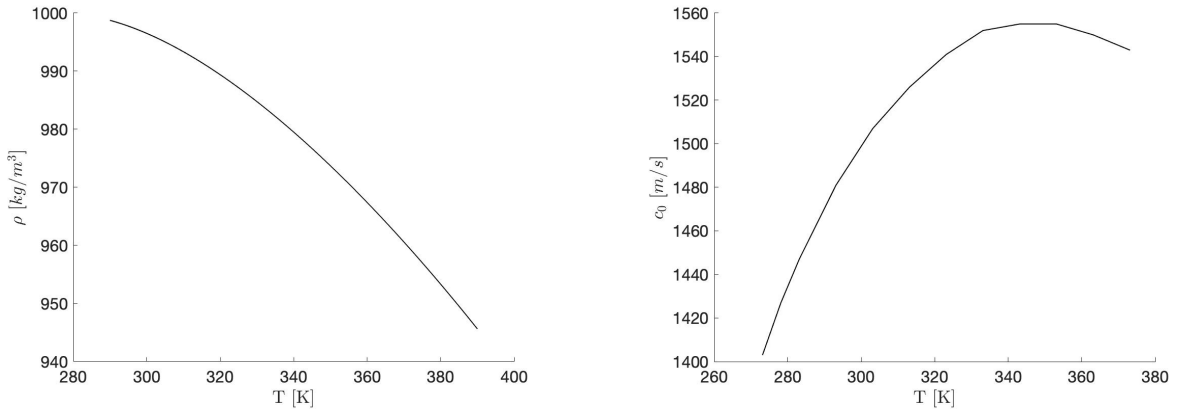
ρ [kg/m^3]	fluid density
$\mathbf{u}$ [m/s]	fluid velocity vector
t [s]	time
p [Pa]	fluid pressure
τ [$kg/m \ s^2$]	fluid viscous stress tensor
$\mathbf{g}$ [m/s^2]	gravitational acceleration.
h [kJ/kg]	fluid specific enthalpy
k [W/mK]	fluid thermal conductivity
T [K]	fluid temperature

Table 2

When dealing with Rayleigh-Bénard convection, the Navier-Stokes equations are usually solved using Boussinesq's approximation. This simplification allows to neglect

any variation of density except the one involved in the buoyancy term of the momentum equation. This last one is considered to vary linearly with temperature, leading to: $(\rho - \rho_0)\mathbf{g} = -\rho_0\mathbf{g}\beta(T - T_0)$ with β [1/K] being the thermal expansion coefficient [34, 35]. As one can see on Figure 8a, the density (of water in this case) changes however consequently with temperature. The approximation is thus compromised and leads to errors when the temperature differences across the fluid become bigger [36]. For water, reference [34] states that a temperature difference of 2 degrees leads to an error of about 1%.

To avoid any errors coming from the Boussinesq approximation, the approximation will not be used in this work. To replace it, the low Mach number approximation will be used. Details concerning this method are explained in the following section.



(a) Variation of water density with temperature [37].

(b) Speed of sound in water as function of the temperature [38].

Figure 8

3.2 Low Mach Number Approximation

Thermal convection enables the motion of a compressible fluid thanks to a buoyancy force. The fluid motion occurs at what can be considered as a low speed, at least compared to the speed of sound [35]. The Mach number is defined as the ratio between the fluid speed and the speed of sound (in the same fluid), see equation 6. The speed of the fluid being low, the Mach number associated to the flow is also low.

$$M = \frac{u}{c_0} [-] \quad (6)$$

In equation 6, u is the velocity of the fluid and c_0 the speed of sound. In the frame of this project, the values of u do not exceed $2.5 * e^{-2}$ [m/s]. Values of the speed of sound in water as function of the temperature can be seen in Figure 8b.

The low Mach number approximation is therefore used to solve the Navier-Stokes equations instead of Boussinesq's approximation, for the reasons described before. The approximation thus consists in assuming that $M \ll 1$ in the whole flow.

To obtain the low Mach number set of equations, one must expand some of the variables as power series [35, 36, 39]:

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

$$\begin{aligned}
\mathbf{u} &= \mathbf{u}^0 + \epsilon \mathbf{u}^1 + \mathcal{O}(\epsilon^2) \\
T &= T^0 + \epsilon T^1 + \mathcal{O}(\epsilon^2) \\
p &= \frac{\rho T}{\gamma M^2} = \frac{1}{\epsilon} p^0 + p^1 + \mathcal{O}(\epsilon)
\end{aligned} \tag{7}$$

where ϵ is defined as $\epsilon = \gamma M^2$ ($\gamma = \frac{C_p}{C_v}$ being the ratio of specific heats).

Since the main assumption is that the Mach number is very low, consequently, $\epsilon \ll 1$ and $\mathcal{O}(\epsilon)$ as well as $\mathcal{O}(\epsilon^2)$ can be neglected. Furthermore, the pressure term can be decomposed into two components: a thermodynamic pressure and a dynamic pressure. As explained in [35], the thermodynamic pressure, p^0 , is spatially invariant: $p^0 = p^0(t)$, while the dynamic pressure $p^1 = p^1(x_i, t)$ varies in space and time. Keeping this information in mind, the pressure appearing in the momentum equation of equations 5 is thus composed of the dynamic part of the pressure field only because the equation refers to the pressure gradient. Meanwhile, the pressure present as a material derivative in the energy equation will be composed mainly of the thermodynamic pressure since $\epsilon \ll 1$ [35, 36, 39].

By incorporating this information into equations 5, we finally obtain the low Mach number equations (the zero subscripts are dropped):

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 \\
\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= -\nabla p'_d + \nabla \cdot \tau + \mathbf{g} \cdot \mathbf{h} \nabla \rho \\
\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho \mathbf{u} h) &= \nabla \cdot (k \nabla T) + \frac{\partial p^0}{\partial t}
\end{aligned} \tag{8}$$

with $p'_d = p^1 - \rho \mathbf{g} \cdot \mathbf{h}$

Equations 8 are actually composed of five equations: one continuity equation, three momentum equation (one for each direction: x , y and z) and one energy equation for 7 unknowns: ρ , u , v , w , p'_d , p^0 and h . Two additional equations must be added to close the system. The first one concerns the thermodynamic pressure p^0 . In this project, one will consider:

$$p^0 = p_{atm} \tag{9}$$

which is correct for an open case and an acceptable hypothesis for a closed one [40]. The last equation will link the density to the temperature field throughout an isobaric equation of state taking the form of a polynomial fit of order N [40]:

$$\rho = \sum_N a_N T^N \tag{10}$$

a_N being the coefficients of the fit. Details on the computation of those coefficients are provided later in section 4.3.2.

3.3 OpenFOAM Solver

The low Mach number equations are thus composed of the five equations, see equations 8, derived from the Navier-Stokes equations to which are added equation 9 for the thermodynamic pressure and the polynomial fit of equation 10 for the density. In this

project, these 7 equations will be solved numerically with OpenFOAM, an open source CFD software [41] by an existing solver called *lowMachBuoyantPimpleFoamWater* [39]. The solver relies on the Finite Volume Method (FVM) to solve the individual equations while it uses the pressure-implicit split-operator algorithm, known as the PISO algorithm, to deal with the coupling of the equations. Both the Finite Volume Method and the PISO algorithm are briefly introduced in the following sections.

3.3.1 Finite Volume Method, FVM

The Finite Volume Method decomposes the geometry under study into a mesh composed of numerous cells or finite elements of various convex shapes with planar surfaces (see Figure 12a for a mesh example). The equations are solved for each one of these cells. The solution for various fields such as velocity, temperature, etc. is computed as the mean value for the cell (collocated arrangement) and is stored at the center of mass of each cell. It happens that the three equations composing the low Mach number system, equations 8 can all be obtained from the general transport equation for a quantity ϕ :

$$\frac{\partial \rho \phi}{\partial t} + \nabla \cdot (\rho \mathbf{u} \phi) = \nabla \cdot (\rho \Gamma \nabla \phi) + S \quad (11)$$

and can therefore be solved in a similar way.

The Finite Volume Method goal is to re-express the equation as a system of linear algebraic equation that can be expressed in a matrix form as in equation 12 by using temporal and spatial discretization over the mesh. The system can therefore be solved, providing the value of ϕ in each cell:

$$\mathcal{M} \Phi = \mathcal{B} \quad (12)$$

with $\mathcal{M}$ being the matrix of coefficients, $\mathcal{B}$ the right hand side term and Φ a vector containing the quantity ϕ at each cell centroid. To obtain this format of the transport equation, several operations need to be performed. These are described hereafter.

Step 1: Integrate the transport equation over one of the cell whose center of mass is denoted by P:

$$\int_{V_P} \frac{\partial \rho \phi}{\partial t} dV + \int_{V_P} \nabla \cdot (\rho \mathbf{u} \phi) dV = \int_{V_P} \nabla \cdot (\rho \Gamma \nabla \phi) dV + \int_{V_P} S(\phi) dV \quad (13)$$

Step 2: Use the Gauss theorem: $\int_V \nabla \cdot \mathbf{a} dV = \oint_{\partial V} d\mathbf{S} \cdot \mathbf{a}$ to convert volume integrals into surface integrals for the convective and diffusion terms. Decompose the source term as $S(\phi) = S_C + S_P \phi$ and integrate it by using a Taylor expansion of ϕ around its center of mass P : $\phi(x) = \phi_P + (x - x_P) \cdot (\nabla \phi)_P$ and by using the fact that P is the center of mass: $\int_{V_P} (\mathbf{x} - \mathbf{x}_P) dV = 0$.

$$\frac{\partial}{\partial t} \int_{V_P} \rho \phi dV + \oint_{\partial V_P} d\mathbf{S} \cdot (\rho \mathbf{u} \phi) = \oint_{\partial V_P} d\mathbf{S} \cdot (\rho \Gamma \nabla \phi) + (S_C V_P + S_P V_P \phi_P) \quad (14)$$

Step 3: Rewrite the surface integral, ∂V , as a sum of surface integrals, S_f , over each face of the cell and use the approximation proposed by [42]: $\oint_{\partial V} d\mathbf{S} \cdot \mathbf{a} = \sum_f \int_f d\mathbf{S}_f \cdot \mathbf{a} \approx \sum_f \mathbf{S}_f \cdot \mathbf{a}_f$

to obtain a semi-discrete equation.

$$\frac{\partial}{\partial t} \int_{V_P} \rho \phi dV + \sum_f \mathbf{S}_f \cdot (\rho \mathbf{u} \phi)_f = \sum_f \mathbf{S}_f \cdot (\rho \Gamma \nabla \phi)_f + (S_C V_P + S_P V_P \phi_P) \quad (15)$$

Step 4: Use a temporal discretization scheme for the partial time derivative as well as spatial discretization schemes to obtain values at the cell faces from the centroid ones. Since several choices are made possible by OpenFOAM for both the temporal and spatial discretization schemes, the ones used as part of this project are described later, in section 4.4.

Once equation 15 is spatially and temporally discretize, the linear algebraic system of equation 12 can be found by applying equation 15 to each one of the cells [43, 44]. The system of linear algebraic equation can thereafter be solved. As several choices are available to solve the system, the ones used within this project are explained later in section 4.5.

3.3.2 PISO Loop

The PISO (pressure-implicit split-operator) loop is an iterative algorithm that aims at solving coupled equations (pressure-momentum usually) of transient flows. The PISO loop used in the *lowMachBuyontPimpleFoamWater* solver is illustrated in Figure 9.

An iteration always begin by solving the momentum equation using the pressure of the previous iteration, to have a first idea of the velocity $\mathbf{u}^*$ (this velocity however does not satisfy the continuity equation). This step is usually called the momentum prediction. Once we have a first idea of the velocity, we can use its value to solve the energy equation and obtain the temperature field. The temperature field enables us to compute the density using the isobaric equation of state (polynomial fit of tabulated data for water density at one atmosphere and over the temperature range of interest).

One must now include the continuity equation in the algorithm. To do so, we rewrite the momentum equation in matrix form, using the Finite Volume Method, as $\mathcal{M}_u \mathcal{U} = \mathcal{B}_u$ with $\mathcal{B}_u$ the right hand side, accounting for $-\nabla p'_d + \mathbf{g} \cdot \mathbf{h} \nabla \rho$. To couple the continuity equation with the momentum equation, one will extract the diagonal components of $\mathcal{M}_u$ and define it as the matrix $\mathcal{A}_u$,

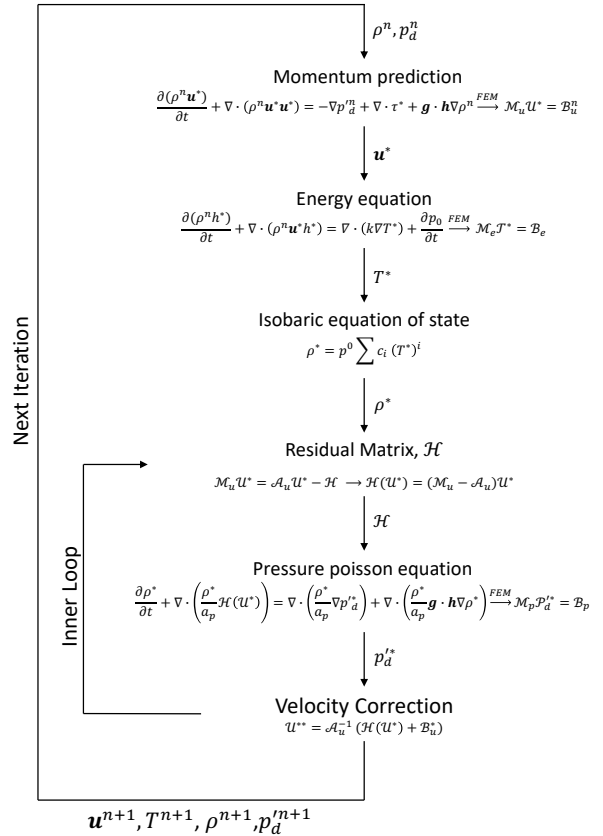


Figure 9: PISO Algorithm.

which can be easily inverted since it is diagonal. We then have:

$$\mathcal{M}_u \mathcal{U} = \mathcal{A}_u \mathcal{U}^* - \mathcal{H} = \mathcal{B}_u \quad (16)$$

with $\mathcal{H}$ being the residual matrix.

Multiplying equation 16 by $\mathcal{A}_u^{-1}$ gives:

$$\mathcal{U} = \mathcal{A}_u^{-1} \mathcal{H} + \mathcal{A}_u^{-1} \mathcal{B}_u \quad (17)$$

Using the divergence of equation 17 and inserting it in the continuity equation gives the Pressure Poisson equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\frac{\rho}{a_p} \mathcal{H} \right) = \nabla \cdot \left(\frac{\rho}{a_p} \nabla p'_d \right) + \nabla \cdot \left(\frac{\rho}{a_p} \mathbf{g} \cdot \mathbf{h} \nabla \rho \right) \quad (18)$$

with a_p being the diagonal component of $\mathcal{A}$.

Equation 18 can thus be solved to obtain the dynamic pressure, and this new dynamic pressure can be used to acquire a better estimation of the velocity, $\mathbf{u}^{**}$. The new velocity can, in turn, enable the computation of a better estimation of the dynamic pressure and so on. An inner loop on the pressure Poisson equation is thus integrated in the PISO algorithm, as one can see on Figure 9, to iterate on the pressure and velocity fields [39, 40, 44, 45].

Various parameter of the algorithm can be modified, such as the linear solvers used to solve the 3 system of equation, the tolerance that must be reached, the number of inner loops,... Information on what is used within this project is given in section 4.5.

3.3.3 Conclusion

This section has put forward the foundation tools on which our spent nuclear fuel pool model relies. Indeed, the existing openFOAM solver is able to directly deal with applications which are governed by the low Mach number equations by using the FVM and a PISO loop. Yet, the case, on which the solver is applied, requires to be correctly configured. The following section will therefore present the case set-up of our specific application.

4 Case set-up

The previous section has introduced the reader to the low Mach number equations, used to describe the natural convection inside a spent nuclear fuel pool. It has also explained how OpenFOAM's *lowMachBuoyantPimpleFoamWater* solver [39] deals with the equations to find a solution numerically. This section continues to work in that direction. Indeed, the solver requires various information, starting with the mesh itself and the boundary conditions (section 4.1), in order for the solver to be applied to our spent nuclear fuel pool. Information about the mesh refinement is then provided in section 4.2. The following section will describe how the fluid properties were computed and built into the case (section 4.3). The discretization schemes as well as the solution parameters will be explained respectively in sections 4.4 and 4.5 before covering the turbulence model used in section 4.6. Finally, since we are only interested in the statistically steady state of the simulation, section 4.7 will explain the choices made to that end.

4.1 Geometry and boundary conditions

The spent nuclear fuel pool is represented, in this case, by a 3D cube of a certain height h centered at the origin, $(0, 0, 0)$. The cube contains three different boundaries. The bottom of the cube (floor on Figure 10) represents the interaction of water with the storage racks containing the fuel while the top of the pool (ceiling on the figure) is the surface that is in contact with air. In this project, the floor of the pool is considered as an isothermal hot fixed wall. The ceiling will either be considered as a fixed wall or a free surface with a cold isothermal temperature. This project aims at comparing the influence of these two types of velocity boundary conditions at the ceiling: fixed wall or free surface, on the flow topology. The sides of the pool are considered adiabatic and fixed walls. Some of these hypothesis are considerable but justified considering the complexity of the interactions happening on those surfaces. The geometry is therefore described by using 8 vertices that compose one block with 6 faces: the floor, four side walls and the ceiling, as shown on Figure 10.

The boundary conditions of temperature, velocity, pressure and dynamic pressure must be defined for the 3 existing boundaries: the floor, the ceiling and the side walls, these conditions are summarized in Table 3. The initial values are fixed for the velocity and the pressure fields, while a linear profile between the isothermal ceiling and floor is computed for the temperature field. The initial values and the temperature profile formula are given in Table 4.

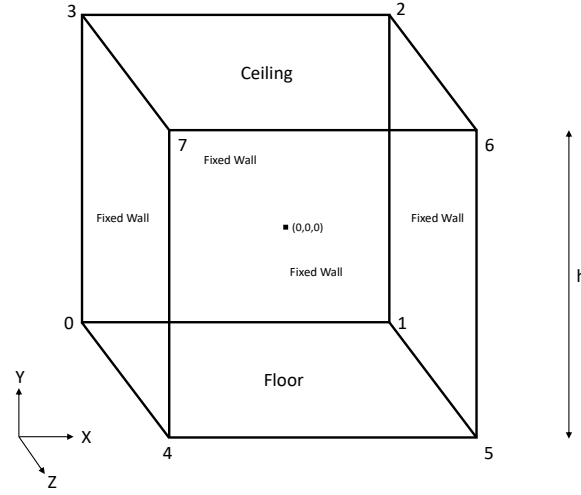


Figure 10: Geometry of the nuclear spent fuel pool, its vertices and boundaries.

Fields		Boundary conditions		
		Ceiling	Floor	Fixed Walls
Temperature	$[K]$	Isothermal: fixed to $T_{cold} = 348.15 [K]$	Isothermal: fixed to $T_{hot} = 358.15 [K]$	Adiabatic
Velocity	$[m/s]$	Fixed wall / Free surface	Fixed walls : zero velocity at walls	
Pressure	$[kg/m s^2]$	Calculated by OpenFOAM based on other information		
Dynamic Pressure	$[kg/m s^2]$	Pressure gradient defined for the flux to satisfy the velocity boundary condition [46]		

Table 3: Boundary conditions of the temperature, velocity, pressure and dynamic pressure fields.

Fields		Initial conditions
Temperature	$[K]$	$-\frac{T_{hot}-T_{cold}}{2} * y + \frac{T_{hot}+T_{cold}}{2}$
Velocity	$[m/s]$	$(0, 0, 0)$
Pressure	$[kg/m s^2]$	10^5
Dynamic Pressure	$[kg/m s^2]$	0

Table 4: Initial conditions of the temperature, velocity, pressure and dynamic pressure fields.

As explained before, the goal of this project is to investigate the influence of a free-slip boundary condition at the ceiling as compared to a fixed wall ceiling boundary condition on the flow characteristics. Two cases will therefore be created, however, they will be entirely similar except for the ceiling's velocity boundary condition. The fixed wall boundary condition will set the velocity at the wall to be zero while the slip boundary condition will keep the tangential component and delete the others [47].

4.2 Mesh refinement

When performing a simulation, one must make sure that the mesh resolution is high enough to resolve all the relevant scales of the flow [48]. To satisfy this, a maximum cell width is computed for both the core mesh and the two boundary layers (B.L.): thermal and kinetic. A refinement is then added near the walls (inside the boundary layer) since the boundary layers require smaller cells compared to the core mesh. A hyperbolic tangent expansion function is used to gradually increase the cell's dimensions from the wall towards the center. Figure 11 illustrates these conditions on a one dimensional mesh. One can see that the cell size increases step by step towards the centre following a hyperbolic tangent expansion. The conditions on the cells width are also detailed for the core and the B.L. Indeed the cells widths must not exceed l and l_{BL} in the core and in the B.L. respectively (when dealing with both the kinetic and thermal boundary layers, the boundary layer having the most constraining condition is used).

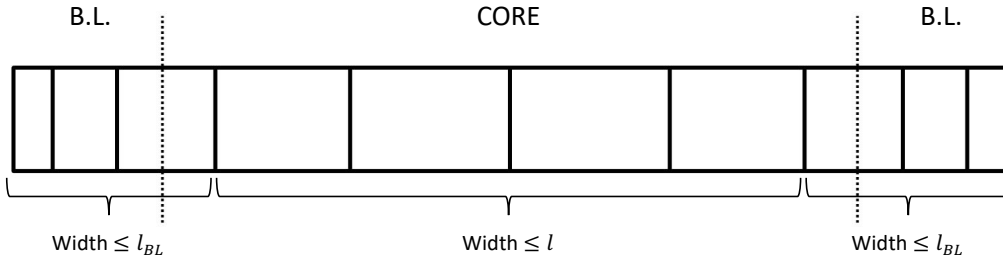


Figure 11: Hyperbolic Tangent Expansion and maximum cell size illustration.

The procedure followed to define the mesh points can be decomposed into 5 steps:

1. The thickness of the kinetic boundary layer, δ_u and the one of the thermal boundary layer, δ_{th} are computed (see equations 19 and 20).
2. The maximum cell sizes are defined for the core mesh, l , the kinetic boundary layer, l_u and the thermal boundary layer, l_{th} (equations 21, 22 and 23).
3. The thicknesses and maximum cell sizes are used to find a first approximation of the number of cells needed, N , equivalent to the case where there would be no expansion.
4. The hyperbolic tangent formula (equation 24) is used to define the mesh points for N cells.
5. The cell sizes, defined by the hyperbolic tangent expansion formula, are verified to ensure that they do not exceed the maximum cell sizes defined in step 2.
 - If the cell sizes are too big, the number of cells is increased by 2: $N = N + 2$ and the process restarts at point 4.
 - If the cell sizes conform to the requirements, the final mesh can be created using these points.

4.2.1 Formulas used

As explained before, the cell dimensions must not exceed a certain value to avoid losing information. However the maximum width permitted depends on the cell location: inside the kinetic B.L., the thermal B.L. or the core mesh. To distinguish these locations, one must compute the thicknesses of the boundary layers [49]:

$$\delta_u = \begin{cases} 0.5 Nu^{-1} Pr^{1/2} A^{-1} \pi^{-1/2} h & \text{for } Pr < 3 \cdot 10^{-4} \\ 0.5 Nu^{-1} Pr^{-0.357-0.022\log(Pr)} h & \text{for } 3 \cdot 10^{-4} \leq Pr \leq 3 \\ 0.5 Nu^{-1} Pr^{1/3} E^{-1} h & \text{for } Pr > 3 \end{cases} \quad (19)$$

$$\delta_{th} = \begin{cases} A \sqrt{\pi} Pr^{-1/2} & \text{for } Pr < 3 \cdot 10^{-4} \\ \delta_u Pr^{-0.357+0.022\log(Pr)} & \text{for } 3 \cdot 10^{-4} \leq Pr \leq 3 \\ Pr^{-1/3} E & \text{for } Pr > 3 \end{cases} \quad (20)$$

Once the domain can be decomposed into the 3 different parts, one can define the conditions inside each one of these: a maximum grid width in the core of the domain, l , a maximum grid width in the thermal boundary layer, l_{th} , and finally a maximum grid width in the kinetic boundary layer, l_u .

For the core of the domain, the maximum grid width is given by [48] for a Direct Numerical Simulation (DNS):

$$l = \begin{cases} \pi h \left(\frac{Pr^2}{Ra Nu} \right)^{1/4} & \text{for } Pr \leq 1 \\ \pi h \left(\frac{1}{Pr Ra Nu} \right)^{1/4} & \text{for } Pr > 1 \end{cases} \quad (21)$$

However since we will not be running a DNS but will use a Large Eddy Simulation (LES), as explained later in section 4.6, values up to 3 to 4 times l can and will be used [25, 48]. For the boundary layers, reference [49] gives the minimum number of nodes required inside the boundary layers, both kinetic and thermal:

$$N_u = \begin{cases} \sqrt{2} a Nu^{1/2} Pr^{-1/4} A^{1/2} \pi^{1/4} & \text{for } Pr < 3 \cdot 10^{-4} \\ \sqrt{2} a Nu^{1/2} Pr^{-0.1785+0.011\log(Pr)} & \text{for } 3 \cdot 10^{-4} \leq Pr \leq 1 \\ \sqrt{2} a Nu^{1/2} Pr^{0.3215+0.011\log(Pr)} & \text{for } 1 \leq Pr \leq 3 \\ \sqrt{2} a Nu^{1/2} Pr^{1/3} E^{1/2} & \text{for } Pr > 3 \end{cases} \quad (22)$$

$$N_{th} = \begin{cases} \sqrt{2} a Nu^{1/2} Pr^{-3/4} A^{3/2} \pi^{3/4} & \text{for } Pr < 3 \cdot 10^{-4} \\ \sqrt{2} a Nu^{1/2} Pr^{-0.5355+0.033\log(Pr)} & \text{for } 3 \cdot 10^{-4} \leq Pr \leq 1 \\ \sqrt{2} a Nu^{1/2} Pr^{-0.0355+0.033\log(Pr)} & \text{for } 1 \leq Pr \leq 3 \\ \sqrt{2} a Nu^{1/2} E^{3/2} & \text{for } Pr > 3 \end{cases} \quad (23)$$

The minimum number of nodes, N_{BL} , can be combined with the thickness of the respective boundary layer to give the maximum cell size required within the B.L.: $l_{th} = \frac{\delta_{th}}{N_{th}}$ and $l_u = \frac{\delta_u}{N_u}$.

One can observe that equations 19 to 23 depend on various parameters. They rely on the Nusselt, the Prandtl, and the Rayleigh numbers, that must be evaluated at a reference temperature and the detail of their calculations is explained in section 4.3. Several constants are also involved and defined in [49] as $a = 0.482$, $A = 0.332$ and $E = 0.982$.

A first approximation of the number of required cells N , can be obtained by combining the maximum cell sizes, the length of the domain and the length of the boundary layers. The value corresponds to the minimum number of cells required if there was no cell expansion between the B.L. and the core mesh.

$$N = \text{roundToEven} \left[\frac{h - 2 * \min(\delta_{th}, \delta_u)}{l} + 2 * \max\left(\frac{\delta_{th}}{l_{th}}, \frac{\delta_u}{l_u}\right) \right]$$

The value must be an even integer to have a symmetric domain.

Once this number is known, the coordinates of the mesh can be computed using the hyperbolic tangent expansion formula:

$$\text{Lower half of the mesh:} \quad p^- = -\frac{h/2}{\tanh(\beta)} \tanh\left(\beta\left(1 - \frac{j}{N/2}\right)\right) \quad (j = 0, \dots, N/2)$$
(24)

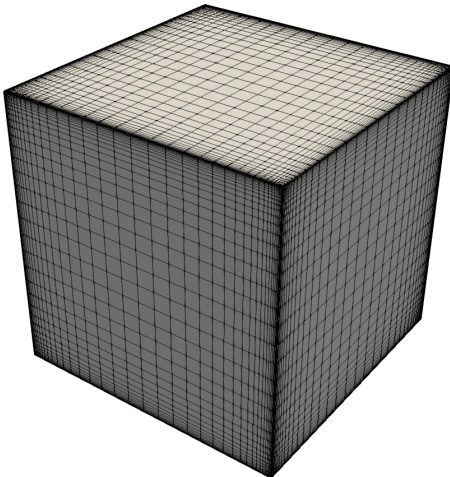
$$\text{Upper half of the mesh:} \quad p^+ = \frac{h/2}{\tanh(\beta)} \tanh\left(\beta\left(\frac{j}{N/2}\right)\right) \quad (j = 0, \dots, N/2)$$

where β is the expansion factor.

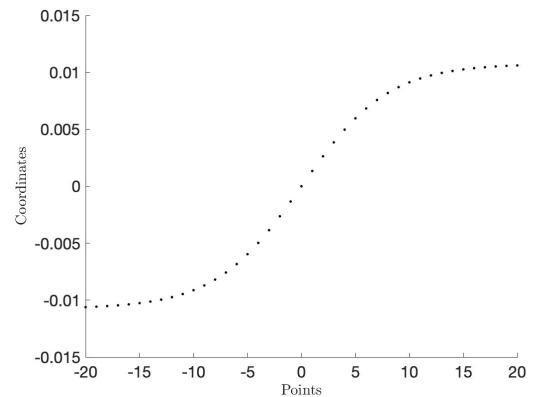
Finally, the distance between two successive coordinates must verify the conditions on the cell size defined before ($\leq l / l_u / l_{th}$ depending on the cell location) or the number of cells, N should be increased until it is the case.

4.2.2 Implementation

The final number of cells required, N , is computed by following the steps described above in a MATLAB function. The mesh refinement is then implemented in the OpenFOAM case for all 3 directions: x , y and z .



(a) Example of a mesh (40 cells) using a hyperbolic tangent expansion.



(b) Mesh coordinates using a hyperbolic tangent expansion.

Figure 12

In order to decrease the simulation time required, we try to avoid having too many cells. To do so, the core cell size (l) will be 3 to 4 times bigger than the one needed for a DNS case, equation 21, while the resolution inside the boundary layers will remain unchanged. Furthermore, the expansion factor β will be chosen to decrease the number of cells. Its value will vary between the different cases analyzed later.

Figure 12a presents a mesh made of 40 cells and using a hyperbolic tangent refinement on its sides. The coordinates of the 40 points, along one direction, are plotted in Figure 12b. One can see that the edges of the domain contain more points than the center, the cells on the edges being smaller than the ones in the center. The distribution of the points is also smooth due to the hyperbolic tangent function.

4.3 Fluid properties

As the properties of water are strongly influenced by temperature, the temperature induced variations of the fluid's properties will be integrated within the cases. They will either take the form of reference values evaluated at a reference temperature or of polynomials that best fit the properties variation with temperature. The reference values will be used inside OpenFOAM in order to compute the Nusselt number [39] and in the MATLAB function computing the mesh refinement as these depend on the Prandtl and Rayleigh numbers (see section 4.2.1). Polynomial fits will be integrated inside OpenFOAM to create a thermophysical model. The model aims at computing certain properties as function of the temperature [50].

4.3.1 Reference temperature properties

A MATLAB function allows to compute the water properties considering the pool temperature. The function computes the average or reference temperature based on the temperatures at the top (cold) and at the bottom (hot) of the pool:

$$T_{ref} = \frac{T_{hot} + T_{cold}}{2}. \quad (25)$$

The function then relies on another function available in the MATLAB File Exchange website: XSteam [37]. The XSteam function can provide multiple properties of water and steam at different pressures and temperatures according to the "International Association for Properties of Water and Steam Industrial Formulation 1997 (IAPWS IF-97)" [37]. The XSteam function is used to find the values of the following properties at the reference temperature and at atmospheric pressure ($p = 1.01325$ [bar]): the density ρ , [kg/m^3], the heat capacity C_p , [$J/kg K$], the thermal conductivity κ , [$W/m K$] and the dynamic viscosity μ , [$kg/m s$]. As the thermal expansion coefficient β , [$1/K$] is not available in the XSteam function, the values of reference [51] were used to approximate its behaviour as a function of temperature.

Once the values of these five properties are known, one can combine them to find:

- the kinematic viscosity:

$$\nu = \frac{\mu}{\rho} [m^2/s], \quad (26)$$

- the thermal diffusivity:

$$\alpha = \frac{\kappa}{\rho C_p} [m^2/s], \quad (27)$$

- and the prandtl number:

$$Pr = \frac{\nu}{\alpha} [-], \quad (28)$$

Figure 13 illustrates the variation with temperature of the different properties of water between 290 and 390 [K]. One can see that some of the properties are not influenced much by temperature changes: density, heat capacity, thermal conductivity and thermal diffusivity. Other properties display a jump in their values at the boiling temperature.

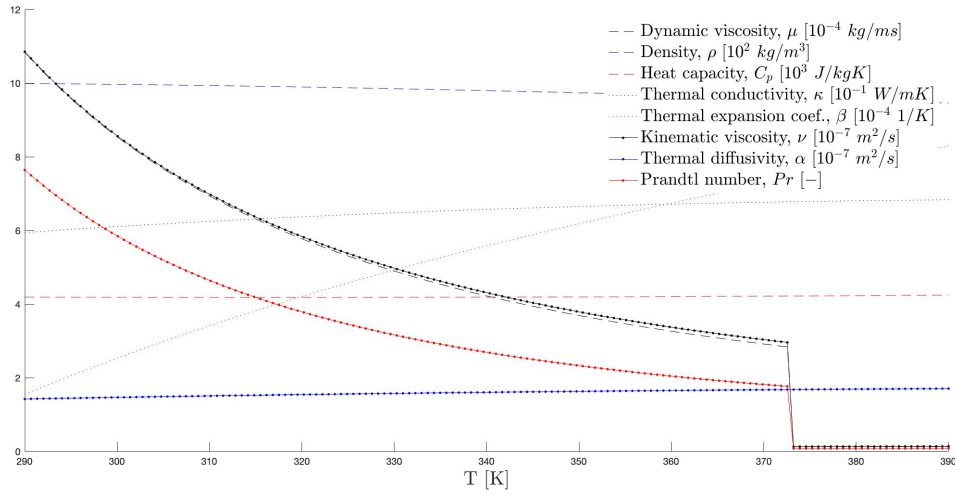


Figure 13: Thermodynamic properties of water as a function of temperature.

By combining these properties with the desired Rayleigh number Ra , one can also obtain the height of the pool:

$$h = \sqrt[3]{\frac{Ra \nu \alpha}{g \beta (T_{hot} - T_{cold})}} [m] \quad (29)$$

and the free-fall velocity:

$$U_f = (\beta (T_{hot} - T_{cold}) g h)^{1/2} [m/s] \quad (30)$$

The Nusselt number is obtained either by using a correlation [52]:

$$Nu = 0.124 Ra^{0.309} [-] \quad (31)$$

or by using the value of a previous simulation.

4.3.2 Polynomial Fits

Since water properties vary with temperature, one will create a thermophysical model inside the OpenFOAM cases. The model will enable some of the fluid properties and the

equation of state to vary with temperature. Seven fields are required by OpenFOAM and can follow different models (see [50] for further details), the ones chosen here are explained in Table 5 [50].

Fields	Model used	Description
type	heRhoThermo	Thermophysical model for fixed composition, based on density ρ .
mixture	pureMixture	Mixture with fixed composition, water in this case.
transport	polynomial	$\mu = \sum_{i=0}^7 a_i T^i$ $\kappa = \sum_{i=0}^7 b_i T^i$
thermo	hPolynomial	$C_p = \sum_{i=0}^7 c_i T^i$
equationOfState	icoPolynomial	Incompressible, polynomial equation of state: $\rho = \sum_{i=0}^7 d_i T^i$
specie	specie	Basic thermophysical properties will be specified: molecular weight.
energy	sensibleEnthalpy	Energy expressed as sensible (does not include the heat of formation) enthalpy.

Table 5

The coefficients a_i , b_i , c_i and d_i allow to compute respectively the dynamic viscosity μ , the thermal conductivity κ , the heat capacity C_p and the density ρ as function of temperature T from a polynomial of order 8. These coefficients are computed from a MATLAB function that interpolates the values given by XSteam [37] to create a polynomial fit using the MATLAB function *polyfit*. As one can see on Figure 14a, the heat capacity is the only property for which a polynomial fit does not give the exact properties due to the "jump" at the boiling temperature. However if this value can be avoided, the fit is very nice, see Figure 14b. In the context of this project, we will use a polynomial fit going from $T_{cold} - 10$ up to $T_{hot} + 10$ which allows to avoid the jump.

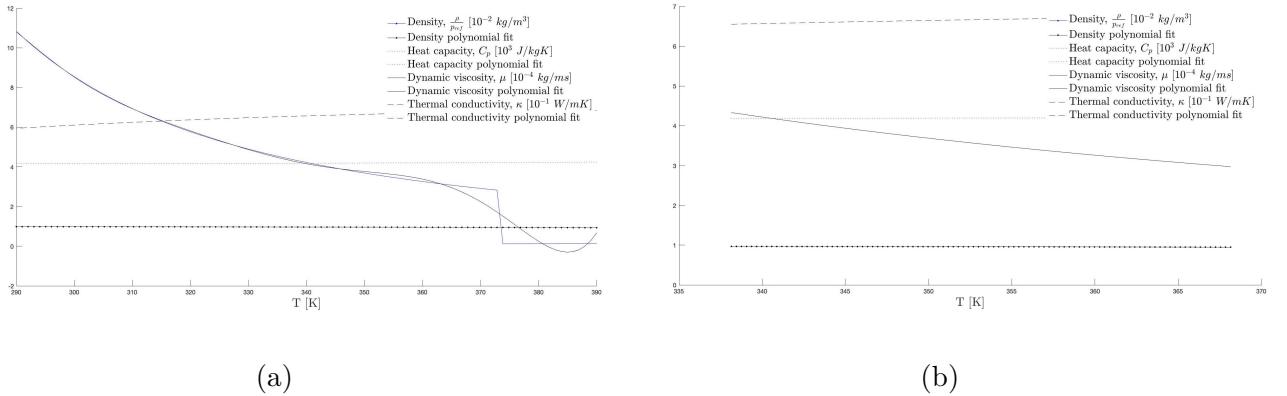


Figure 14: Polynomial fits of the properties of water over different temperature ranges.

4.4 Discretization schemes

We have now defined the mesh, its refinement and boundary conditions as well as the influence of temperature on the fluid. In order to solve the system of equation that governs the flow and its heat transfer inside the pool, we must now make choices concerning the Finite Volume Method as well as the PISO Loop.

As explained in section 3.3.1, the low Mach number equations, which describe our spent nuclear fuel pool problem, must be discretized spatially and temporally in order to provide a system of linear algebraic equations that can be solved. The "universal" discretization is explained in section 3.3.1, however, specific choices for this particular case need to be made. Table 6 summarizes the choices made and encoded in the OpenFOAM case.

Scheme	Model
Time discretization	
Time discretization	backward
Spatial discretization	
Gradient term discretization	Gauss linear
Divergence terms discretization	Gauss linear
Laplacian terms discretization	Gauss linear orthogonal
Interpolation (from cells to face)	linear
Surface normal vector (from cells to face)	orthogonal

Table 6

The time discretization is performed using the backward scheme: this scheme is a transient, second order implicit method and is defined, for a field ϕ as

$$\frac{\partial \phi}{\partial t} = \frac{1}{\Delta t} \left(\frac{3}{2} \phi - 2\phi^0 + \frac{1}{2} \phi^{00} \right) \quad (32)$$

where ϕ is the field at the current time step while ϕ^0 and ϕ^{00} are for the two previous time steps [40, 44, 50, 53].

The spatial discretization, involving gradients, divergences and Laplacians relies on the Gauss theorem: $\int_V \nabla \cdot \mathbf{a} dV = \oint_{\partial V} d\mathbf{S} \cdot \mathbf{a}$ (which is the only existing choice for the divergence and Laplacian schemes since they were already used in the Finite Volume Method, section 3.3.1). Once the Gauss theorem is applied, various quantities as well as surface normal gradients must be computed at the face separating 2 cells, see Figure 15a.

The interpolation scheme describes how to compute face quantities from cell-center ones. A linear interpolation is used here. A linear interpolation for a field ϕ , illustrated in Figure 15b computes the quantity at the face, ϕ_f using the cell-center values of adjacent cells, ϕ_1 and ϕ_2 :

$$\phi_f = f_x \phi_1 + (1 - f_x) \phi_2 \quad \text{with} \quad f_x = \frac{\overline{fP_2}}{\overline{P_1P_2}} \quad (33)$$

f_x taking into account the grading [44, 50].

Surface normal gradients are computed using the orthogonal scheme which can be used only when the line connecting the adjacent cell centers is perpendicular to the face it intersects with, which is always our case. The orthogonal scheme for a field ϕ is given by:

$$\mathbf{S} \cdot (\nabla \phi)_f = |\mathbf{S}| \frac{\phi_2 - \phi_1}{P_1 P_2} \quad (34)$$

and illustrated in Figure 15c [44, 50, 54].

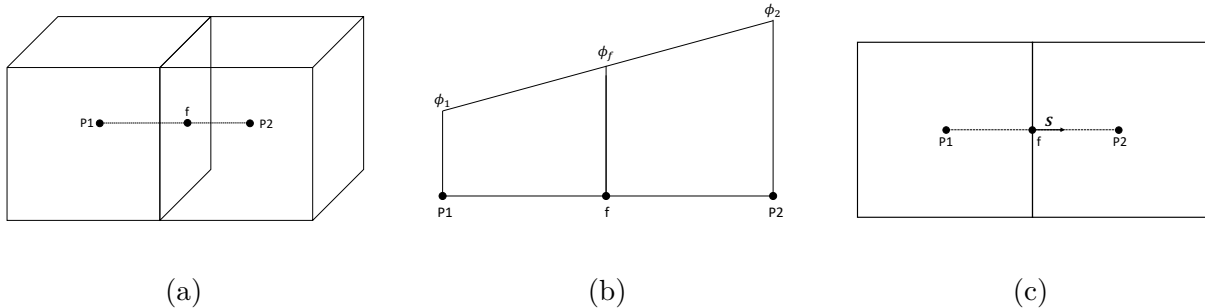


Figure 15: Illustration of interpolation schemes from cell center to face center [44].

Gradients, divergences and Laplacian terms of the initial equations are thus primarily simplified as functions of face-center values using the Gauss theorem and Jasak's hypothesis see section 3.3.1. Their face center values can afterwards be re-expressed using cell-center values by using the linear interpolation for quantities and the orthogonal scheme for surface normal gradients (appearing only in Laplacian terms). Performing all these manipulations enables to transform a transport type equation into a system of linear algebraic equations that can be expressed in a matrix form as $\mathcal{M}\Phi = \mathcal{B}$ and solved according to the information given in the next section.

4.5 Solution and algorithm control

Two types of information are needed for OpenFOAM to resolve the low Mach number equations. The first one concerns the system of linear algebraic equation, $\mathcal{M}\Phi = \mathcal{B}$, obtained by using the Finite Volume Method. At each iteration, multiple systems of equations must be solved for $\mathbf{u}$, T or p'_d using a linear-solver. The solver works using multiple iterations in order to reach a specific tolerance. One must thus define the type of solver to use and the tolerance to reach. As we are using the most common one, we will not describe each of them here. The second information requested relates to the PISO Loop. The number of inner loops, see Figure 9 in the algorithm must be defined. Is is in our case set to 3. We also specify that we are using a momentum predictor, Figure 9 [50].

4.6 Turbulence

As the natural convection phenomena happening in the pool is turbulent, this section describes the model used to incorporate the turbulent effects to the case. A turbulent flow is an irregular flow within which fields at each point change randomly in magnitude and direction [55, 56]. These fluctuations can have different sizes and timescales [57]. Turbulent flow are thus composed of many eddies, defined in [55] as "macroscopic fluid

element in which the microscopic element composing the eddy behave as a unit". Eddies can be themselves composed of smaller eddies and so on. The more turbulent the flow is, the largest the range of size of the eddies and the more complex it is to calculate it [55]. There are three methods usually used to deal with turbulence:

- Direct Numerical Simulation (DNS): resolves all the eddies, regardless of their size without using any type of model. The mesh size must thus be smaller than the smaller scales that should be resolved, which leads to enormous computational costs for the type of application that we are studying here [58, 59].
- Reynolds Averages Navier Stokes (RANS): turbulent fluctuations are averaged by a time-filter in order to decompose the instantaneous quantities as mean values and fluctuations: $u = \bar{u} + u'$. The fluctuations are then replaced by an additional viscosity term for all the domain. Consequently, all the eddies are modeled [58, 57].
- Large Eddy Simulation (LES): the large scale is solved directly (as in DNS) while the smaller scales are parametrized /modeled [59, 25].

In this project we will use a LES model. It has the advantage of being less computationally expensive than a DNS since it does not resolve all the small scales, and the benefit of still resolving the large scales which is not feasible with RANS. In a LES, the small scales are removed using a spatial filter to allow the large scales to be resolved, while these small scales are taken into account via models. The initial laminar Navier-Stokes with low Mach number approximation equations, see equations 8, become the filtered equations 35 :

$$\begin{aligned} \frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\mathbf{u}}) &= 0 \\ \frac{\partial (\bar{\rho} \bar{\mathbf{u}})}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\mathbf{u}} \bar{\mathbf{u}}) &= -\nabla \bar{p}_d + \nabla \cdot \bar{\boldsymbol{\tau}} + g \cdot h \nabla \bar{\rho} - \nabla \cdot \boldsymbol{\tau}^{SGS} \\ \frac{\partial (\bar{\rho} \bar{h})}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\mathbf{u}} \bar{h}) &= \nabla \cdot (k \nabla \bar{T}) + \frac{d\bar{p}^0}{dt} - \nabla \cdot \mathbf{q}^{SGS} \end{aligned} \quad (35)$$

where

- the overbar represents the filtering operation
- $\boldsymbol{\tau}^{SGS}$ is the subgrid scale stress tensor and
- $\mathbf{q}^{SGS}$ is the subgrid scale heat flux vector.

The subgrid scale (SGS) stress tensor and the subgrid scale heat flux account for the unresolved subgrid scales and must be modeled [59, 58, 25]. The simulation performed here uses a dynamic one-equation eddy-viscosity model, called *DynamicKEqn* in OpenFOAM. The next paragraphs first explain what type of spatial filter is used, then how this one-equation eddy-viscosity model defines the SGS stress and the SGS heat flux. Finally, a brief description of the dynamic procedure and its features will be given.

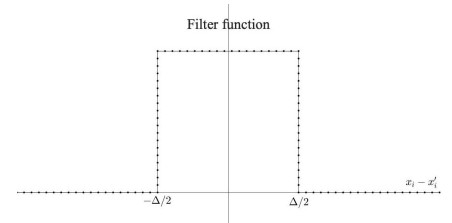


Figure 16: Top-hat filter [58].

4.6.1 Filter

The type of filter used can be chosen inside OpenFOAM when using the *DynamicKEqn* model. We here choose to use the basic one, called simple. The spatial filtering will thus be performed with a simple top-hat filter [60], shown in Figure 16 while the spatial filter length Δ will be the grid itself since only scales larger than the mesh can be resolved.

4.6.2 One-equation eddy-viscosity model

The one equation eddy-viscosity model defines (as most models) the SGS stress tensor as

$$\tau_{ij} = -2 \nu_t \overline{S_{ij}} \quad (36)$$

with

- $\overline{S_{ij}} = \frac{1}{2} \left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right)$, the resolved rate of strain
- ν_t , the turbulent viscosity

The turbulent viscosity, in the framework of this model, is defined as the product of the characteristic length, l with the square root of the kinetic energy: $\nu_t = l k^{1/2}$. The characteristic length is given by $l = C_v \Delta$ where C_v is a parameter of the model and Δ is the filter width. Using the kinetic energy allows to account for non-local and history effects [58]. The turbulent viscosity is thus:

$$\nu_t = C_v \Delta k^{1/2} \quad (37)$$

To obtain the kinetic energy, a transport equation for k must be solved, involving two additional parameters: C_ϵ and C_k [58]. The transport equation used by OpenFoam is given in [61].

Concerning the energy equation, the SGS heat flux can be modeled as [59, 58]:

$$q^{SGS} = \alpha_t \nabla T$$

where α_t is the turbulent diffusivity that can be obtained from the turbulent Prandtl number, defined as:

$$Pr_t = \frac{\nu_t}{\alpha_t}$$

We thus end up with 4 parameters to define: C_v , C_ϵ , C_k and Pr_t . As suggested by [59] and [58], a value of 0.4 will be used for the turbulent Prandtl number, Pr_t . The default value proposed by OpenFOAM will be used for $C_\epsilon = 1.048$. The model parameter C_v will be computed dynamically (see below) and C_k will be considered equal to C_v [58].

4.6.3 Dynamic model

Even though the model could be used as such by defining a constant value for C_v , a dynamic procedure can be used to determine its value. Dynamic means that the parameter of the base model: one-equation eddy-viscosity model, C_v can be calculated thanks to the smallest resolved scale. A second filter of width $\tilde{\Delta} (> \Delta)$ is used to compute an approximate value of C_v that can then be used, as described in the previous paragraph, to find the SGS stresses and heat flux.

4.7 Steady-state

To be sure that the data that we will analyse later in this report have reached a statistically steady-state, we first run a simulation for $200 T_f$. T_f being the free-fall time unit, defined as:

$$T_f = \frac{h}{U_f} [s]$$

with h the height and U_f the free-fall velocity defined respectively in equations 29 and 30. This first run has the initial conditions of Table 4 and thus a linear temperature profile along the vertical axis. The mesh refinement is defined using a correlation for the Nusselt number, see equation 22. Once the first simulation is done, a second simulation is created. This one has a mesh based on the Nusselt number of the first simulation and its initial conditions are mapped to the latest time computed in the first simulation by using OpenFOAM's mapFields utility.

4.8 Conclusion

The simulation performed in this report aim at comparing two Rayleigh-Bénard convection cases representing spent fuel nuclear pools. The two cases investigate different velocity boundary conditions at the top of their geometry. To do so, a solver is used to solve the Navier-Stokes equation with the low Mach number approximation on a cube heated from below and cooled from above. The solver was presented in section 3. However, the case set-up still needed to be determined. In summary, the geometry representing the pool is cube made of 6 walls. The bottom wall is a cold fixed wall and the sides ones are adiabatic fixed wall. The upper plane is a hot surface with a fixed wall boundary condition or a free-surface. The mesh is properly refined in order to resolve all the necessary scales and a LES turbulence model is used to account for the turbulence phenomena happening inside the geometry. The reliance of the water's properties to temperature is taken into account by either evaluating these at a reference temperature or by using polynomial fits.

5 Results

Numerical simulations to model the natural convection inside nuclear spent fuel pools have been performed and their results are analyzed hereafter. As explained in detail above, we model the pool as a cube with a constant uniform "hot" temperature at the floor and a "cold" one at the ceiling. The sidewalls as well as the bottom part are fixed and thus have a no-slip velocity boundary condition. The upper velocity boundary condition, which represent the surface of the pool will either be considered as a fixed wall or a free surface. The two cases will respectively be referred to as classical Rayleigh-Bénard convection (RBC) and free-slip. This report attempts to compare the influence of these two boundary conditions on the flow topology.

The flow inside the cube representing the pool is computed using the low Mach number equations. As the equations are coupled, a PISO algorithm is used to solve the system of equations. The equations involved in the PISO Loop are solved using finite volumes. The spatial discretization relies on second order central differences while the time-integration scheme takes into account the current and the two previous time steps. Furthermore, turbulence is added to the model by means of a LES, large eddy simulation. LES allows to resolve the large scales eddies while the small scales are parametrized. Finally, in order to have a good mesh resolution, a hyperbolic tangent refinement is added to the cube to allow more cells in the boundary layers than in the core of the domain.

The following two sections present the results obtained by these simulations and compare the respective influence of the no-slip and free-slip boundary conditions. The first section focuses on the flow topology and the flow statistics for varying Rayleigh numbers, while the second section compares the re-orientations of the classical RBC and the free-slip case for a moderate Rayleigh number of $Ra = 2 * 10^7$.

5.1 Influence of a free-slip upper boundary condition on the flow properties

The classical Rayleigh-Bénard convection (no-slip boundary condition) and the free-slip cases are here analyzed for various Rayleigh numbers, Ra . The cases considered are included in Table 7. The Rayleigh number as well as the upper boundary condition and the number of cells composing the mesh are referenced. The time- and volume-averaged Nusselt number is given. Other parameters such as the non-dimensional root mean square value of the vertical velocity, the eddy turnover time and the free-fall time unit are also listed. The non-dimensional root mean square value of the vertical velocity is computed using probes (their specific locations are explained in section 5.2). The value of v_{rms} allows us to compute the eddy turnover time by using the following relationship: $T_{eddy} = \frac{h}{v_{rms}}$.

Ra	Upper boundary condition	$N_x \times N_y \times N_z$	Nu	v_{rms}	T_{eddy}	T_f
$2 * 10^7$	no slip	$60 \times 60 \times 60$	22	$1.67e^{-3}$	16.02	$6.546e^{-1}$
$2 * 10^7$	free slip	$60 \times 60 \times 60$	29	$2.72e^{-3}$	9.83	$6.546e^{-1}$
$5 * 10^7$	no slip	$72 \times 72 \times 72$	29	$2.06e^{-3}$	17.62	$7.627e^{-1}$
$5 * 10^7$	free slip	$72 \times 72 \times 72$	38	$2.53e^{-3}$	14.34	$7.627e^{-1}$
10^8	no slip	$88 \times 88 \times 88$	36	$1.78e^{-3}$	25.71	$8.56e^{-1}$
10^8	free slip	$88 \times 88 \times 88$	46.9	$2.04e^{-3}$	22.41	$8.56e^{-1}$

Table 7: Parameters of various case set up: Rayleigh number, Ra [–], upper boundary condition for the velocity field: no slip or free slip, mesh size, Nusselt number, Nu [–], Root mean square value of the vertical velocity, v_{rms} , eddy turnover time T_{eddy} and free-fall time, T_f .

The Nusselt numbers from classical RBC simulations can be compared to the values of reference [33] and [62], given in Table 8. The values obtained within this report are comparable to the ones coming from these previous studies. It is important to note that the simulations performed as part of these studies have some differences in comparison with ours and must therefore be considered carefully. Reference [33] performs a LES simulation using the Boussinesq approximation for air having a Prandtl number of $Pr = 0.7$ while [62] uses a DNS and the Boussinesq approximation on a fluid of $Pr = 4.38$. Unfortunately, no comparative study can be found for the free-slip case. We can, nevertheless, see that the Nusselt number values are always higher than in classical Rayleigh-Bénard convection meaning that the convection is probably increased by this new boundary condition.

Ra	10^7	$3 * 10^7$	$5 * 10^7$	10^8
Nu of reference [33]	16.4	22.4	/	31.6
Nu of reference [62]	16.1	22.6	26.2	32.2

Table 8: Nusselt numbers for various Rayleigh numbers from existing references.

To make sure that the data analyzed are in a statistically steady-state, each case runs a first time for $200 T_f$ [s] on a coarse mesh, starting from a linear temperature profile between the floor and the ceiling. Once this first simulation is performed, the final mesh of Table 7 is computed using the Nusselt number of this first simulation (see section 4.3 for more details). A second simulation is then performed on the appropriate mesh with initial conditions mapped from the latest time of the first simulation. The flow properties presented in Table 7 and hereafter are the result of the second simulation only and can thus be considered as being in a statistically steady-state. The results presented in this section (5.1) are averaged over $300 T_f$ [s].

In the following information to come, all the fields have been normalized to become non-dimensional. The time average of a field, ϕ will be denoted by $\bar{\phi}$ while an area-averaging (in the horizontal plane) by $\langle \phi \rangle_{xz}$.

5.1.1 Large Scale Circulation

Figures 17a and 17b present 3D plots of the time-averaged velocity streamlines that compose the flow respectively for the classical RBC and the free-slip cases. The color

represents the non-dimensional temperature, $\theta = \frac{T-T_{ref}}{\Delta T_{ref}}$, averaged over time. The numbers present at each visible corner of both cubes (2,3,7,6 at the top and 1,5,4 at the bottom) refer to the vertices used to describe the geometry in OpenFOAM, see Figure 10. They are useful to understand the figures to come, representing several planes, sections, etc. of the cubic samples.

As it has already been observed in previous studies for turbulent Rayleigh-Bénard convection, the flow creates a large-scale circulation, LSC or mean wind. This LSC is known to be aligned to a vertical diagonal plane for square cross section geometries. For the classical RBC and the free-slip cases, one can see on Figures 17a and 17b that the LSCs are aligned to one diagonal plane. For both cases, this diagonal plane contains vertices 2 and 7. However, the direction of the classical RBC case, as seen from the top, is from 7 to 2 while it is from 2 to 7 for the free-slip case. In the LSC plane, one can also observe small re-circulations on the edges. In the perpendicular plane (the other diagonal), counter-rotating vortices are formed, going from the corner of the geometry towards the center. All these characteristics have already been observed in other LES: [25, 33, 63] as well as in some DNS: [40, 64].

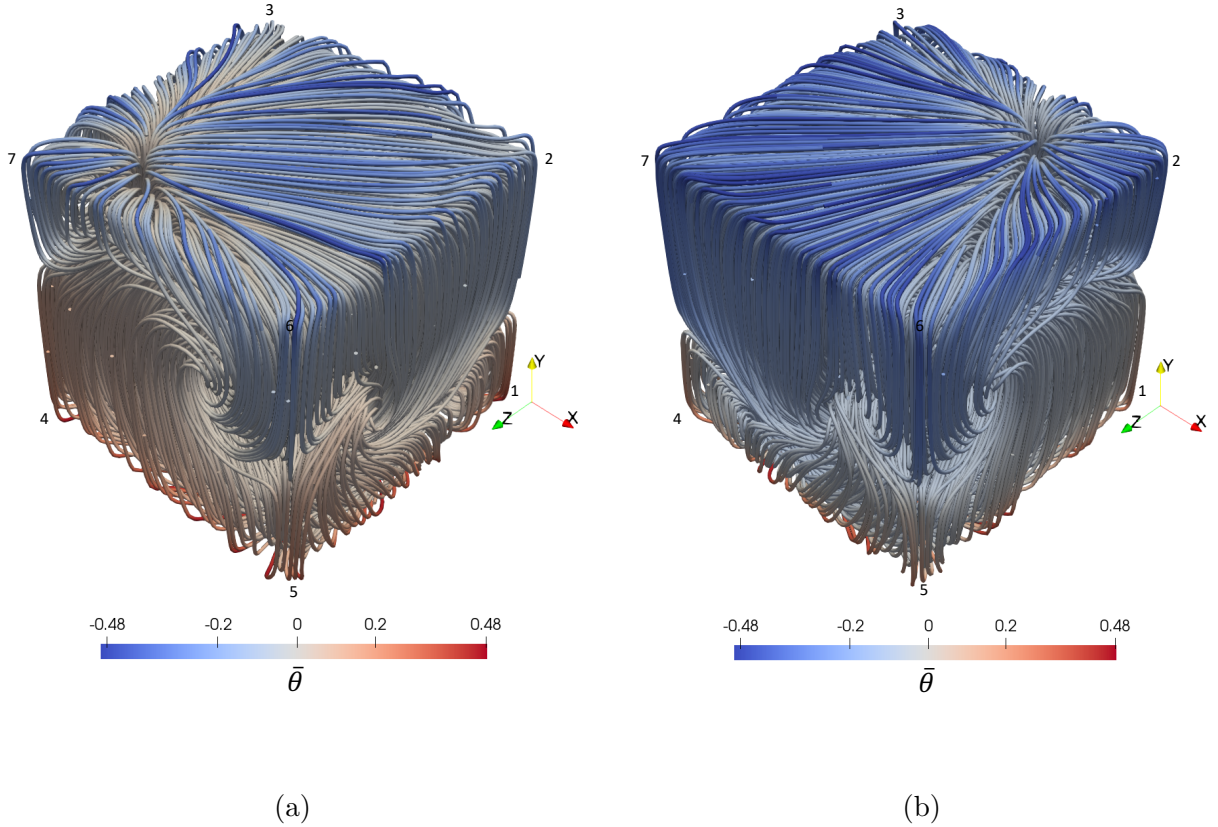


Figure 17: 3D velocity streamlines colored with $\bar{\theta}$ for $Ra = 10^7$. (a) Classical Rayleigh Bénard Convection. (b) Free-slip upper boundary condition.

As we will see later on, the LSC in Rayleigh-Bénard convection re-orientates itself randomly in time. The difference of LSC orientation of the two cases under study is therefore not linked to the upper boundary condition. If another time range was analyzed, one may

observe other orientations of the LSCs. It should however be noted that, over the $300 T_f$ time range, the flows are fixed in the orientations presented before. More details about these re-orientations will be given in section 5.2.

Figure 18 showcases diagonal cuts of the cube for the classical RBC (18a) and the free-slip (18b) cases. The coloring corresponds to the magnitude of the time-averaged non-dimensional velocity, $\bar{U}$ (with $U = \frac{U_{dim}}{U_f}$) while the black arrows represent the time-averaged velocity vectors. The top figure displays the diagonal cut aligned to the LSC while the lower one is perpendicular to it. In both cases, one can clearly observe, in the upper plot, a convection cell around the diagonal which corresponds to the Large Scale Circulation. In these LSCs, the flow rises on one side and reaches the cold upper plate. It follows the plate until it reaches the other side of the diagonal, where it sinks back to the hot bottom surface. One can clearly observe that in both cases, the LSC is oriented in the vertical plane containing vertices 7,2,1 and 4 but with opposite directions. Besides the LSC itself, the LSC plane also contains re-circulations. These are present in corner 1 and 7 for classical RBC and in corner 2 and 4 for the free-slip case. Counter-rotating vortices can be observed at the corners of the diagonal perpendicular to the LSC (lower figure).

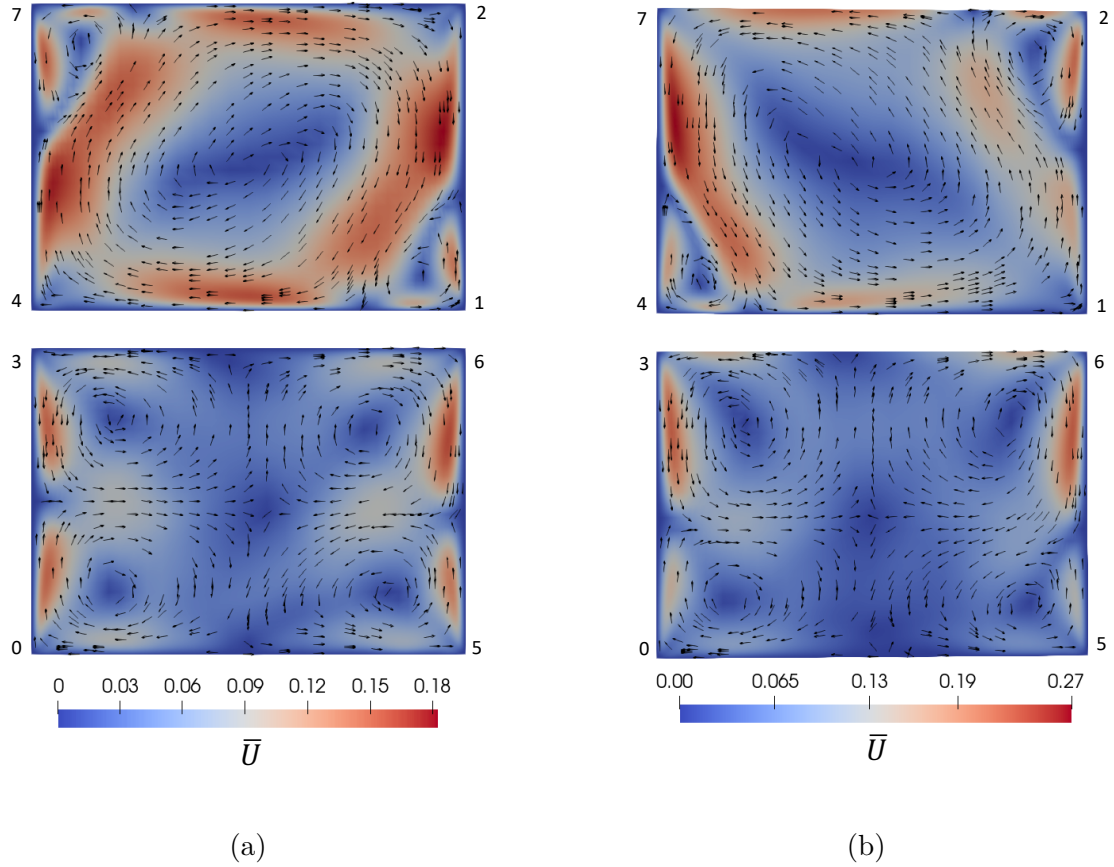


Figure 18: Colour plot of $\bar{U}$ with superimposed velocity vectors on diagonal cuts for $Ra = 10^7$. (a) Classical Rayleigh Bénard Convection. (b) Free-slip upper boundary condition.

Horizontal cuts were performed near the top, at the middle and at the bottom of the cube and are shown in Figure 20a and 20b for the classical RBC and the free-slip cases.

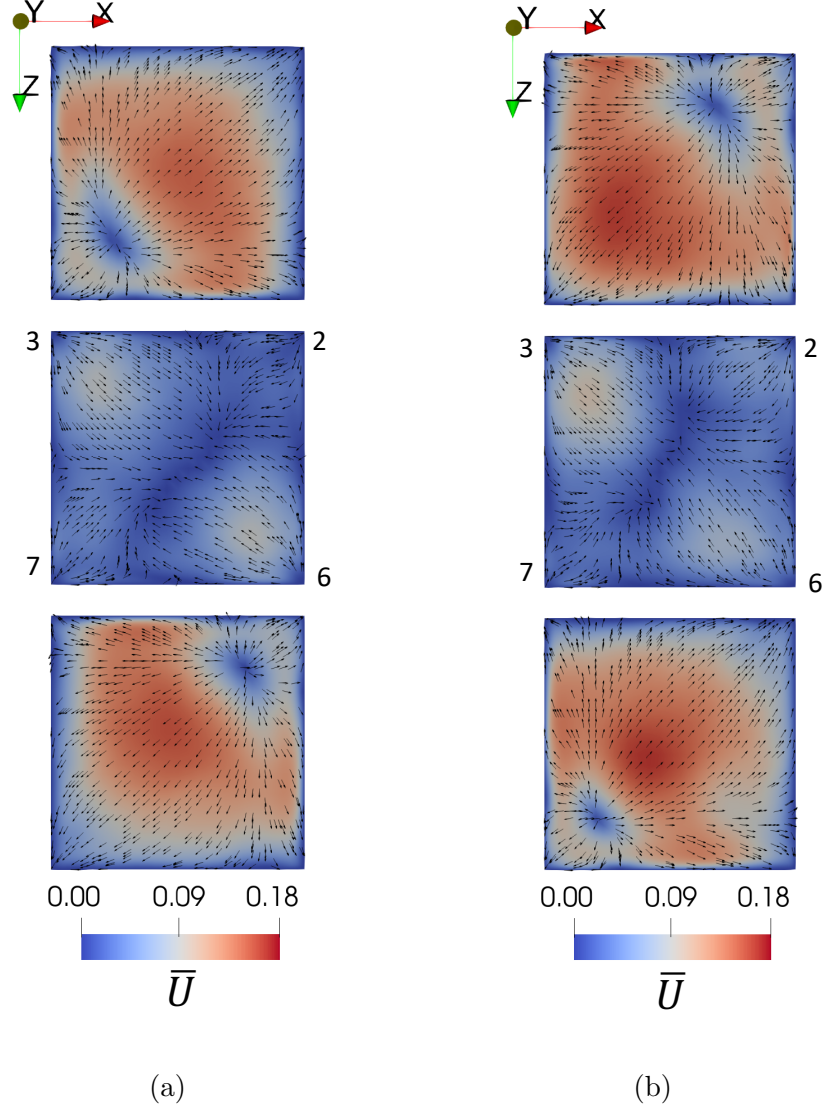


Figure 19: Colour plot of $\bar{U}$ with superimposed velocity vectors on horizontal cuts at $0.05 h$ (bottom), $0.5 h$ (middle) and $0.95 h$ (top) for $Ra = 10^7$. (a) Classical Rayleigh Bénard Convection. (b) Free-slip upper boundary condition.

The cuts are seen from above and are taken at a distance of $0.05 h$ from the floor and the ceiling as well as at middle height. The figures feature the time-averaged velocity vector components that are parallel to the plane in question (as arrows) and the non-dimensional velocity averaged over time throughout the color. The upper and lower figures respectively display the top and bottom cuts. These are in a mirror symmetry with each other. Both cases have an upward/downward jet of plume at one of the top/bottom corner. From these impingements, the flow then extends mainly to the opposing corner to create the large-scale circulation but also to the two other corners, forming the counter-rotating vortices. Part of the flow also moves "behind", towards the corner it has emerged from, creating the re-circulations. For example, in the classical RBC case, the flow rises near corner 7, the impingement thus occurs near it (see Figure 20a, top). The flow then extends mainly to

corner 2 but also to corners 3 and 6 to form the counter-rotating vortices. Finally, part of the flow from the impingement moves to corner 7 and creates a re-circulation. The same approach can be used for the free-slip case as well as for the bottom plane. In the middle plane, one can observe both the counter-rotating vortices and the re-circulations all aiming towards the center of the geometry.

One final important point is the temperature distribution across the volume. On Figure 20, one can observe the mean temperature in a diagonal cut, aligned to the LSC. The perpendicular cut is not shown as they are identical. In both cases, the bulk has a constant temperature, only the sides show different temperatures. The main difference between the two cases is the bulk temperature which is colder in the free-slip case compared to the classical one.

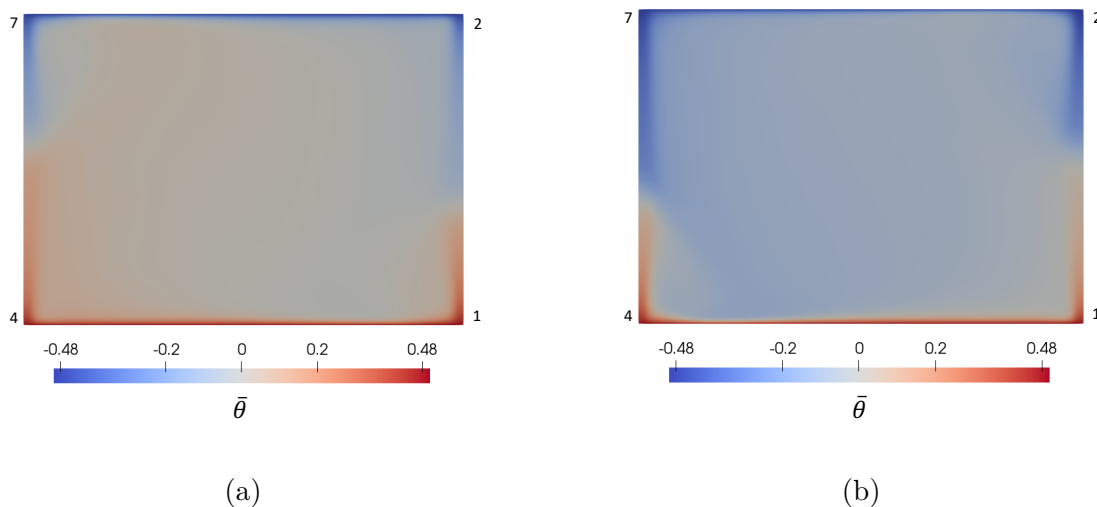


Figure 20: Colour plot of $\bar{\theta}$ on a diagonal cut aligned to the LSC for $Ra = 10^7$. (a) Classical Rayleigh Bénard Convection. (b) Free-slip upper boundary condition.

The figures presented in this section have shown us that the change in the upper velocity boundary condition does not impact the structure taken by the flow. In both cases, the LSC and the counter-rotating vortices can be identified easily. Even though the global structures seem very similar to each other, some variations between the two samples exist. Indeed, the temperature and velocity profiles are very similar for the two boundary condition investigated but their magnitudes are not the same. The velocity is higher and the bulk temperature lower in the free-slip case.

5.1.2 Flow statistics

In this section we analyse various flow statistics as function of the height of the domain. These statistics have been obtained by averaging the studied fields over a time range of $300 T_f$. The fields are analyzed using two different means. First of all we look at the fields value along the center line, which is the vertical line passing by the origin. Then we compute area-averages in the xz plane and display them as a function of the height, y. The area-averages are computed at the center of each cell constituting the mesh. The temperature profiles are first presented. Focus is thereafter placed on various velocity profiles before ending with the turbulent heat flux.

The profiles are compared to those obtained in references [65], [66] and [28] for the

upper no-slip boundary condition. Article [65] performs a DNS using the Boussinesq approximation and periodical horizontal boundaries. The fluid under study has a Prandtl and a Rayleigh numbers respectively of $Pr = 0.7$ and $Ra = 2 * 10^7$. Paper [66] provides the same type of simulation than the previous one. However it is done for $Pr = 1$ and for $Ra = 2.5 * 10^6$ and it focuses on the influence of rotation. Finally, experiments on water at $Pr = 4.3$ and $Ra = 3.2 * 10^{11}$ within a rectangular cell can be found in reference [28]. The paper, nevertheless, deals exclusively with temperature profiles. The free-slip upper boundary condition sample, on the other side, will be compared against the no-slip case as well as to reference [40]. The latter performs a DNS and a LES, using the low Mach number approximation on a rectangular cavity with a periodic boundary along one of the horizontal directions. The Prandtl and Rayleigh number are respectively $Pr = 3$ and $Ra = 10^7$.

Temperature Profiles

Figure 21 displays the non-dimensional temperature, θ , averaged over time and taken along the center-line (21a) as well as its time and area-averaged along the vertical axis (21b). The classical RBC case (solid line), presents a plateau at the averaged value and the profile follows a mirror symmetry. The small variations between the center-line and the area-averaged profiles are probably due to the influence of the side walls (see Figure 20). However, very close to the upper and lower walls, the temperature changes greatly in a very thin layer of the geometry then transitions quickly to the core temperature. These observations are in good agreement with previous theories [28, 67, 68, 66, 65], that have found the thermal boundary layer to be composed of three different parts. Closer to the wall, the temperature changes considerably and varies linearly with the height. In this thin layer, conduction is the main heat transfer. Then, a transition phase occurs before reaching a constant value in the core of the domain where heat is predominantly carried by convection.

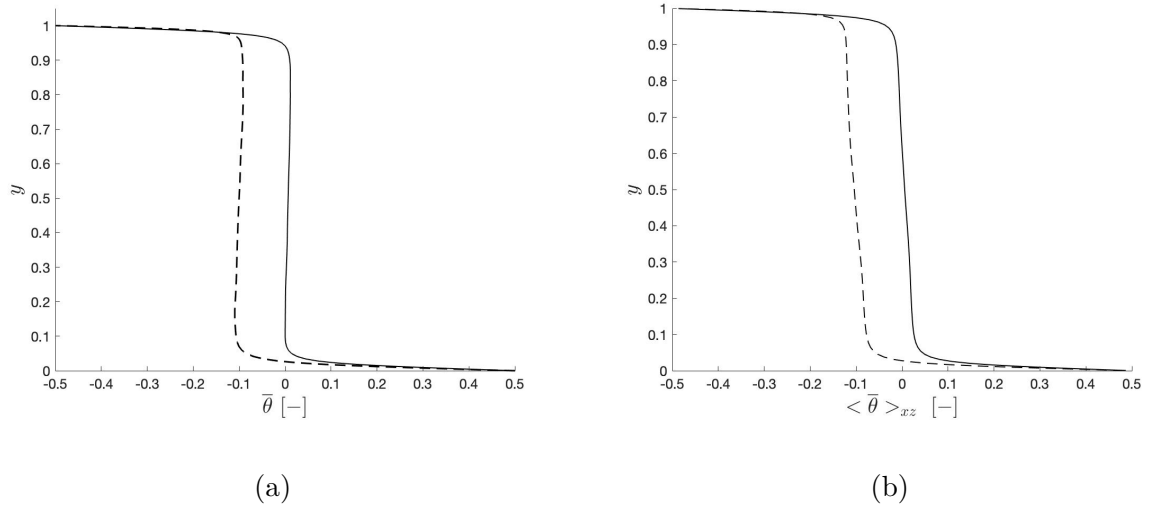


Figure 21: Non-dimensional temperature, θ for $Ra = 10^7$. (a) Averaged over time and plotted along the center-line. (b) Time and area-averaged. The legend is as follows: classical RBC (solid line) and free-slip upper boundary condition (dotted line).

The free-slip case (dotted lines on Figures 21a and 21b) presents the same shape as classical RBC shifted to the left. The temperature profile is therefore not in symmetry and the core value of the field is not equal to the mean value anymore but is cooler. This shift of the core temperature had already been observed in Figure 20 as well as in reference [40].

Zooms on the boundary layers of Figure 21a are displayed in Figures 22a and 22b for classical RBC and the free-slip case respectively. An estimation of the thermal boundary layer thickness can be obtained by computing the intersection between the core temperature (vertical gray line) and an extrapolation of the linear part of the profile (inclined gray line), as illustrated in Figure 22. Table 9, columns 2 and 3, contains the values of the thermal boundary layers, $\delta_{\bar{\theta}}$, defined using the averaged temperature at the top and bottom of the geometry along the center-line. One can see that the top and bottom thicknesses are approximately equal in the classical case while the top boundary layer thickness is smaller than the bottom one for the free-slip upper boundary condition.

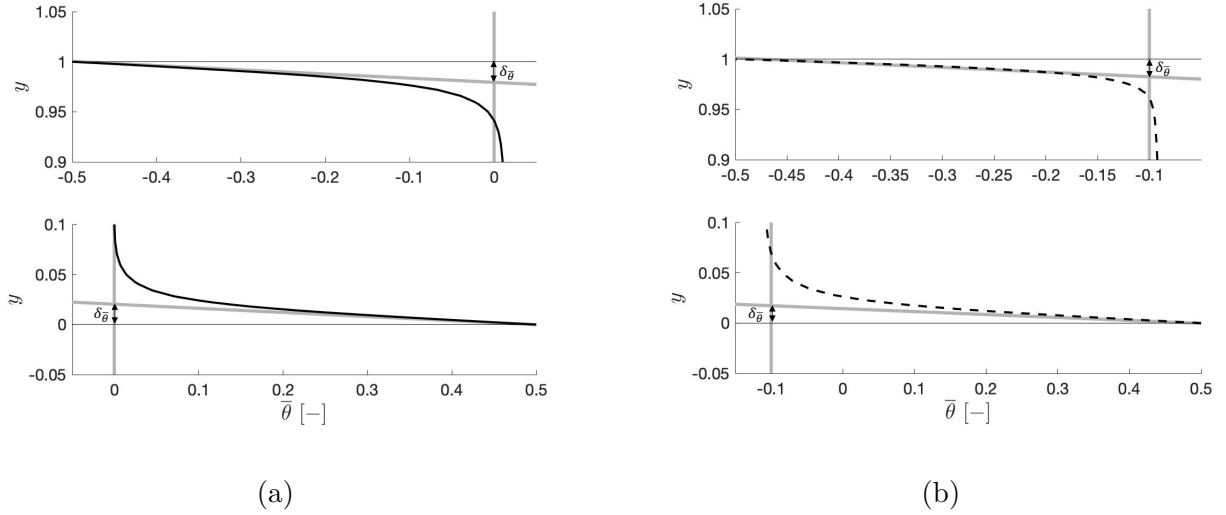


Figure 22: Zoom of Figure 21a in order to define the thermal boundary layer thickness. (a) Classical RBC. (b) Free-slip upper boundary condition.

	$\delta_{\bar{\theta}}$		$\delta_{\theta_{rms}}$	
	RBC	Free-slip	RBC	Free-slip
Top B.L.	0.0247	0.0176	0.022	0.014
Bottom B.L.	0.0244	0.0242	0.022	0.022

Table 9: Values of the thermal boundary layer thickness defined using either the time-averaged temperature or the rms temperature.

Another interesting field is the non-dimensional root mean square (rms) temperature, $\theta_{rms} = \sqrt{\overline{\theta'\theta'}}$, where θ' is the fluctuating component of the non-dimensional temperature field [55]. The rms value tells us about the intensity of the non-dimensionnall temperature field compared to its mean value [69]. Plots of θ_{rms} can be found on Figures 23a and 23b. As expected, when the cube has an upper no-slip boundary condition (solid line), the profile is symmetric. Starting from 0 at the wall, since the temperature is constant in time and uniform over the whole surface, it increases strongly and linearly as the distance

from the wall increases. It reaches a maximum at the end of the thermal boundary layer derived from the temperature root mean square [28, 65]. It then decreases to reach a small value, however not null, in the center of the geometry. Since the peaks seems to represent a "natural scale", the rms derived thermal boundary layer, $\delta_{\theta_{rms}}$, is usually preferred to the one computed using the time-averaged temperature field [28]. In classical RBC, as the profile is symmetric, the top and bottom boundary layer are equal, see Table 9. The free-slip boundary layer (dotted line) is again not symmetric. The upper peak is much lower than the bottom one. The peak distances from the wall, i.e. the thermal boundary layers, are not the same at the top and the bottom. Indeed, the upper boundary layer is thinner than the lower one, values are given in Table 9.

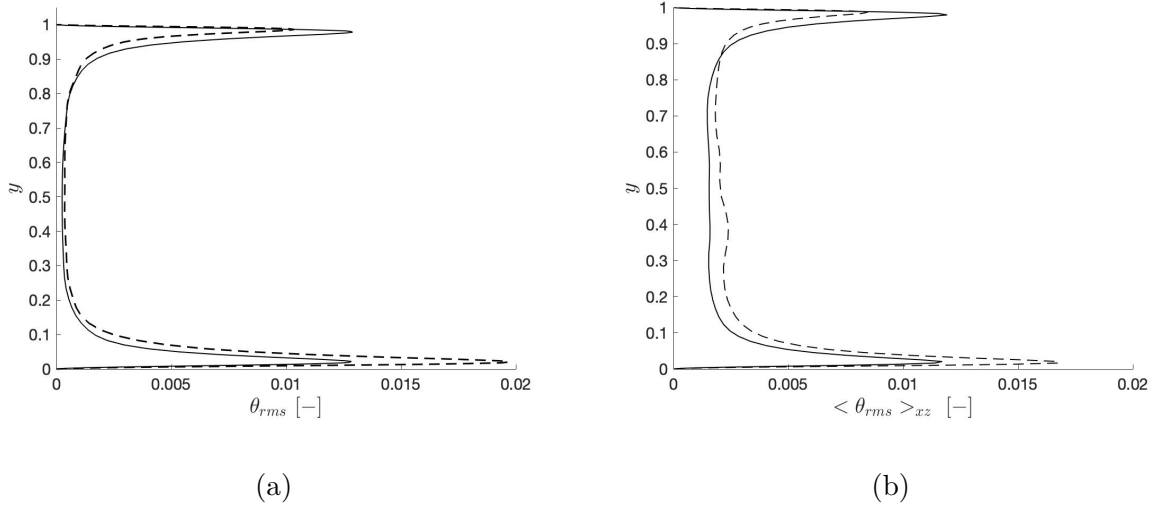


Figure 23: Root Mean Square temperature, θ_{rms} for $Ra = 10^7$. (a) Along the center line. (b) Area-averaged. The legend is as follows: classical RBC (solid line) and free-slip upper boundary condition (dotted line).

The profiles presented in Figures 21 and 23 are in good agreement with previous studies. Indeed similar temperature profiles are presented in references [28, 66, 65] for classical Rayleigh-Bénard convection while paper [40] obtains similar results for the slip-case even though differences between these studies and ours subsist.

The free-slip velocity boundary condition seems to induce two types of differences to the temperatures profiles. Firstly, the bulk temperature inside the whole structure is decreased, removing the symmetry. Secondly, the top thermal boundary layers is decreased meaning that the core temperature is reached within a smaller distance from the wall.

Velocity Profiles

In this section we analyze velocity profiles. First of all, Figure 24 plots the time-averaged non-dimensional velocity profiles along the center-line for all three directions. The area-averaged profiles will not be shown as they are very similar to the center line ones for the horizontal directions and not relevant for the vertical one.

Concerning the horizontal directions, in classical RBC (solid line) we can see that the curves are in mirror symmetry with respect to the half-height of the cube, see Figures 24a and 24c. This is due to the large scale circulation pattern taken by the flow. Indeed, we

had already seen this in Figure 19. The free-slip case (dotted line) seems to more or less follow this symmetry in its core. However, since the wall horizontal velocity is not set to zero at the ceiling of the cube due to the free-slip boundary condition, the velocity is different than zero at the top while it is null at the bottom. The x and z velocities have the opposite signs at all heights for both cases (RBC and free-slip). This is due to the various orientations taken by the flow in the $300 T_f$ time range for which the fields are averaged. As a matter of fact, the orientations taken by the two cases are not the same and therefore lead to this sign difference.

The vertical velocity, Figure 24b, goes upward in the upper half of the domain and downward in the lower one. Both the classical RBC and the free-slip curves are in agreement with what was previously observe on the diagonal cuts of Figure 18.

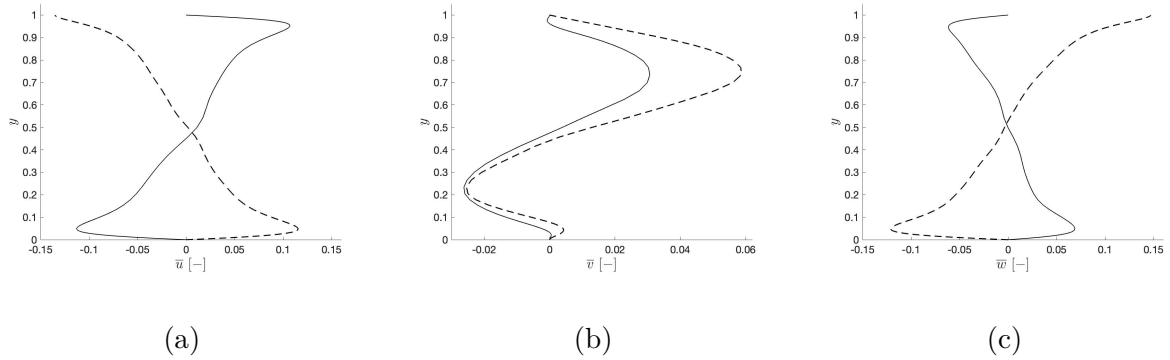


Figure 24: Time-averaged non-dimensional temperature along the center-line for $Ra = 10^7$. (a) In the x direction. (b) In the y direction. (c) In the z direction. The legend is as follows: classical RBC (solid line) and free-slip upper boundary condition (dotted line).

The horizontal root mean square velocity is computed as follows:

$$u_{rms} = \sqrt{u'u' + w'w'} \quad (38)$$

Again, the plot is symmetric for classical RBC while the free-slip case has a very similar shape except at the upper wall due to its specific boundary condition that allows non-zero horizontal velocity, see Figure 25. As the profiles present peaks near the horizontal boundaries, the maximum position of u_{rms} can be used to define the kinetic boundary layer exactly as what was done to obtain the root mean square derived thermal boundary layer [65]. The values of the boundary layer thicknesses are available in Table 10. One can see that the upper and lower thicknesses are equal for classical RBC. For the free-slip case, one can only define a lower boundary thickness whose value is smaller than for classical RBC.

	$\delta_{U_{rms}}$	
	RBC	Free-slip
Top B.L.	0.0421	/
Bottom B.L.	0.0421	0.0341

Table 10: Values of the kinetic boundary layer thickness defined using the rms horizontal velocity.

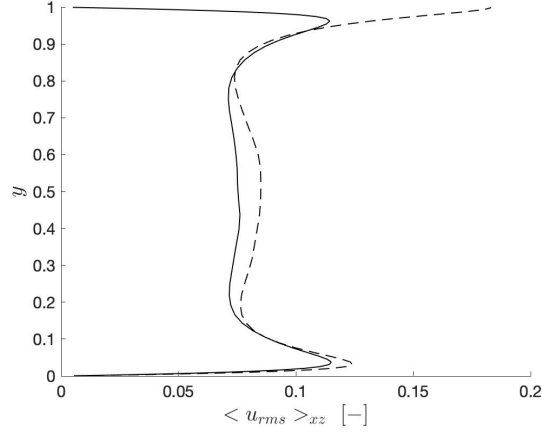


Figure 25: Root Mean square horizontal velocity, u_{rms} for $Ra = 10^7$, area-averaged. The legend is as follows: classical RBC (solid line) and free-slip upper boundary condition (dotted line).

Figure 26 exhibits the non-dimensional root mean square vertical velocity, $v_{rms} = \sqrt{v'v'}$ area-averaged along the height of the geometry. In this case, both types of boundary conditions, no-slip and free-slip, impose a vertical rms velocity of zero at the upper and lower boundary. The area-average profile has a parabolic shape that reaches a maximum in the center. The shape is characteristic of Rayleigh-Bénard convection and has previously been observed in references [65, 66] for classical RBC and in [40] for Rayleigh-Bénard convection with a free-slip boundary condition at the top. Even though v_{rms} does not reach a core value, one can see that it changes more near the boundaries than in the core.

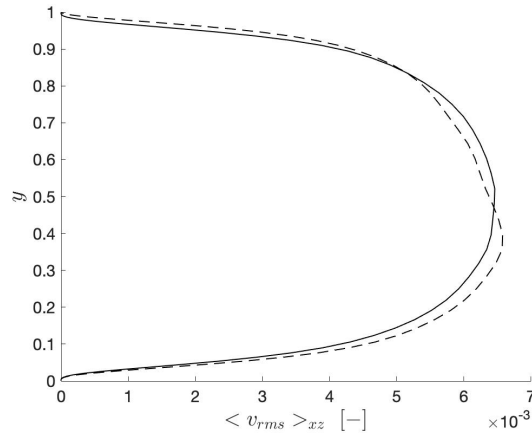


Figure 26: Root Mean square vertical velocity, v_{rms} for $Ra = 10^7$, area-averaged. The legend is as follows: classical RBC (solid line) and free-slip upper boundary condition (dotted line).

The 5 velocity profiles investigated in this section, that is, $\bar{u}$, $\bar{v}$, $\bar{w}$, u_{rms} and v_{rms} are coherent with the streamlines and velocity vectors displayed in the previous section as well as with previous studies. The root mean square velocities of the free-slip case present similar values and its lower kinetic boundary layer is thinner.

Turbulent Heat Flux

The last statistic that we focus on is the turbulent heat flux, $\overline{\theta'v'}$, area-averaged. This field combines temperature and velocity. A high value of turbulent heat flux implies that the non-dimensional temperature as well as the non-dimensional vertical velocity are affected by the same cause. The area-averaged profile is symmetric for both cases and present a sharp increase near the boundaries and a plateau in the core of the domain, similarly to what is plotted in [40]. The free-slip case, however, has a constant value in the bulk higher than the one from Rayleigh-Bénard convection. As the overall Nusselt number is also higher, see Table 7, we can conclude that convection is enhanced by the free-slip upper boundary condition which causes $\overline{\theta'v'}$ to increase as well.

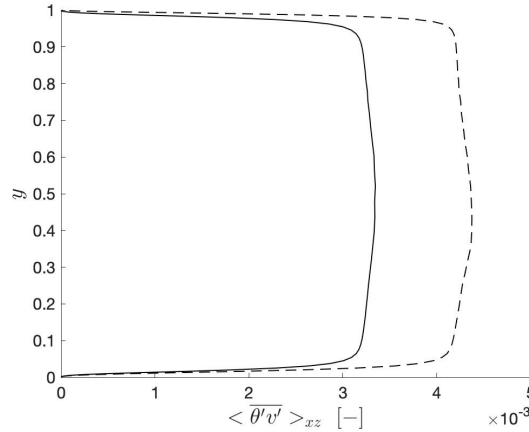


Figure 27: Turbulent heat flux, $\overline{\theta'v'}$, for $Ra = 10^7$ area-averaged. The legend is as follows: classical RBC (solid line) and free-slip upper boundary condition (dotted line).

5.1.3 Higher Rayleigh numbers

As we have established the main differences between classical RBC and a free-slip case for $Ra = 2 * 10^7$, we now focus on analyzing the same profiles for higher Rayleigh numbers. We here compare the temperature and velocity statistics for the six cases detailed in Table 7. Three different Rayleigh numbers are used: $2 * 10^7$, $5 * 10^7$ and 10^8 and we investigate the influence of the no-slip and the free-slip upper boundary condition for each.

Table 7 contains the time and volume averaged Nusselt number. One can see that an increase of Rayleigh number can be associated with an increase of Nusselt number. Furthermore, the free-slip case always present a higher Nusselt number than classical Rayleigh-Bénard convection for an equivalent Rayleigh number.

Temperature Profiles

Figures 28 and 29 plot the time-averaged non-dimensional temperatures and the non-dimensional root mean square temperatures over the center-line for $Ra = 2 * 10^7$ in black, $Ra = 5 * 10^7$ in red and $Ra = 10^8$ in blue. Classical RBC cases are presented by solid lines while the free-slip ones use dotted lines.

The profiles of $\bar{\theta}$ are very similar for the cases having the same boundary conditions. The classical RBC cases for the three Rayleigh numbers under study, all present a bulk

temperature equal to the mean temperature while the plateaus in the free-slip cases have a value colder than the mean value, see Figure 28a. Figures 28b and 28c present enlargement of the previous figure near the top and the bottom of the geometry. This allows us to notice the decrease of boundary layer thickness (defined using the mean temperature) with increasing Rayleigh number. Table 11 contains the value of the boundary layer for each case and we can see that for the three Rayleigh numbers investigated, the boundary layer is always thinner in the respective free-slip case. Furthermore, in the free-slip cases, the upper thermal boundary layers are thinner than the lower ones due to the specific velocity boundary condition of those samples.

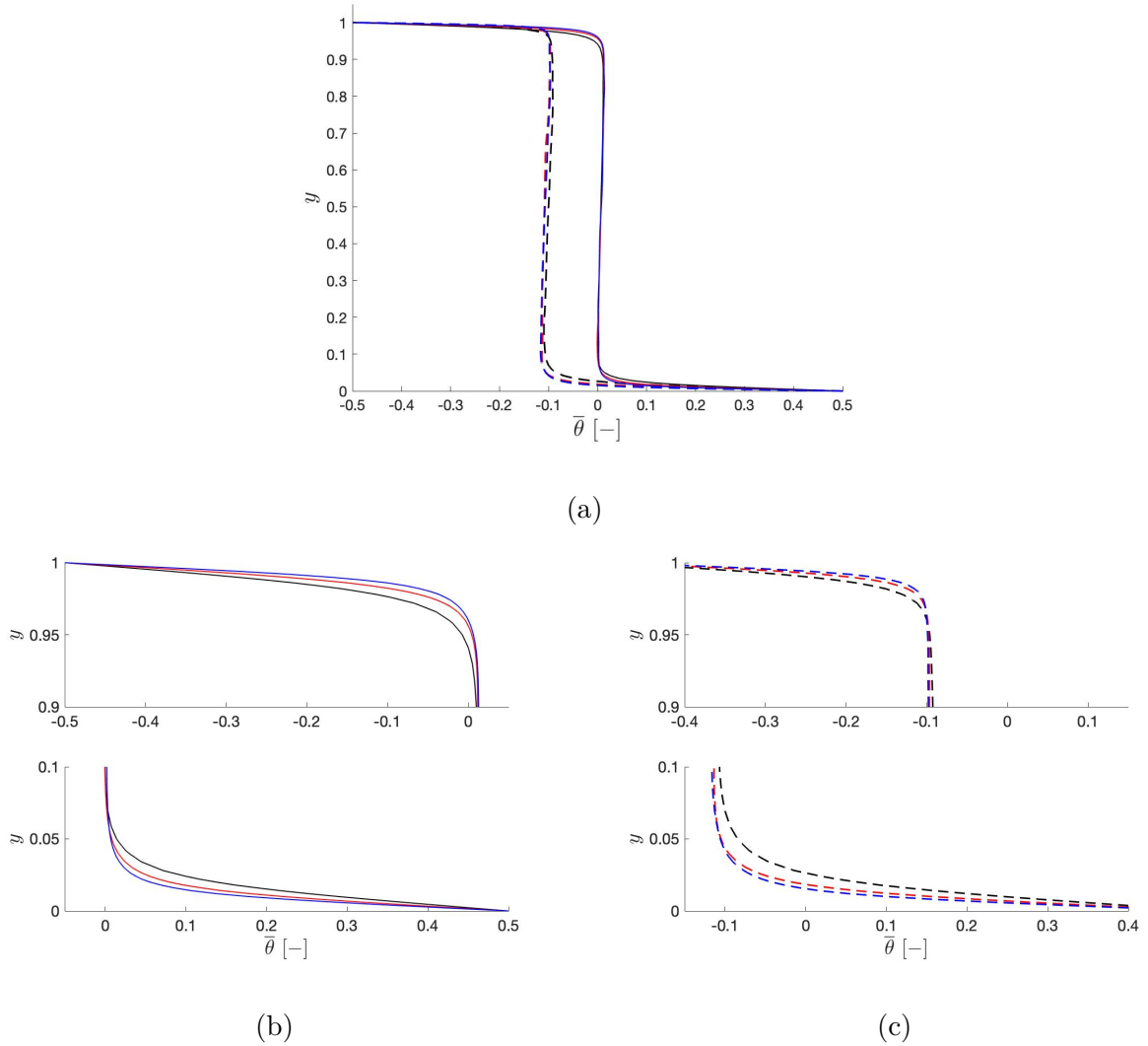


Figure 28: (a) Non-dimensional temperature, θ averaged over time along the center-line. (b) Zooms on the B.L. of the classical RBC cases. (c) Zooms on the B.L. of the free-slip cases. The legend is as follows: classical RBC (solid line) and free-slip upper boundary condition (dotted line) as well as $Ra = 2 \times 10^7$ (black), $Ra = 5 \times 10^7$ (red) and $Ra = 10^8$ (blue).

Rayleigh Number		$\delta_{\bar{\theta}}$		$\delta_{\theta_{rms}}$	
		RBC	Free-slip	RBC	Free-slip
$2 * 10^7$	Top B.L.	0.0247	0.0176	0.022	0.014
	Bottom B.L.	0.0244	0.0242	0.022	0.022
$5 * 10^7$	Top B.L.	0.02	0.015	0.016	0.01
	Bottom B.L.	0.019	0.018	0.015	0.014
10^8	Top B.L.	0.017	0.014	0.012	0.008
	Bottom B.L.	0.017	0.016	0.012	0.012

Table 11: Values of the thermal boundary layer thicknesses defined using either the averaged temperature or the rms temperature for various Rayleigh numbers.

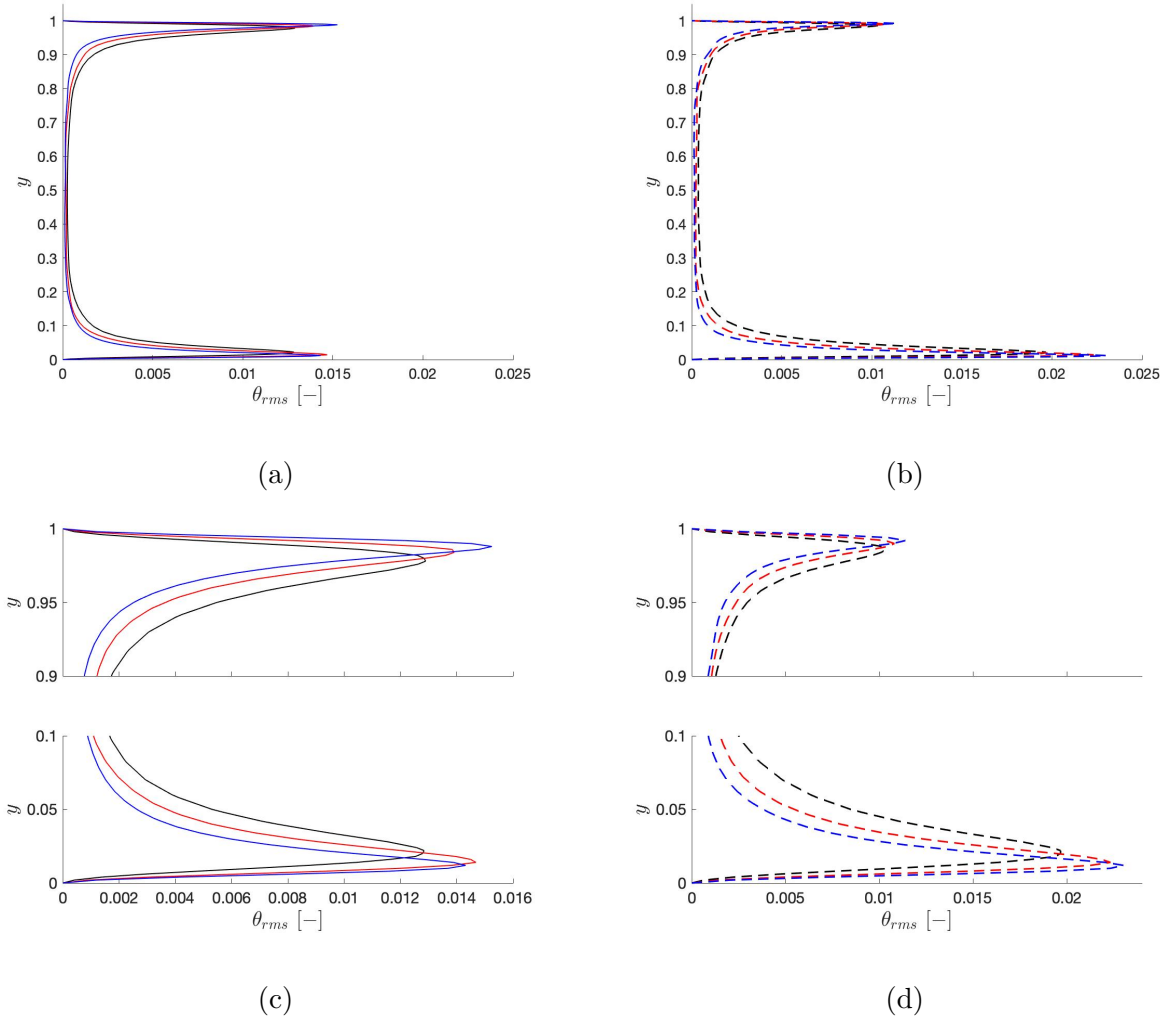


Figure 29: Non-dimensional rms temperature, θ_{rms} along the center-line. (a) Classical RBC (b) Free-slip upper boundary condition. (c) Zooms on the B.L. of the classical RBC cases. (d) Zooms on the B.L. of the free-slip cases. The legend is as follows: classical RBC (solid line) and free-slip upper boundary condition (dotted line) as well as $Ra = 2 * 10^7$ (black), $Ra = 5 * 10^7$ (red) and $Ra = 10^8$ (blue).

The root mean square temperatures, θ_{rms} of Figure 29 have higher peaks but lower mean values with increasing Rayleigh. The free-slip cases always present a lower peak at the top and a higher one at the bottom, suppressing the symmetry of the profile. Values of the boundary layer derived from θ_{rms} are presented in Table 11. The same observations as the one from earlier are seen: the thickness decreases with increasing Rayleigh and the free-slip cases have thinner thermal B.L. at the top.

RMS Velocity Profiles

For the velocity statistics we analyse the area-averaged horizontal and vertical root mean square velocities. It is important to note that the normalization used in this section is different than the one used before in order to allow a comparison between the Rayleigh numbers. Indeed, previously we used the free-fall velocity, U_f to define the non-dimensional velocity while we here use $\frac{\alpha}{h}$ where α is the thermal diffusivity.

As expected, the rms values increase when the Rayleigh number increases since the later measures the turbulence intensity. For the horizontal rms velocity, Figure 30a presents similar shapes for the various Rayleigh numbers. However, the free-slip cases do not come back to zero at the ceiling, making the classical RBC and the free-slip profiles different, especially at the ceiling of the cube. The vertical profile, on the other side, always shows a parabolic shape as one can see on Figure 30b. The free-slip case is however a bit flatter for higher Rayleigh numbers.

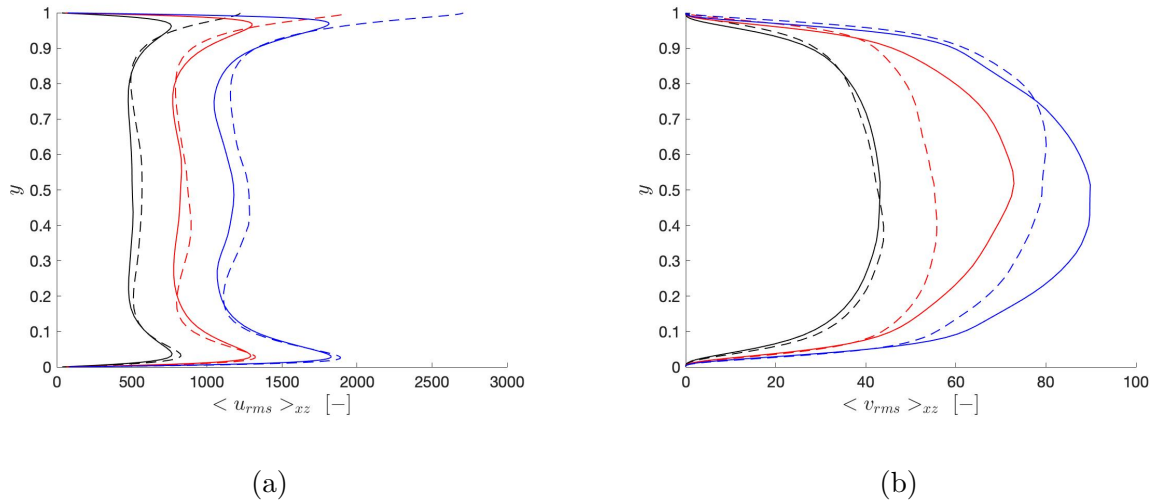


Figure 30: (a) Non-dimensional rms horizontal velocity, u_{rms} time and area-averaged. (b) Non-dimensional rms vertical velocity, v_{rms} time and area-averaged. The legend is as follows: classical RBC (solid line) and free-slip upper boundary condition (dotted line) as well as $Ra = 2 * 10^7$ (black), $Ra = 5 * 10^7$ (red) and $Ra = 10^8$ (blue).

Turbulent Heat Flux

Finally, the turbulent heat fluxes for the 6 cases analyzed are plotted in Figure 31. As expected, an increase of the Rayleigh number allows to increase the flux. The free-slip boundary condition has the same effect. The shape is identical for all 6 cases as well as

the zero value at the top and bottom walls.

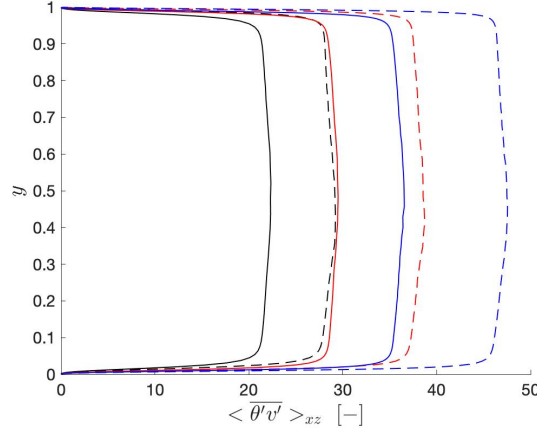


Figure 31: (a) Turbulent heat flux, $\overline{\theta'v'}$ area-averaged. (b) Zooms on the B.L. of the classical RBC cases. (c) Zooms on the B.L. of the free-slip cases. The legend is as follows: no-slip boundary condition (solid line) and slip boundary condition (dotted line) as well as $Ra = 2 \times 10^7$ (black), $Ra = 5 \times 10^7$ (red) and $Ra = 10^8$ (blue).

5.1.4 Conclusion

The temperature statistics, velocity statistics as well as the combination of temperature and velocity are in good agreement with previous studies for all the samples analyzed. Differences between the classical Rayleigh-Bénard and the free-slip cases were however noticed. Indeed, the type of boundary condition at the ceiling of the pool influences some of the profiles. First of all, the bulk temperature is colder when a free-slip upper boundary condition is used and the thickness of the thermal boundary layer is decreased. The horizontal velocity profiles have similar shapes except at the ceiling where the velocity comes back to zero for classical RBC while it does not with the free-slip condition. The horizontal and vertical rms velocities have similar values for both boundary conditions. Finally, the Nusselt number is enhanced by the free-slip condition as well as the turbulent heat flux in the bulk.

On the other side, an increase of Rayleigh number does not influence the mean and rms temperature profiles much. It only decreases the thermal boundary layer and increases the peaks of θ_{rms} . The rms velocities maintain the same shape but their magnitude is increased. The same is true for the turbulent heat flux.

5.2 Influence of a free slip upper condition on flow re-orientations

5.2.1 Introduction

Turbulent Rayleigh-Bénard convection leads to the formation of a large scale circulation, LSC, as discussed in section 5.1.1. In a cubic container, the LSC is oriented along a vertical plane containing one of the diagonals. The fluid rises on one side of the plane and sinks on the other, see Figures 17, 18 and 19. The perpendicular plane, containing the second diagonal, contains counter-rotating vortices.

It has been observed, both experimentally and numerically, that the large scale circula-

tion can spontaneously change its orientation. One of the first to discover this characteristic of turbulent Rayleigh-Bénard convection was [70] in 1996, in a cylinder containing mercury ($Pr = 0.025$). Analysis of this phenomenon has evolved since then and has been observed in different fluids within containers of various geometries. To cite a few, re-orientations have been observed in air within a cylinder [71] and in a cube [25], as well as for water inside a cylindrical container [27, 72], and in 2D rectangular geometries [73, 74]. This spontaneous change is often invoked either as re-orientation or reversal of the flow.

Experiments have allowed to distinguish two different ways for the large scale circulation to change its orientation. The most frequent one is called a rotation. It involves a rotation of the whole LSC during a certain amount of time, estimated to be around $10 T_{eddy}$. During this rotation, the LSC keeps a velocity of the same order of magnitude as when it is in a stable orientation. The other possibility is a momentary cease of the velocity of the LSC and its re-initiation from a different orientation just after. This type of reorientation is called a cessation. It is known to be quicker than a rotation, less than $1 T_{eddy}$, but also much less frequent than rotations [27, 72]. Even though both these phenomena have been observed for air and water inside cylindrical containers. Cessations have not yet been observed in cubical containers, nor for air nor for water.

While the range of possible orientations in a cylinder container is continuous, it is limited in a cubic enclosure due to the presence of angles. In a cube, the LSC can choose between 4 different orientations: alignment with one or the other diagonal and up-welling and down-welling plumes at either side of both diagonals.

The previous experiments for the various fluids and geometries have led to the discovery of several properties. First of all, the re-orientations are spontaneous and thus do not happen periodically but occur in a completely random way. By the same reasoning, the duration time of an orientation is not constant [25]. Successive rotations have been found to be independent of each other. However, it has been observed that slower rotations as well as smaller re-orientations are more frequent [27, 72]. Cessations, on the other hand, are known to be less common than rotations and the orientation following such an event is completely random. The LSC seems to have a loss of memory during a cessation.

This section therefore looks into re-orientations and aims at comparing the classical RBC case with the free-slip case for $Ra = 2 * 10^7$. The following section starts by introducing the reader to the different methods that can be used to analyze this phenomenon. Then, the results of the two cases are analyzed.

5.2.2 Measurements

The experiments and numerical simulations of previous studies have interpreted flow re-orientations by using several means. Three methods are presented here. They either use streamlines or probes.

Re-orientation of the large-scale circulation can be observed by comparing plots of instantaneous streamlines over different time ranges, supposing that a re-orientation took place in between these times. It can also be of great help to understand the transition between the two different orientations. However this does not allow to get an overview of the re-orientations happening over a long period of time.

The second method implies the use of probes. Indeed, an analysis of the vertical velocity field (or the temperature field) can also tell us about the orientation of the LSC. The LSC orients itself in one vertical diagonal plane. In this plane, the fluid rises on one

side and sinks on the other, see the upper part of Figure 18. While in the perpendicular plane, lower part of Figure 18, the counter-vortices are formed leading to vertical velocities of the same direction and magnitude on both sides of the diagonal plane. So as to identify re-orientations, a certain number of probes will be placed inside the cubical container. These probes will record the evolution of the non-dimensional vertical velocity, v , with time. This technique has been used both in experiments with thermistors [27, 72] as well as in numerical simulations [25, 73, 75]. The probes are placed at the same locations than the one used in reference [25]. Namely, 24 probes spread over 3 horizontal plane, as shown on Figure 32a. The upper and lower planes are located respectively at $y = h/4$ and $y = -h/4$ while the mid-plane corresponds to $y = 0$. Figure 32b shows one of the horizontal plane. The 8 probes are located around the azimuth at angles of $\frac{i\pi}{4}$ for $i = 1 \dots 8$ and at a distance of $0.1 h$ from the vertical walls.

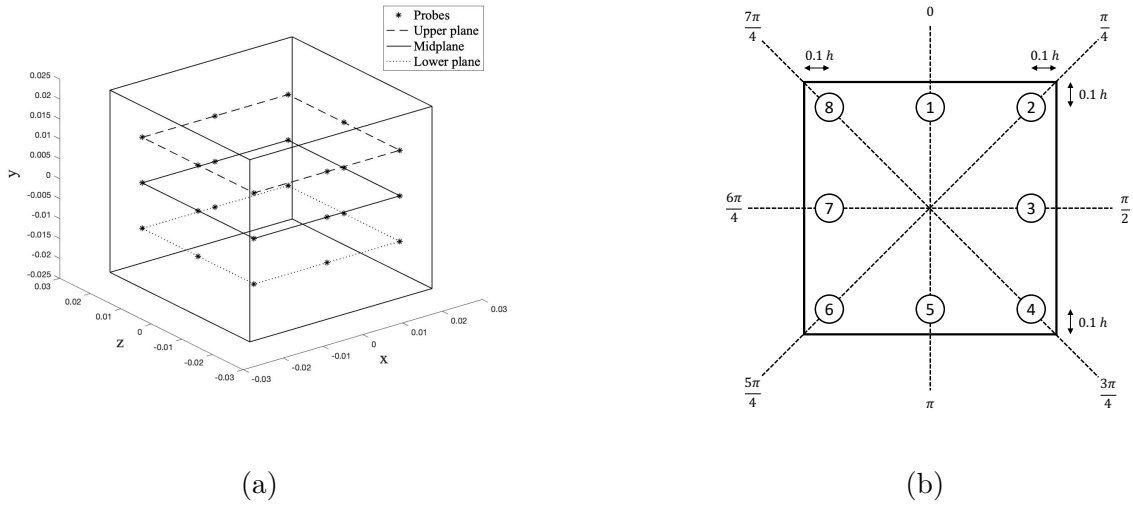


Figure 32: (a) Positions of the 24 probes inside the cube. (b) Probes position in a horizontal plane [25].

As explained before, the values of vertical velocity recorded by the probes can be directly interpreted to identify re-orientations but they can also be used to compute the angular orientation, ϕ , of the LSC and its amplitude, δ , at every time. Several models exist to compute ϕ and δ . As part of this project we use a method based on azimuthal Fourier transform, initially presented in [75] than adapted by [25]. This is the third method used to investigate flow re-orientation. Using the non-dimensional vertical velocity of each probe, v_i , and their respective azimuthal angle, θ_i , one can compute at each time t :

$$\begin{aligned}
 A_1(t) &= \frac{1}{2} \sum_{j=1}^8 v_j(t) \cos(\theta_j) & B_1(t) &= \frac{1}{2} \sum_{j=1}^8 v_j(t) \sin(\theta_j) \\
 \delta(t) &= \sqrt{A_1^2(t) + B_1^2(t)} & \phi(t) &= \text{sgn}(B_1(t)) \arccos\left(\frac{A_1(t)}{|\delta(t)|}\right)
 \end{aligned} \tag{39}$$

Changes of ϕ as function of time depict any re-orientation of the LSC while δ gives information about the amplitude of the flow.

The next section presents results for different case set ups. The results are analyzed following the methods explained hereby.

5.2.3 Results

In order to identify the various orientations of the flow, we first focus on the dynamics of the re-orientations. To do so, one can use the instantaneous vertical velocity plot as function of time at several probes, see Figure 33a for classical RBC and 33b for the free-slip case at $Ra = 2 * 10^7$. The probes used here are located in the midplane and are presented as pairs. Indeed, probes P2 and P6 are located at the tips of one diagonal plane while P4 and P8 are on the edges of the perpendicular one (see Figure 32b). Whenever the LSC is in one diagonal, the probes located on this same diagonal should record vertical velocities of the same order of magnitude but of opposite signs as illustrated on the diagonal cut of the upper part of Figure 18. The probes positioned on the perpendicular one should, on the other hand, show vertical velocities of equal magnitude and zero mean. This is characteristic of the counter-rotating vortices [25].

Using the instantaneous vertical velocity profile as a function of time for several specific locations enables us to have a first glimpse at the flow dynamics. As a matter of fact, it allows one to identify the orientations and their directions during the range of time analyzed. However, using only the data presented on Figure 33 does not allow to define correctly the starting and ending points of the re-orientations. To overcome this, a computation of the orientation ϕ and the amplitude δ of the LSC, using equation 39 based on azimuthal Fourier transform, is used. It provides another way of identifying the orientations. Moreover, this method uses the eight mid-plane probes instead of only the four diagonal ones. This should allow us to gain insight. Figure 34 therefore plots the amplitude and orientation of the LSC as a function of time for both classical RBC (34a) and the free-slip case (34b).

The combination of Figure 33 with Figure 34 helps identifying the various orientations. As part of this project, the orientations are analyzed over a bit less than 500 [s] of simulated time. This time range corresponds to 765 T_f for the cases analysed here, namely classical Rayleigh-Bénard convection and the free-slip case for $Ra = 2 * 10^7$. This time-range is relatively low compared to similar studies since this project was constraint in time. The results presented here should therefore be taken with care and longer simulations should be performed to improve the results and draw more certain conclusions.

In the classical Rayleigh-Bénard convection case (Figures 33a and 34a), we were able to identify two time-ranges during which the orientation was fixed in one of the diagonal of the cube, with a precise direction. These two are highlighted on Figure 33a by black boxes. The same was done for the free-slip case for which we could also identify two time-ranges. Figure 34 shows that there is, for both cases, a variation of 90° between the two orientations noticed. This observation is coherent with Figure 33, as in both cases, the flow changes of diagonal with a quarter twist. Previous papers, [25, 27, 72], have observed that the orientation are not happening periodically in time, that they seem to take place in a random way. They also saw that the duration of a specific orientation as well as the one of the re-orientations in between these vary over time. Finally, they observed that there does not seem to be any link between successive orientations of the LSC. Even though, we do not have results over a sufficient time range to clearly observe all these characteristics of the flow re-orientation, we can still see that our results agree with them.

On Figure 33a, the first orientation highlighted by a black box is going from $t \approx 0$ to 200 [s]. During this period, the LSC is in the vertical diagonal plane containing probes P2 and P6, as they record a vertical velocity of the same order of magnitude but of opposite

signs. The direction, as seen from the top, is going from probe P6 to probe P2. Indeed, the flow has an upward (positive) velocity at probe P6 while it is going downward (negative) at probe P2. At the floor of the cube, the flow is obviously going in the opposite direction, from P2 to P6. The same kind of reasoning can be used to define the flows orientation at different time as well as for the free-slip case.

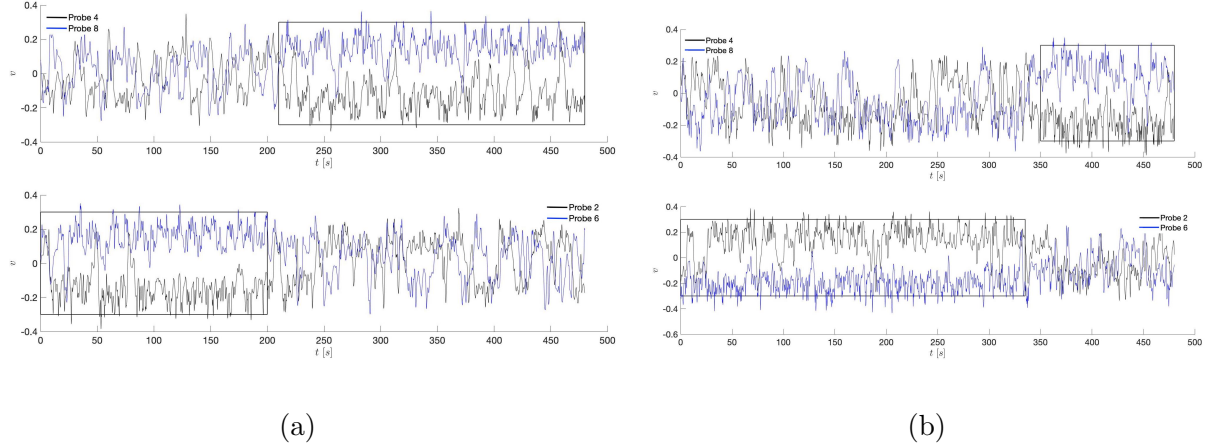


Figure 33: Instantaneous non-dimensional vertical velocity as function of time for four mid-plane diagonal probes. (a) Classical Rayleigh-Bénard convection. (b) Free-slip boundary condition.

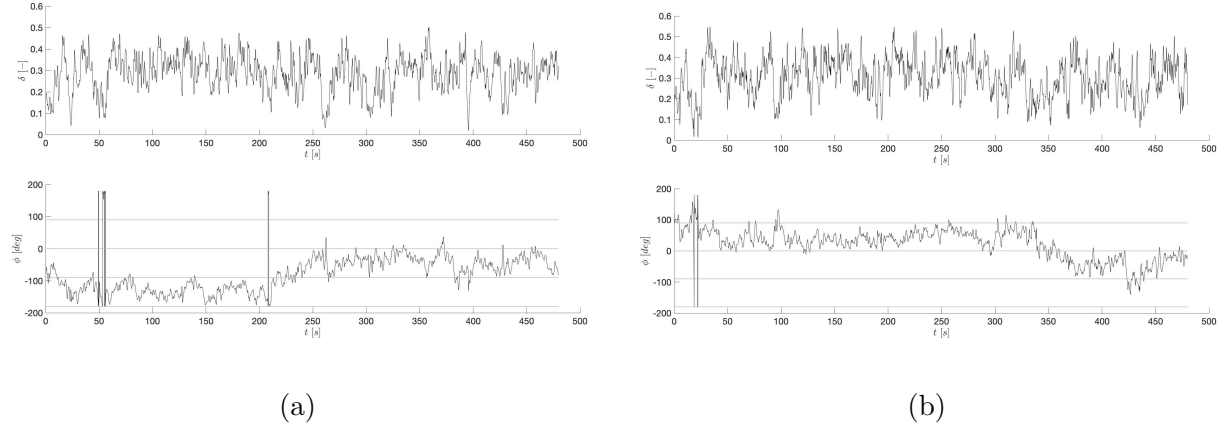


Figure 34: Amplitude δ [–] and angular orientation ϕ [deg] of the LSC as function of time (computed using equation 39). (a) Classical Rayleigh-Bénard convection. (b) Free-slip boundary condition.

The lower and upper probes can be used to further analyze the flow over time. Indeed, on Figures 35 and 36, one can see, respectively probes P4 and P8 as well as probes P2 and P6 in the upper ($y = h/4$) and lower ($y = -h/4$) planes for classical RBC (a) and the free-slip case (b). In the upper plane, one can see that the flow has a value oscillating between -0.2 and 0 , while in the lower plane the value fluctuates between 0 and 0.2 . In the upper plane, sometimes positive peaks take place, while negative ones are present in the lower one. These peaks are due to the impingement of the LSC at the top or the bottom of the geometry. Peaks are therefore mainly present on the probes positioned in the LSC plane.

Once again, the time ranges of probable orientations have been highlighted by black boxes for the diagonal plane containing the LSC. The first one of the classical RBC case, going from $t \approx 0$ to 200 [s], is investigated more deeply in Figure 36a. As discussed previously, the LSC presents a mirror symmetry across the height of the cube. The impingement of the LSC at the top is therefore near probe P6 with an upward velocity while it is not far from probe P2 with a downward velocity at the bottom. Peaks are therefore present in Figure 36a for the time-range of interest while nothing remarkable takes place in Figure 35a as the LSC is not passing by probes P4 and P8.

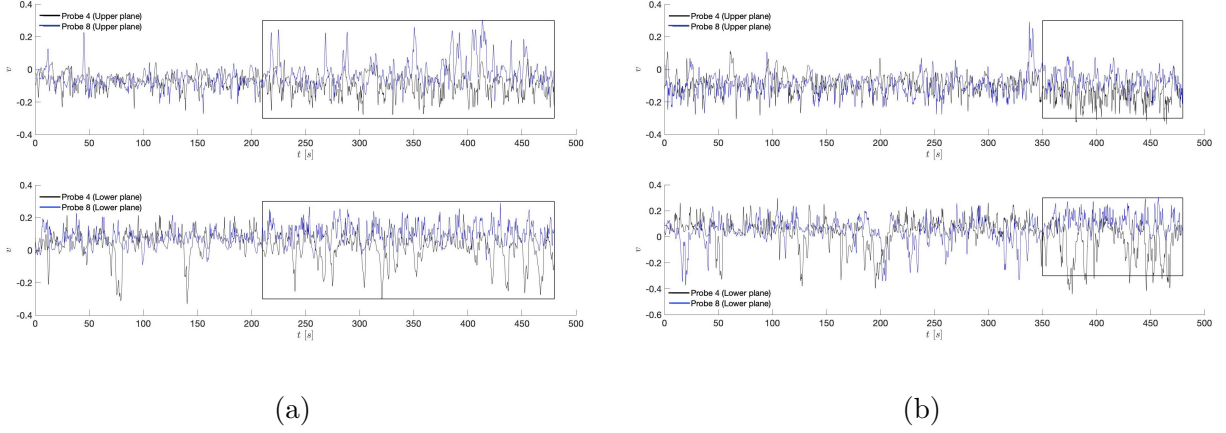


Figure 35: Instantaneous non-dimensional vertical velocity as function of time for upper and lower probes P4 and P8. (a) Classical Rayleigh-Bénard convection. (b) Free-slip boundary condition.

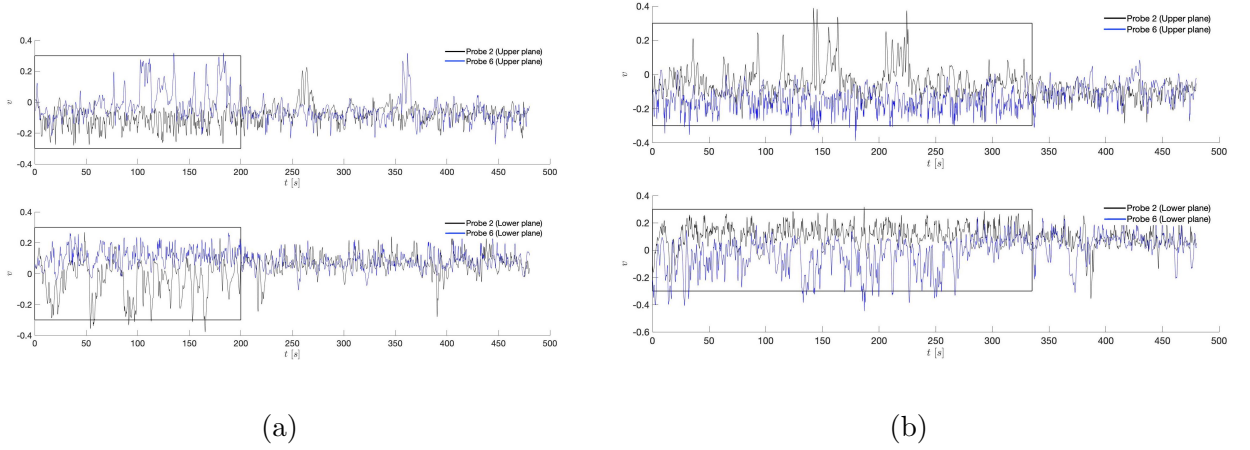


Figure 36: Instantaneous non-dimensional vertical velocity as function of time for upper and lower probes P2 and P6. (a) Classical Rayleigh-Bénard convection. (b) Free-slip boundary condition.

Finally, streamlines representing the velocity over the time-ranges identified hereby allow for a better understanding of the flow. Indeed, Figure 37 plots streamlines, viewed from the top of the cube for the two orientations of the classical RBC case (37a and 37b) and the ones of the free-slip case (37c and 37d). The corner are marked with the corresponding probes numbering. As a matter of fact, one can see that the flow for classical RBC from 0 to 200 [s] comes in near corner P6, extends mainly to P2 and a bit less to P4

and P8 (to form the counter-rotating vortices). This corresponds to the analysis performed with the mid-plane probes. Similar observations can be seen for the other orientation as well as the ones from the free-slip case.

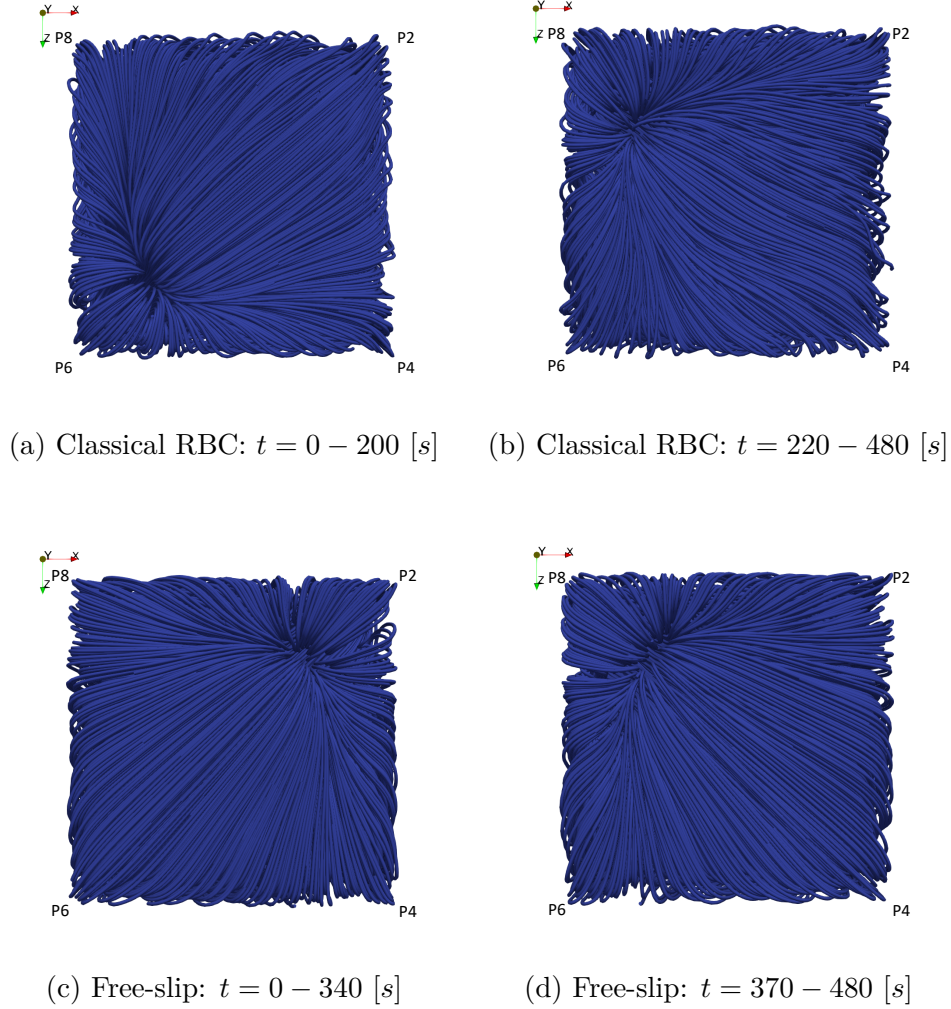


Figure 37: Time-averaged velocity streamlines seen from the top of cube for different orientations of the flow. (a) and (b) Classical RBC. (c) and (d) Free-slip boundary condition.

One can also see that between the 1st and 2nd orientations taken by the flow, the structure performs a 90° clockwise and anticlockwise rotation respectively for the classical RBC and the free-slip case which is in accordance with Figure 34. The velocity streamlines during these rotations are plotted in Figure 38. One can see that the transition between two different orientations involves an impingement line instead of a spot. This line is in-between probes P6 and P8 for classical RBC while it is between P2 and P8 for the free-slip case. At the tip of the line, two small back-eddies are formed [25].

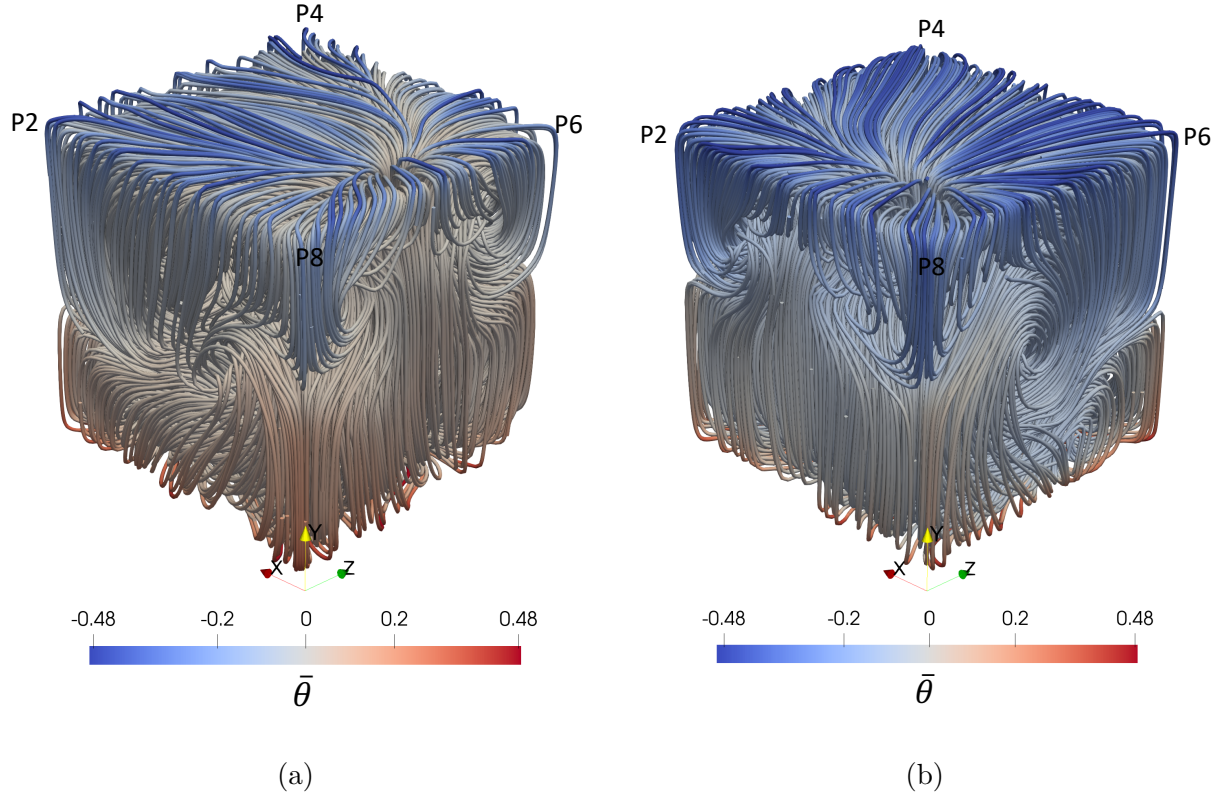


Figure 38

Even though, the analysis concerning re-orientations is not definitive due to a restricted simulation time, we were able to observe one re-orientation in the two cases under study. It is important to point out that such a phenomenon had never been observed in Rayleigh-Bénard convection with an upper free-slip boundary condition. Three different methods were used to numerically measure the orientation of the flow: measurement of the vertical velocity using probes, use of the azimuthal Fourier transform to obtain ϕ , the angular orientation of the LSC and plots of the flow streamlines. The outcomes from these three techniques were coherent with each other. As flow re-orientations are still poorly understood today, further investigation will be needed to better understand the phenomenon.

6 Conclusion

This paper has investigated the natural convection of water in nuclear spent fuel pools by means of numerical study. It started by pointing out the hazards linked to nuclear spent fuel pools. Indeed, as long as nuclear energy is used, nuclear spent fuel is created. This spent fuel generates heat and radioactivity during years after it is removed from the nuclear reactor. The nuclear spent fuel must therefore be managed thoroughly for some considerable time. Spent nuclear fuel pools play an important role in this management as they enable to store the spent fuel underwater. The water acts as a shield against the radiation emitted by the fuel and as a coolant to evacuate the heat given off by the fuel. However, the pool itself necessitates maintenance which is performed throughout a cooling and cleanup system. If anything was to happen that would lead to a decrease of the pool water level (leak, shut-down of the cooling system, etc.), the consequences would be dramatic. Such catastrophes have happened in the past, the most well-known being the Fukushima disaster.

In order to gain insight on the flow of water as well as the heat transfer taking place inside the pool, a simplified model of the pool was developed. The major simplifications are: the evaporation at the surface was neglected, the fuel rods were replaced by a flat hot plate at the bottom of the pool, the lateral walls were considered as perfectly insulated while the geometry was assumed to be a perfect cube.

This simplified model was used to run several simulations using OpenFOAM. The goal of those simulations was to compare the influence of a classical Rayleigh-Bénard convection case with a free-slip case (closer to the spent nuclear fuel pool). The classical Rayleigh Bénard Convection case has a no-slip boundary condition at the upper wall which corresponds to having a fixed horizontal wall at the ceiling of the cube while the free-slip case allows one to model a free-surface at the top of the pool. The two cases were compared in terms of the formation of a Large Scale Circulation, their statistical profiles and their re-orientation characteristics. The statistical profiles of both cases were also analyzed for increasing Rayleigh numbers.

The simulations were performed using an existing OpenFOAM solver, *lowMachBuyont-PimpleFoamWater*, which uses a PISO algorithm to solve the low Mach number equations. Turbulence was added to the case using a Large Eddy Simulation.

Both the classical RBC case (no-slip upper boundary condition) and the free-slip one presented a Large Scale Circulation in one of the vertical diagonal plane with counter-rotating vortices in the perpendicular plane for $Ra = 2 * 10^7$. Even though the two cases seemed to have the same flow structure, the magnitude of the velocity was higher for the free-slip case while the temperature in the bulk of the cube was lower.

A statistical analysis of $\bar{\theta}$, θ_{rms} , $\bar{u}$, $\bar{v}$, $\bar{w}$, u_{rms} , v_{rms} and $\overline{\theta'v'}$ along the center-line or area-averaged over horizontal slices, allowed us to notice several differences between the two types of boundary conditions. First of all, the free-slip upper boundary condition influences the bulk temperature inside the geometry, which becomes colder than the mean temperature, while the classical RBC has a bulk temperature equal to its mean temperature. The thermal boundary layer is also thinner at the top compared to the bottom while they are similar in classical RBC. Furthermore, the rms temperature presents peaks, near the edges, of the same order of magnitude in classical RBC while the upper one is decreased and the lower one increased with the free-slip condition. The horizontal

velocities and rms velocities have similar shapes except at the ceiling where they are allowed to have a non-zero value in the free-slip sample. All the profiles mentioned so far presented a symmetry along the mid-height axis in classical RBC. This symmetry is lost when the free-slip condition is applied. The rms vertical velocity keeps a similar shape and magnitude in both cases. The turbulent heat flux has an analogous profile but a higher magnitude and finally, the Nusselt number is increased in the free-slip case as compared to classical RBC.

An increase of the Rayleigh number, on the other hand, does not influence the profiles shape, neither in classical RBC nor with a free surface. The bulk temperature is similar for all Rayleigh numbers having the same boundary conditions. Concerning the mean temperature profiles, however, a reduction of the thermal boundary layer with increasing Rayleigh number is noticed as well as an increase of the rms peaks. The rms horizontal and vertical velocities are increased as the turbulence rises. Similar conclusion can be drawn for the turbulent heat fluxes and Nusselt numbers.

Finally, an analysis of the flow re-orientations for classical RBC and the free-surface case was done. Both flows presented one rotation of 90° over a time-range of about 500 [s]. It should be noted that re-orientations had never been observed in Rayleigh-Bénard convection with a free-slip upper boundary condition before. However, the knowledge concerning such phenomenon must still be enhanced to gain a better understanding of it.

Some improvements could be added to this work. Indeed, the pool model could be improved to be even closer to reality by removing some of the assumptions made in this project. Furthermore, a longer time-range should be used for the re-orientation analysis in order to be able to draw more consistent conclusions. Indeed, a computation of the mean re-orientation time as well as the determination of the existence of a preferred orientation would be a first step into a better comprehension of the phenomenon.

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