

École polytechnique de Louvain

Numerical study of turbulent thermal convection in water pools of different aspect ratios and different heat loadings

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1 Conventions of writing

ρ	Density [$\frac{kg}{m^3}$]
T	Temperature [$^{\circ}C$]
P	Pressure [Pa]
h	Enthalpy [$\frac{J}{kg}$]
μ	Dynamic viscosity [$\frac{kg}{m.s}$]
ν	Kinematic viscosity coefficient [$\frac{m^2}{s}$]
k	Conductivity constant [$\frac{W}{m.K}$]
$\hat{\phi}$	dimensional value of ϕ
u	Horizontal velocity [$\frac{m}{s}$]
v	Vertical velocity [$\frac{m}{s}$]
w	Depth velocity [$\frac{m}{s}$]
<u>vector</u>	Vector (single underscore)
<u>tensor</u>	Tensor (double underscore)
$\underline{v}$	velocity vector [$\frac{m}{s}$]
$\hat{n}$	Base vector for the direction of the boundary
c_p	Constant pressure calorific capacity [$\frac{W}{kg.K}$]
c_v	Constant volume calorific capacity [$\frac{W}{kg.K}$]
γ	[$\frac{c_p}{c_v}$]
H	Height of the geometry [m]
g	Constant of gravitation on earth [$\frac{m}{s^2}$]
$\underline{\underline{I}}$	Identity matrix
$\underline{\underline{S}}$	the strain rate tensor $\frac{1}{2} (\nabla \underline{v} + (\nabla \underline{v})^T)$
$\underline{\underline{S}}^d$	deviatoric part of the strain rate tensor $\frac{1}{2} (\nabla \underline{v} + (\nabla \underline{v})^T - \frac{2}{3} (\nabla \cdot \underline{v}) \underline{\underline{I}})$
$\underline{\underline{\tau}}$	Tensor of constraints [$\frac{kg}{m.s^2}$]
Re	Reynolds number [-]
Pr	Prandtl number [-]
Gr	Grashov number [-]
Ray	Rayleigh number [-]
Nu	Nusselt number [-]
Ri	Richardson number [-]
C	Courant number [-]

2 Introduction

Natural convection is a fundamental process that plays a significant role in various engineering and environmental scenarios. Such a flow is present in nature (e.g. atmospheric convection) and employed in industrial applications. One important application is the phenomenon of natural convection occurring in a spent fuel pool, a key component of nuclear power plants. A spent fuel pool serves as a temporary storage facility for nuclear fuel assemblies that have been used in reactor cores. These assemblies generate intense heat due to the residual radioactivity of the fuel, necessitating effective heat removal mechanisms to ensure both safety and optimal pool operation. This work is linked with the thermal convection occurring in a spent fuel pool. In this Master thesis we propose a numerical study of turbulent thermal convection in domains of different aspect ratios. A software code is used to solve the Navier Stokes equation applied to natural convection. Different aspect ratios will be investigated for two different Rayleigh number: $Ra = 10^7$ and $Ra = 5 \cdot 10^7$. This work is separated in three parts. First some context around spent fuel pool, a loss-of cooling accident and the phenomena of Rayleigh natural convection is provided. A second part will present the model we will use, the equations involved and give a presentation of the numerical algorithm that is applied. A third part will present the numerical results.

3 Context

3.1 Nuclear Energy Use in the World and Future Development

Nuclear energy is mainly used to produce electricity through nuclear power plans. As shown in Figure 1, it produces about 10% of the electricity generated in the world. Looking at his development history (Figure 2), it shows a strong development after the 1970s corresponding to the reaction of the oil shocks which had a large impact on countries like France who had relied heavily on oil for electricity production. The Chernobyl disaster of 1986 altered the development of nuclear power plants. The total production of nuclear electricity has remained quite stable since the early 2000s. While some countries like Germany have decided to reduce their electricity generation with nuclear power plants, other countries like China are investing a lot, with 24 units under construction [3], they lead the world in building nuclear power plants today.

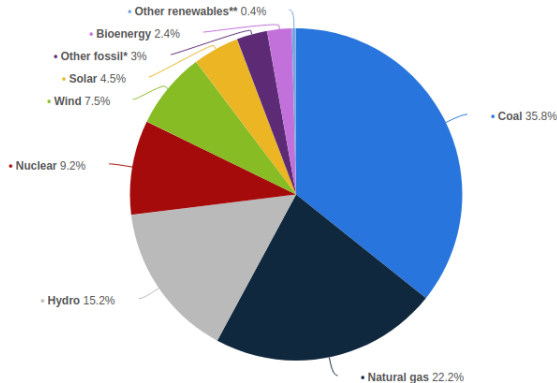


Figure 1: World gross electricity production by source [1]

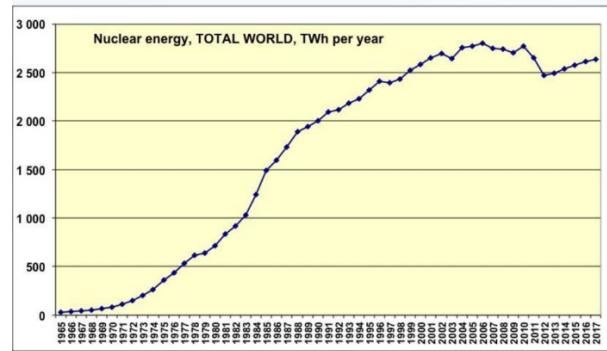


Figure 2: Nuclear production in the world per year [2]

Despite this slow down in development, nuclear energy has some major advantages to consider

regarding future developments: it is a low CO₂ emission and controllable energy source, and it doesn't require a lot of space and materials as it is an extremely dense energy source. For this reason, nuclear can be an interesting tool to reduce climate change. Most mitigation scenarios of the group III of IPCC [4] include an increase in nuclear electricity production. Despite its advantages, nuclear energy has its drawbacks: it produces nuclear waste which need long term treatment, it needs high investments and is a very long term industry. It also requires a lot of safety rules and expertise to be safe. As producing nuclear energy is complex and mainly used to produce electricity, it can't replace all the uses of fossil fuels but is mainly a competitor of coal. But if the world would like to use nuclear energy much more massively in a long term sustainable way, some technological gaps need to be closed. Indeed almost all reactors use the isotope 235 of uranium which is present at a concentration of 0.7% in the natural uranium extracted from the mines, but the amount on earth can eventually become a limit. Future reactors under development called Generation IV reactors aim at also using the isotope 238 or thorium as nuclear fuel. This would in theory increase the amount of potential nuclear energy by a lot, more than all fossil fuels available on earth.

3.2 Nuclear Power Plan Cycle

Nuclear power plan produces electricity from the fission of uranium. Today, most of them use the technology of PWR (pressurized water reactor). Schematically it has three main circuits of water. First the fuel is made by uranium enrichment using a centrifuge to have a higher concentration of U-235 uranium. In the reactor neutrons will cause the fission of the uranium atoms which will release heat and other neutrons which will cause the fission of other atoms of uranium keeping the reaction going. In order to provoke this fission of other atoms those neutrons need to be slowed down by a moderator, usually by water of the primary circuit which is used as both the coolant and neutron moderator. The heat will warm up the water of the primary circuit and this water is pressurized to stay liquid, the liquid of the primary circuit then flows to a steam generator, where it transfers its thermal energy to a lower pressure water of a secondary circuit system where steam is generated. As the water of this primary circuit goes through the reactor, it becomes radioactive by neutron activation [6], the reactor and the steam generator are thus in a containment structure (see figure 3). The secondary circuit undergoes a steam cycle: it receives heat from the steam generator, heats up isobarically from liquid to steam then undergoes an expansion producing mechanical work to drive a turbine which spins an electric generator. The water is then cooled down in a condensor and once cooled liquid is brought back to a higher pressure through a pump. The third circuit will evacuate the heat from the condensor. In case of using a river as cooling source, a cooling tower is used to release as much heat as possible to the air before putting the water back in to the river.

3.3 Waste Management and Spent Fuel Pool

There is a large variety of radioactive waste from nuclear power plan broadly classified into three categories [7](see Figure 4): low-level waste, such as tools and clothing used by employees, which contain small amounts of mostly short-lived radioactivity, intermediate-level waste (ILW), like steel components from within the reactor. These are more dangerous because they contain higher amounts of radioactivity and require some shielding, and finally high-level waste (HLW), which is highly radioactive and warm, so it requires shielding but also cooling. This high-level waste represents only a small volume of the total radioactive waste but contains the majority of the total radioactivity. This comes mostly from the spent nuclear fuel and is produced mainly by two processes : the product of fission created after the fission of the uranium U-235 and actinides created

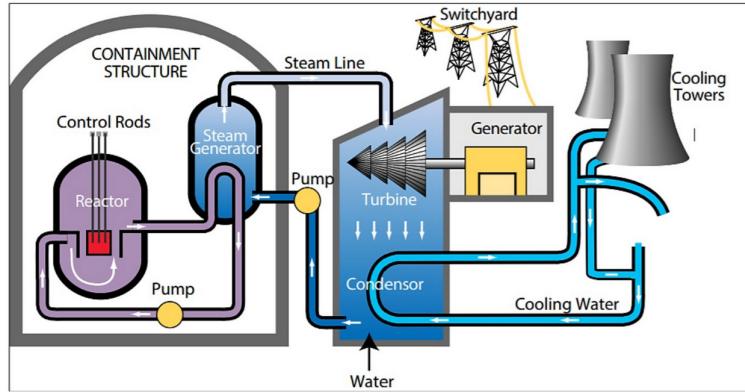


Figure 3: Nuclear power plan [5]

by neutron capture [8]. The fuel assemblies are made by long tubes (see figure 5). The fuel rod cladding is made with zirconium alloy because of its low neutron capture and resistance to corrosion properties. Inside the tubes the fuel is pelleted, a large pressurized water reactor typically has 150-250 fuel assemblies, each containing 200-300 fuel rods.

Types of Nuclear Waste

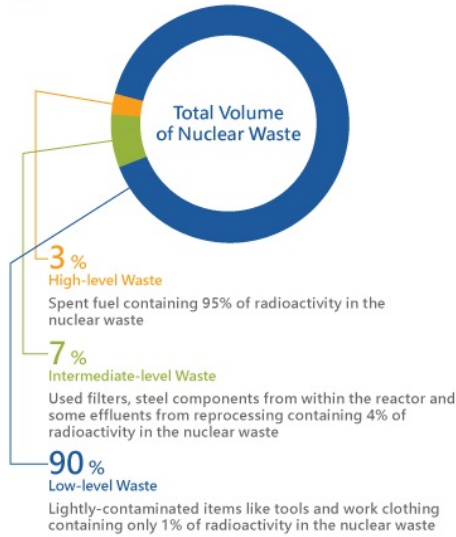


Figure 4: classification of nuclear waste [9]

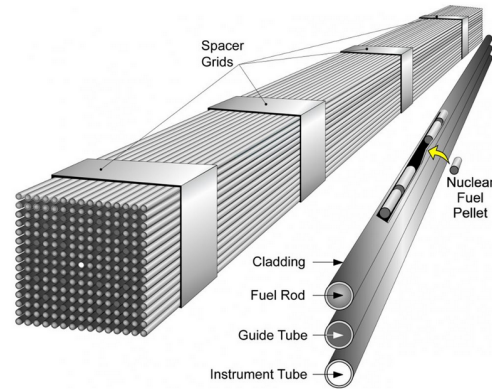


Figure 5: Fuel assembly composed mainly with fuel rods and few guide tubes for mechanical strength and one instrument tube in the middle to insert measurement instruments. [10]

Once used in the reactor, then removed this spent fuel releases thus still a lot of heat and radioactivity that make it dangerous and necessitate storage in a spent fuel pool first for at least one year. These pools are located directly on the site of nuclear power plan to make it possible to transfer this dangerous spent fuel from the reactor to the pool directly. They are used for short-term cooling of the fuel rods to allow the short-lived isotopes to decay and thus reducing the radiation and decay heat emanating from the rods. It is then possible to move the spent fuel to another location where the waste can be treated, melted and stored in dry containers and eventually stored geologically at high depth. The water of the pool acts both to cool and protect from radioactivity as water is an efficient shield against radioactivity. The water of the pool is constantly being cooled

actively to maintain it below $50\text{ }^{\circ}\text{C}$ using pumps and heat exchangers so it needs electrical power supply. The bottom is equipped with metal storage racks (see Figure 7) at the bottom to hold fuel assemblies that are removed from the reactors in a vertical position.

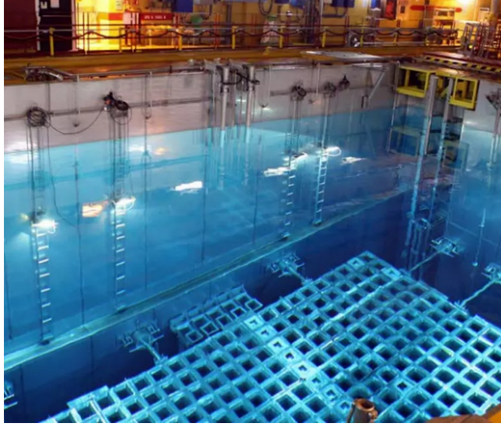


Figure 6: spent fuel pool [11]

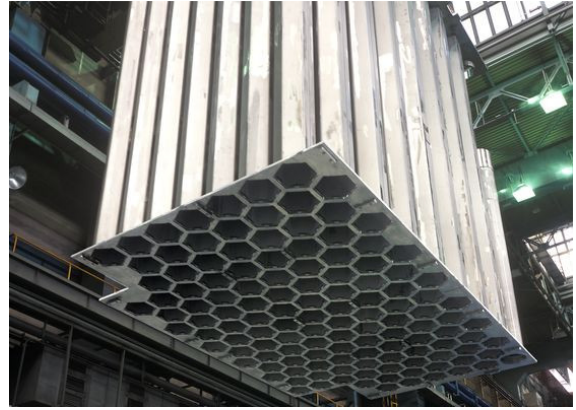


Figure 7: racks disposed at the bottom of the pool [12]

Several designs of storage racks have been used, nowadays to store a high density of fuel assemblies. Power plants employ solid stainless steel holder walls with plates of neutron absorbers based on inserted bore to prevent criticality issues of uncontrolled fission chain reaction (definition of criticality in [18]). There is a hole at the bottom and the top of the storage rack to allow convection of water but it doesn't allow cross-flow.

3.4 Loss-of-cooling Accident in a Spent-fuel-pool

The management and safety of spent nuclear fuel plays a crucial role in the operation of nuclear power plants. Accidents such as loss-of-coolant accident can occur either by sudden leakage loss of the pool water inventory or by loss of Cooling Accident (LOCA) if the cooling system stops working or is not efficient enough. The LOCA accident is a slower process and this work is related with this type of accident. It can be partitioned into three temporal phases showed in Figure 8.

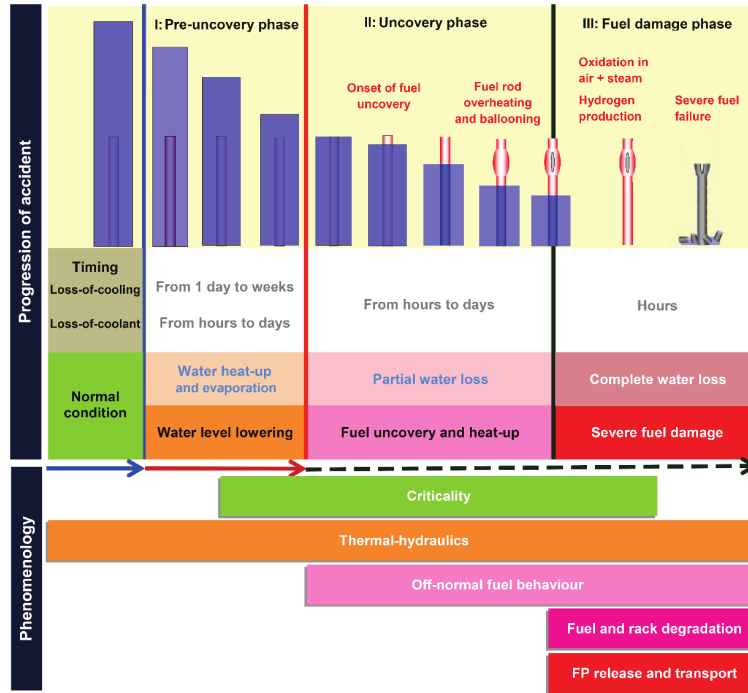


Figure 8: Temporal phases and phenomenology of SFP loss-of-cooling/coolant accidents [15]

During the pre-uncovery, phase, the spent fuel assemblies (FAs) are still covered with water but the water heats up and natural convection loops develop in the pool, the evaporation rate increases at the free surface and as a result the level of water decreases. Several safety issues are concerned during this phase. Boiling mechanism can occur, mainly by wall heterogeneous nucleation on heated structures at the top of the fuel assemblies (see Figure 9). The boiling phenomena has several potential consequences. It increases the production of hydrogen from the pool water because hydrogen produced by radiolysis of water increases in boiling compared with non-boiling conditions [16]. The bubbles breaking the free surface increase the release rate of radionuclides contaminants coming from activated corrosion products deposited on the spent fuel, leaking fuel rods or tritium carried over from the reactor cooling circuit to the pool during refueling. Subcriticality may also eventually be lost (critical accident phenomenology is explained in [17]) especially if the pool contain fresh fuel. The increase void fraction by boiling or a decrease of soluble boron concentration (in case of refueling the pool with non bored water for example) reduces the subcriticality margin. Furthermore the increase in water temperature promotes cavitation phenomena in the pumps of the cooling system and the drop of water level may increase the radiation field around the pool that would access to the spent fuel pool building which makes the accident more and more difficult to handle over time.

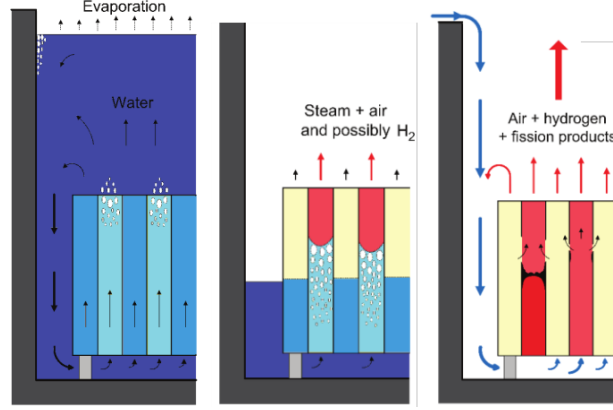
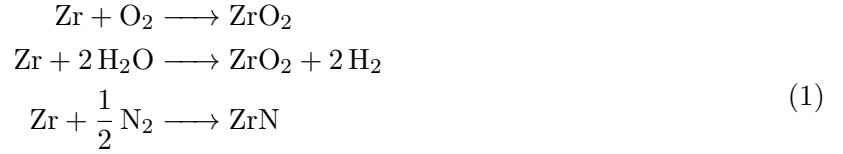


Figure 9: From left to right: Pre-uncovery phase, Uncovery phase and Fuel damage phase [15]

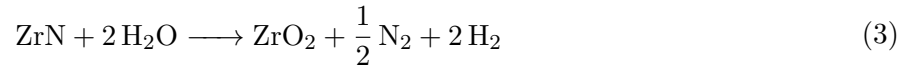
During the Uncovery Phase, parts of the rods start to be uncovered but the steam flow from the evaporation will still cool the uncovered parts but as the water level drops, the peak temperature of the cladding at the top of the uncovered part increases because less steam is produced by boiling in the bottom part and the steam overheating is increased along the uncovered length. The higher temperature during the uncovery phase will accelerate the cladding creep under the internal gas overpressure in the fuel rod and the temperature will also promote the cladding oxidation of the Zirconium alloy. It undergoes the following oxydation reactions in parallel [15]:



The last two above equations mainly occur in the absence of oxygen or oxygen starvation. If oxygen recovery occurs, the additional so-called back reactions will take place:



Under presence of steam without oxygen the zirconium nitride ZrN will be oxidised:



We can thus observe that during the oxidation, hydrogen is released and deflagration of this hydrogen is a risk of explosion in the building of SPF. This oxidation is exothermic so it is also an extra source of heat release and at high temperature it can become self sufficient leading to the fully consuming of fuel rod cladding in a short time period if sufficient oxygen is available. This is called zirconium cladding fire [14]. Critical risk is also increased for the same reasons as the pre-uncovery phase but also because some racks are made with neutron absorbing materials that can degrade at a lower temperature than the stored fuel assemblies. Once all the water has evaporated natural convection of air will still provide some cooling to the spent fuel. A large scale flow pattern develops in the building, air goes from below the racks and by heating up moves to the ceiling (see Figure 8). The integrity of the ventilation inside the pool building is crucial to evacuate the hot air on the ceiling to enhance the effect of the natural convection. But overall the natural air convection cooling is not sufficient [13], as can be seen on figure 8 when only natural convection occur the

LOCA enter in the fuel damage phase which has an order of magnitude of hours length so it is in any case an absolute emergency. Furthermore, the end of the uncover phase is a very dangerous moment, when the water nearly completely uncovers the storage racks, when only the bottom inlets of the rack cells are immersed. At this specific stage the water is no longer in direct contact with the heat loading so the water heats up less and generates less steam to cool the above fuel assembly but also the water prevents the circulation of air. So, at that moment the fuel temperature increases very quickly. This situation can also happen when refilling a complete empty SFP during a loss of cooling accident.

Finally during the fuel damage phase rod integrity is lost by cladding creep rupture and excessive oxidation (see Figure 8) and debris will relocate downward and obstruct the natural convection flow of air. Volatilisation of fission products will occur. The more heated the fuel assembly, the more fission volatile those products are and it will be maximum if the fuel assembly melts. Further contamination of these fission products to the environment outside the pool building are different for an SFP located inside the reactor containment building than for a SFP outside the containment building. Overall a loss of cooling accident in a spent fuel pool is slower and less immediately urgent than an accident in the reactor. This explains why before the Fukushima disaster, relatively little attention had been paid to SFPs and research was more focused on accidents in the reactor. The Fukushima disaster of 2011 has raised awareness concerning the security of nuclear spent fuel pools.

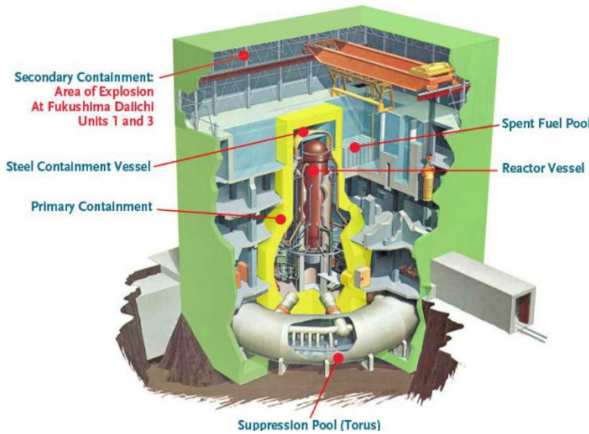


Figure 10: Schematic of the reactor building at Fukushima [20]

On March 11, 2011, an earthquake occurred on the east coast followed by a tsunami. During the earthquake the rods stopped the reaction in the reactor, the electricity supply from the network grid was lost, diesel generator took over to supply the electricity needed to cool the plant but the tsunami drowned them and produced a station blackout from unit 1 to unit 4. Fuel melting appeared in 3 unit reactors (unit 4 was in maintenance and thus shut down), hydrogen was generated in the reactors and moved out of the containment structure and exposed in the reactor building (see Figure 10) damaging the ceiling (hydrogen explosion in unit 4 may have come from hydrogen leaking from unit 3). Emergency action was first focused on cooling the reactor but quickly the loss of cooling of the spent fuel pools also became an issue and emer-

gency water injection was conducted by using a helicopter, a concrete pump truck and a fire truck, the water decreased up to about 1.5 meter above the storage racks [14]. With the damaged ceiling open to air environment, extra dramatic release of radioactivity coming from the pool was avoided by a small margin. So, the Fukushima accident brought to the forefront that accidents in SFP also pose major risks to the environment and need more safety. More research was needed highlighted by [15] to fully understand the accident phenomenology to improve safety. At UCLouvain, SFP LOCA [19] is a research project to advance the state of the art in the modelling and simulation of the phenomena that take place during a Loss of Coolant Accident (LOCA). This work is linked with the natural convection of water occurring above the racks during the pre-uncovery phase.

3.5 Rayleigh Natural Convection in a Spent Fuel Pool

In the context of a loss of cooling accident, Rayleigh natural convection phenomena plays a vital role in maintaining temperature safety within the spent fuel pool.

Natural convection is the situation for which there is no forced velocity but a free convection current exists within the fluid due to a body force (usually the gravity) acting on the fluid in which there are density gradients (usually due to a temperature gradient). Generally, density of liquid and gases decreases with temperature: $\frac{\partial \rho}{\partial T} < 0$ which is usually expressed with the thermal expansion coefficient $\beta = -\rho \frac{\partial \rho}{\partial T} \Big|_p$ [1/K]. Natural convection is driven by buoyancy forces that must overcome the viscous forces of the fluid in order to create the convection movement, to characterize the phenomena we use the Grashof number that is defined as the ratio between buoyancy forces and viscous forces:

$$Gr = \frac{g\beta\Delta TL^3}{\nu^2} \quad (4)$$

Where g [m/s^2] is the gravitational acceleration, β [1/K] is the thermal expansion coefficient, ΔT [K] the temperature difference L [m] the characteristics length and ν [m^2/s] the kinematic viscosity. This number is obtained by nondimensionalizing the momentum equation along the vertical in a laminar boundary layer flow and taking into account the gravity term in, as in the book [21] (dimensional variables have been denoted with a hat symbol $\hat{\cdot}$ and dimensionless variables without it, as during the main part of the work dimensionless variables are used the simple notation is kept for them):

$$\hat{\rho}\hat{u}\frac{\partial \hat{v}}{\partial \hat{x}} + \hat{\rho}\hat{v}\frac{\partial \hat{v}}{\partial \hat{x}} = -\frac{d\hat{p}}{d\hat{y}} - \hat{\rho}g + \hat{\mu}\frac{\partial^2 \hat{v}}{\partial^2 \hat{y}} \quad (5)$$

and then using the approximation of Boussinesq by simplifying $\hat{\rho}(\hat{T}) \approx \hat{\rho}_\infty - \beta(\hat{T} - \hat{T}_\infty)$ for the density in the gravity term, the other density keeping constant $\hat{\rho}_\infty$ and approximating $-\frac{d\hat{p}}{d\hat{y}} \approx \hat{\rho}_\infty g$ we have :

$$\hat{u}\frac{\partial \hat{v}}{\partial \hat{x}} + \hat{v}\frac{\partial \hat{v}}{\partial \hat{y}} = g\beta(\hat{T} - \hat{T}_\infty) + \hat{\nu}\frac{\partial^2 \hat{v}}{\partial^2 \hat{y}} \quad (6)$$

Then by nondimensionalizing we obtain:

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = \frac{g\beta(T_s - T_\infty)L}{u_{ref}^2}\theta + \frac{1}{Re_L}\frac{\partial^2 u}{\partial^2 y} \quad (7)$$

It is convenient to choose $u_{ref} = \sqrt{g\beta(T_{hot} - T_{cold})L}$, so that the term multiplying θ^* becomes unity (so from the course of Fluid Mechanics I at UCL [22] it corresponds to the case where the buoyancy is counterbalanced by the inertia of the fluid). Then, Re_L becomes $[g\beta(T_s - T_\infty)L^3/\nu^2]^{1/2}$ and thus $Gr = Re_L^2$. The Grashof plays the same role in free convection as the Reynolds number plays in forced convection. The ratio $\frac{Gr}{Re_L^2}$ is used to compare the effects of free and forced convection (Re_L is calculated using the characteristic speed of the forced convection), when $\frac{Gr}{Re_L^2} \ll 1$ the natural convection can be neglected, when $\frac{Gr}{Re_L^2} \gg 1$ the forced convection can be neglected and when $\frac{Gr}{Re_L^2} \approx 1$ both effects need to be taken into account. Usually in practice, it is the Rayleigh number that is used instead of the Grashof number. The Rayleigh number is defined as the product of the

Grahsof number with the Prandtl number (which is defined as the ratio between the momentum diffusivity and thermal diffusivity and equal to $\frac{\mu/\rho}{k/(\rho c_p)}$):

$$Ra = \frac{g\beta\Delta TL^3}{\alpha\nu} \quad (8)$$

Thermally driven convection occurs in many geophysical, astrophysical and industrial processes. In the Earth's atmosphere and oceans, the thermally driven convection is a major source of determining weather patterns and currents in the ocean. Rayleigh-Bénard convection is a case of natural convection occurring in a horizontal layer of fluid heated from below and cooled from above. The Rayleigh number of natural convection will characterize three main regimes. The Rayleigh number uses $L = H$ where H is the height of the convection domain and $\Delta T = T_{hot} - T_{cold}$. At a very low Rayleigh number the buoyancy forces don't overcome the viscous forces and the fluid does not present a movement convection, it is stable and the heat transfer occurs by conduction. When the Rayleigh increases convection starts to take place in a laminar form and presents a pattern of circular convection cells (see Figure 11), first discovered by Henri Bénard, that can take various shapes.

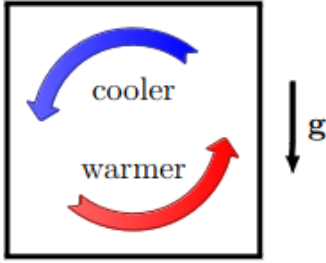


Figure 11: Schematic of a Rayleigh-Bénard convection cell [24]

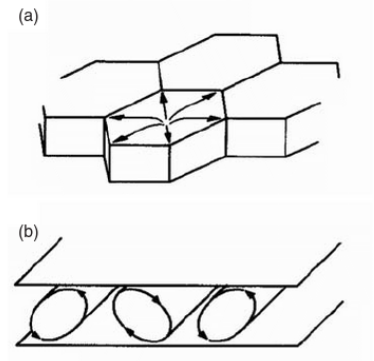


Figure 12: a) Hexagonal convection cells and b) Convection rolls [25]

The specific pattern and organization of the convection cells also called large scale circulation (LSC) depend on various factors, including the physical properties of the fluid, the temperature gradient applied, the geometry of the domain and the boundary conditions. The primary pattern observed by Bénard in his experiment in 1900 [23] is a regular arrangement of hexagonal cells. Each cell consists of an upward flow of fluid in the center, surrounded by a downward flow along the cell boundaries. These cells form a repeating pattern across the entire fluid layer. However, depending on the parameters of the system, different patterns can emerge like rolls (see Figure 12). If the Rayleigh number is further increased, the convection becomes turbulent but the average flow can still present large scale circulation. In this work we are interested in the turbulent natural convection during a loss of cooling accident (see figure 13). A simplified model of the pool will be used to focus on the large scale circulation above the racks for different aspect ratios of the pool.

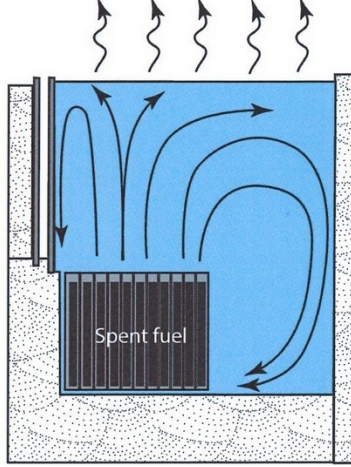


Figure 13: natural convection above the racks [19]

4 Model and Presentation of the Code

4.1 Case Setup

The spent nuclear fuel pool is represented, in this work, by a cuboid. The objective of this work is to vary the aspect ratio of the dimensions. The center $(0,0,0)$ is at a corner of the floor (see Figure 14). The dimensions are the height H along the axis y , the width W along the axis x and the length L along the axis Z . The cube contains three different types of boundaries.

- The floor represents the interaction of water with the storage racks containing the fuel and is thus at a high temperature T_{hot} (Dirichlet boundary conditions). Regarding the velocity it is considered a fixed wall so $\underline{v} = 0$ (Dirichlet boundary conditions).
- The ceiling representing the surface of the pool is thus a fixed temperature T_{cold} (Dirichlet boundary conditions). The velocity boundary condition is a free slip so $\frac{\partial u}{\partial y} = 0$, $\frac{\partial w}{\partial y} = 0$ and $v = 0$.
- The sidewalls are considered adiabatic so $\frac{\partial T}{\partial x} = 0$ on the sides perpendicular to the x axis and $\frac{\partial T}{\partial z} = 0$ on the sides perpendicular to the z axis (Von Neuman boundary conditions).

As a result of these boundary conditions there are three hydrodynamic boundary layers (one on each vertical side and one on the floor) and two thermal boundary layers (on the floor and

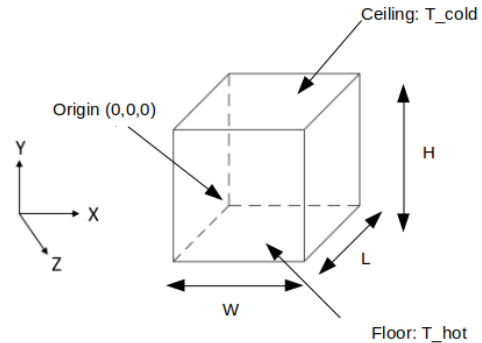


Figure 14: Schematic of the model

on the ceiling). About the initiale temperature distribution it is simply linearized $T(x, y, z) = T_{hot} - \hat{x} \frac{T_{hot} - T_{cold}}{W}$

4.2 Governing Equations and Low Mach Number Approximation

The objective is to simulate a RBC occuring in a Rectangular cuboid representing the model of a spent fuel pool heated from below and cooled from above. Classically the RBC is modeled using oberbeck-boussinecq simplification like in 3.5 where the density variations are neglected except for the term of the buoyancy in the momentum equation where the density varies linearly with the temperature starting from a reference (ρ_0, T_0) and with a coefficient $\beta = -\frac{1}{\rho_0} * \frac{\partial \rho}{\partial T}$ in [1/K] such that $\rho = \rho_0 * (1 - \beta(T - T_0))$. However, the simulations done in this work uses a more precise model, the low-Mach number approximation explained in [28] which is presented here. First, we remind the continuity, momentum and energy equation:

$$\frac{D\hat{\rho}}{D\hat{t}} + \hat{\rho} \nabla \cdot \hat{\underline{v}} = 0 \quad (9)$$

$$\hat{\rho} \frac{D\hat{\underline{v}}}{D\hat{t}} = -\nabla \hat{P} + \nabla \cdot \hat{\underline{\underline{\tau}}} + \hat{\rho} \underline{\underline{g}} \quad (10)$$

$$\hat{\rho} \frac{D\hat{h}}{D\hat{t}} = \frac{D\hat{P}}{D\hat{t}} + \hat{\underline{\underline{\tau}}} : \hat{\underline{\underline{S}}} + \nabla \cdot (\hat{k} \nabla \hat{T}) \quad (11)$$

with $\hat{h}$ the enthalpie equal to $\hat{c}_p \hat{T}$

By nondimensionalization these three equations using $x = \frac{\hat{x}}{l_{ref}}$, $v = \frac{\hat{v}}{v_{ref}}$, $\rho = \frac{\hat{\rho}}{\rho_{ref}}$, $T = \frac{\hat{T}}{T_{ref}}$, $\mu = \frac{\hat{\mu}}{\mu(T_{ref})}$, $c_p = \frac{\hat{c}_p}{c_p(T_{ref})}$, $c_v = \frac{\hat{c}_v}{c_v(T_{ref})}$, $P = \frac{\hat{P}}{P_{ref}}$ such that $P_{ref} = \rho_{ref} T_{ref} \frac{R}{M_r}$ with R the perfect gas constant and M_r the molar mass we recall that $\frac{R}{M_r} = c_p - c_v$, $\gamma = \frac{c_p}{c_v}$ the reference Mach number is $M = \frac{v_{ref}}{c_{ref}}$ with c the speed of sound which is equal to $\sqrt{\gamma \frac{p}{\rho}}$ for an isentropic process of an ideal gas and $\hat{t} = \frac{t}{l_{ref}/v_{ref}}$ we obtain:

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \underline{v} = 0 \quad (12)$$

$$\rho \frac{D\underline{v}}{Dt} = -\frac{1}{\gamma M^2} \nabla P + \frac{1}{Re} \nabla \cdot \underline{\underline{\tau}} + \frac{l_{ref}}{v_{ref}^2} \rho \underline{\underline{g}} \quad (13)$$

$$\rho \frac{DT}{Dt} = \frac{\gamma - 1}{\gamma} \frac{DP}{Dt} + \frac{(\gamma - 1)M^2}{Re} \underline{\underline{\tau}} : \underline{\underline{S}} + \frac{1}{Pr Re} \nabla \cdot (k \nabla T) \quad (14)$$

We can see that reference Mach number appears in the nondimensionalized equations. At low mach number we can analyse those equations by considering the Mach number as a perturbation parameter. As the Mach number is at the denominator in the momentum equation it implice a singular perturbation analysis. We define the perturbation parameter $\epsilon = \gamma M^2$ and we expanding the flow variables in power series of $\epsilon = \gamma M^2$ to expand the equations around the point of singularity :

$$P = P^0 + \epsilon P^1 + O(\epsilon^2) \quad (15)$$

$$v = v^0 + \epsilon v^1 + O(\epsilon^2) \quad (16)$$

$$\rho = \rho^0 + \epsilon \rho^1 + O(\epsilon^2) \quad (17)$$

$$T = T^0 + \epsilon T^1 + O(\epsilon^2) \quad (18)$$

We replace those expansions in equations (12),(13) and (14) and taking into account that $\epsilon \ll 1$ so we neglect $O(\epsilon)$ and $O(\epsilon^2)$ and that γM^2 already appears in these equations. In (13) γM^2 is at the denominator of ∇P so this means that at order $O(1/\epsilon)$ equation (13) yields $\nabla P^0 = 0$, P^0 is thus invariant in space, it is the thermodynamic pressure spatially uniform which will be equal to $P_{atm} = 1013$ hPa in this work, the term P^1 is the dynamic pressure and will remain in equation (13) at order $O(1)$. P^0 is called thermodynamique pressure because by insterting the expansions in the equation of state only P^0 will remain at low mach number. In (14) as there is no M^2 appearing next to $\frac{D\hat{P}}{Dt}$ it is mainly the thermodynamic pressure which appears. The term $\underline{\tau} : \underline{S}$ is multiplied by M^2 so it is neglected. We finally obtain the following low Mach approximation:

$$\frac{D\rho^0}{Dt} + \rho^0 \nabla \underline{v}^0 = 0 \quad (19)$$

$$\rho^0 \frac{D\underline{v}^0}{Dt} = -\nabla P^1 + \frac{1}{Re} \nabla \cdot \underline{\tau}^0 + \frac{l_{ref}}{v_{ref}^2} \rho^0 \underline{g} \quad (20)$$

$$\rho^0 \frac{DT^0}{Dt} = \frac{\gamma - 1}{\gamma} \frac{DP^0}{Dt} + \frac{1}{PrRe} \nabla \cdot (k \nabla T^0) \quad (21)$$

Which are the equations that will be solved numerically as we will investigate an open domain P^0 will be equal to the ambient pressure and $\frac{DP^0}{Dt} = 0$ and will be removed in the rest of this work. Strictly speacking this derivation has been obtained assuming an ideal gaz law of state but the general analysis can also be done for different law of state, ?? derived using a more general approache. Overall intuitively the low mach number approximation neglect the vriations of density due to pressure but not due to temperature.

As a last remark, the code stores a referential pressure equal to $\rho_{ref} u_{ref}^2$ which isn't equal to the above P_{ref} but it still make sense because we have to keep in mind that the expansion variables in equations (15), (16), (17) and (18) are dimensionless so the total pressure is : $\hat{P}_{total} = \hat{P}_{ambient} + \epsilon P_1 P_{ref}$ but $\epsilon = \frac{\rho_{ref} u_{ref}^2}{P_{ref}}$ so the code will solve the dimensionless P^1 that we can use with the stored $\rho_{ref} u_{ref}^2$ to have :

$$\hat{P}_{total} = \hat{P}_{ambient} + \rho_{ref} u_{ref}^2 P^1 \quad (22)$$

4.3 Fluid and Reference Properties

The fluid properties μ, ρ, c_p, k and the thermal varies with temperature, they are calculated using a polynomial fit $\sum_{i=0}^7 a_i T^i$ over the range of temperature $(T_{hot} - 5)$ to $T_{hot} + 5$. The coefficients a_i are obtained using a small python script and the module XSteam [30]. The reference temperature is taken as $T_{ref} = \frac{T_{hot} + T_{cold}}{2}$. With this reference temperature we can obtain the references $\mu_{ref} = \mu(T_{ref})$, $\rho_{ref} = \rho(T_{ref})$, $c_{p,ref} = c_p(T_{ref})$, $k(T_{ref})$ and $\beta(T_{ref})$ with them we obtain the Prandtl:

$$Pr = \frac{\mu_{ref} / \rho_{ref}}{k_{ref} / (\rho_{ref} c_{p,ref})} \quad (23)$$

The free-fall velocity as explained in section 3.5:

$$U_f = \sqrt{\beta_{ref}(T_{hot} - T_{cold})gH} \quad (24)$$

And the free fall time T_f

$$T_f = \frac{H}{U_f} \quad (25)$$

4.4 Finite Volume Method

In order to solve the equations we will use in this work the finite volume method for a collocated grid. Let us briefly remind ourselves of the finite volume method for a collocated grid. The domain is subdivided into a finite number of small control volumes for a collocated grid where both the scalars and velocity values are stored in the center of each control volume cells. The method uses the integral form of the conservation equations. The three equations (mass, momentum and energy) can be expressed in the form of the general transport equation integrated over a domain Ω for a quantity ϕ :

$$\int_{\Omega} \frac{\partial \rho \phi}{\partial t} d\Omega + \underbrace{\int_{\Omega} \nabla \cdot (\rho \phi \underline{v}) d\Omega}_{\text{convective term}} = \underbrace{\int_{\Omega} \nabla \cdot (\Gamma \nabla \phi) d\Omega}_{\text{diffusive term}} + \int_{\Omega} \text{Source}(\phi) d\Omega \quad (26)$$

Where Γ is the diffusion coefficient and Source_{ϕ} the source term. The solution domain uses a grid to divide the domain into a finite number of control volumes cells, and the conservation equations are applied to each one.

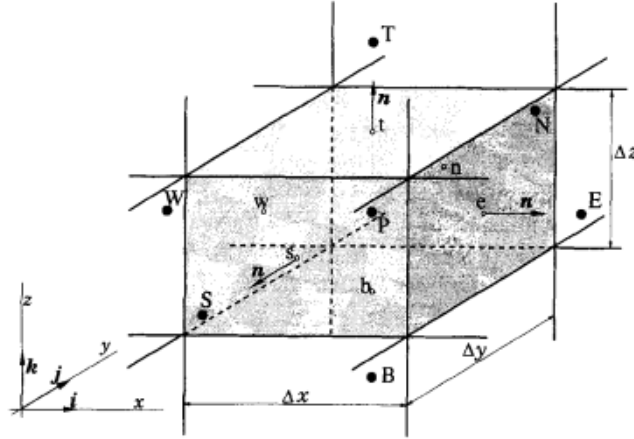


Figure 15: A typical Control Volume (CV) cell and the notation used for a Cartesian 3D grid [26]

The variable ϕ is calculated at a computational node P situated at the centroid of each control volume representing the average value over the control volume V_c :

$$\phi_P = \frac{1}{V_c} \int_{V_c} \phi(x) dV_c \quad (27)$$

By applying the divergence theorem on the convective and diffusive term we obtain:

$$\int_{V_c} \frac{\partial \rho \phi}{\partial t} dV_c + \underbrace{\int_{S_c} \rho \phi \underline{v} \cdot \underline{n} dS_c}_{\text{convective term}} = \underbrace{\int_{S_c} \Gamma \nabla \phi \cdot \underline{n} dS_c}_{\text{diffusive term}} + \int_{V_c} \text{Source}(\phi) dV_c \quad (28)$$

Where S_c is the total surface of the boundary of the control volume. The net flux through this surface is the sum of integrals over V_c faces (there are six faces in the case of Figure 15):

$$\int_{S_c} \underline{f} \cdot \underline{n} \, dS_c = \sum_k \int_{S_{c_k}} \underline{f} \cdot \underline{n} \, dS_{c_k}, \quad (29)$$

where the vector $\underline{f}$ is either the convective term $(\rho\phi\underline{v})$ or diffusive term $(\Gamma\nabla\phi)$ and $\underline{n}$ the normal to the V_c face surface. To calculate the surface integral in equation (29) exactly, we would need to know the value of $\underline{f}$ everywhere on the surface S_c . But only the volume center values at P are calculated so a double approximation must be introduced. We approximate the surface integral as a product of the cell-face center value $\underline{f}_{S_{c_k}-center} \cdot \underline{n}_{S_{c_k}-center}$:

$$\int_{S_{c_k}} \underline{f} \cdot \underline{n} \, dS_{c_k} \approx \underline{f}_{S_{c_k}-center} \cdot \underline{n}_{S_{c_k}-center} S_{c_k}. \quad (30)$$

So we also need to further approximate $\underline{f}_{k-center}$ with an interpolation of the known nodal values at the V_c 's center. Several ways exist for this approximation, the most common are presented in the book [26]. More detail for the approximation used for the simulation of this work is presented in section 4.6. An approximation is also needed for the integrals over V_c of equation (28), a simple approximation of the term on the left is $\int_{V_c} \frac{\partial\rho\phi}{\partial t} dV_c \approx (\frac{\partial\rho\phi}{\partial t})_P V_c$ and the source term is often approximated as $\int_{V_c} Source_\phi dV_c \approx Source_C V_P + Source_P V_P \phi_P$ (which is obtained by a double approximation, first $Source(\phi) \approx Source_C + Source_P \phi$ and then using approximation of Taylor $\phi(\underline{x}) \approx \phi_P + (\underline{x} - \underline{x}_P) \cdot \nabla\phi_P$ and taking advantage that the point P is at the center of mass of V_c so $\int_{V_c} (\underline{x} - \underline{x}_P) dV_c = 0$, combining those results we obtain $\int_{V_c} Source dV_c \approx Source_C V_c + Source_P V_c \phi_P$). As a result for one cell control volume of the grid we obtain:

$$\begin{aligned} & \left(\frac{\partial(\rho\phi)}{\partial t} \right)_P V_P + \sum_k (\rho\phi\underline{v})_{S_{c_k}-center} \cdot \underline{n}_{S_{c_k}-center} S_{c_k} = \\ & \sum_k (\Gamma\nabla\phi)_{S_{c_k}-center} \cdot \underline{n}_{S_{c_k}-center} S_{c_k} + (Source_C V_P + Source_P V_P \phi_P) \end{aligned} \quad (31)$$

Furthermore for a rectangular parallelepiped cartesian 3D grid with each cell of dimension Δx , Δy and Δz like in figure 15 we have $V_c = \Delta x \Delta y \Delta z$ and (using the notations e,w,n,s,t and b like on figure 15) $\sum_k \underline{f}_{S_{c_k}-center} \cdot \underline{n}_{S_{c_k}-center} \cdot S_{c_k} = (\underline{f}_e - \underline{f}_w) \cdot \underline{e}_1 \Delta y \Delta z + (\underline{f}_n - \underline{f}_s) \cdot \underline{e}_2 \Delta x \Delta z + (\underline{f}_t - \underline{f}_b) \cdot \underline{e}_3 \Delta x \Delta y$ so we can divide left and right sides of equation 31 by V_c to obtain :

$$\begin{aligned} & \left(\frac{\partial(\rho\phi)}{\partial t} \right)_P + \frac{(\rho\phi\underline{v})_e - (\rho\phi\underline{v})_w}{\Delta x} \cdot \underline{e}_x + \frac{(\rho\phi\underline{v})_n - (\rho\phi\underline{v})_s}{\Delta y} \cdot \underline{e}_y + \frac{(\rho\phi\underline{v})_t - (\rho\phi\underline{v})_b}{\Delta z} \cdot \underline{e}_z = \\ & \frac{(\Gamma\nabla\phi)_e - (\Gamma\nabla\phi)_w}{\Delta x} \cdot \underline{e}_x + \frac{(\Gamma\nabla\phi)_n - (\Gamma\nabla\phi)_s}{\Delta y} \cdot \underline{e}_y + \frac{(\Gamma\nabla\phi)_t - (\Gamma\nabla\phi)_b}{\Delta z} \cdot \underline{e}_z + (Source_C + Source_P \phi_P) \end{aligned} \quad (32)$$

Which is the final form that we will use in this work. By applying this result to each control volume cell, one obtains an algebraic equation for each control volume, and by further using the spatial discretization in each equation, a number of neighbor nodal values appear in each equation, we put all those equations into a linear system $\mathcal{A}\Phi = \mathcal{B}$ that we can resolve using linear algebra. More details about the spatial and time discretization and the inter cell face center interpolation (at points e, w, n, s, t and b) used in this work and the general algorithm is provided in section 4.6.

4.5 Mesh Refinement

In order to solve the previous equations and obtain the field values of all the flow elements, the pool model is modeled by a cuboid form which is discretized using a rectangular mesh. As explained in section 4.1 the convection presents boundary layers at the boundaries, so the mesh needs to be small enough to capture correctly this physical phenomena. In order to achieve this, the grid is non-uniform and finer near the boundaries and to calculate the coordinates of the corners of the grid along one axis with a resolution of N cells along this axis the code uses an hyperbolic tangent expansion function which gradually increases the cell's dimensions from the wall towards the center with the following formula for a certain length (which is the height H in our case):

$$\begin{aligned} coordinate_j &= -\frac{length}{2} \frac{\tanh(\beta_{grid} \frac{round_{down}(N/2)-j}{round_{down}(N/2)})}{\tanh(\beta_{grid})} + \frac{length}{2} \quad \text{for } j=0,1,\dots,round_{down}(N/2) \\ coordinate_j &= \frac{length}{2} \frac{\tanh(\beta_{grid} \frac{j-round_{up}(N/2)}{round_{up}(N/2)})}{\tanh(\beta_{grid})} + \frac{length}{2} \quad \text{for } j=round_{up}(N/2),\dots,N \end{aligned} \quad (33)$$

By using this formula, we ensure that the first coordinate of corners of the grid will start at zero, and finish at the end of the length. The higher the constant β_{grid} will be the smaller the cells close to the boundaries will be and the larger the cells in the center will be. The cells of the cooling pool domain are in blue on Figure 16 with the coordinates of their corners calculated with formula (33) and we also add one extra layer of cells (in red in Figure 16) which has the same dimensions as the adjacent blue cell. These red virtual cells in Figure 16 are used to implement the boundary conditions explained in section 4.1. More details about their implementation is provided in section 4.6.

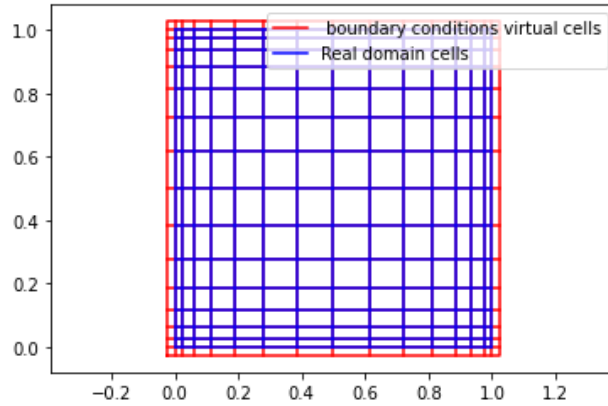


Figure 16: example image of the mesh in 2D when $\beta_{grid} = 1.5$ and $N=14$

To create the grid we need thus to decide the number of points N and the expansion constant coefficient β_{grid} , for this we created a small python script that gives us the β_{grid} which follows the same procedure as in [32]. The procedure is explained below:

1. calculate an approximation of the boundaries layer width using formulas from [31] which approximate the boundaries layers turbulent Rayleigh–Bénard (RB) convection :

$$\begin{aligned}
& 0.5 \, Nu^{-1} \, Pr^{1/2} \, A^{-1} \, \pi^{-1/2} \, H & \text{for } Pr < 3 * 10^{-4} \\
\delta_u = & 0.5 \, Nu^{-1} \, Pr^{0.357-0.022\log(Pr)} \, H & \text{for } 3 * 10^{-4} \leq Pr \leq 3 \\
& 0.5 \, Nu^{-1} \, Pr^{1/3} \, E^{-1} \, H & \text{for } Pr > 3 \\
& \delta_u \, A \, \sqrt{\pi} \, Pr^{-1/2} \, A & \text{for } Pr < 3 * 10^{-4} \\
\delta_{th} = & \delta_u \, Pr^{-0.357+0.022\log(Pr)} & \text{for } 3 * 10^{-4} \leq Pr \leq 3 \\
& \delta_u \, E \, Pr^{-1/3} & \text{for } Pr > 3
\end{aligned} \tag{34}$$

With $A \approx 0.332$ and $E \approx 0.982$ and H the height of the domain. The Prandtl Pr used is calculated at T_{ref} as said in section 4.3. As we don't know the Nusselt Nu in advance we use a correlation [32]: $Nu = 0.178Ra^{0.301}$.

2. Again from [31] we approximate the minimum number of cells required in the boundary layers:

$$\begin{aligned}
& = \sqrt{2} \, a \, Nu^{1/2} \, Pr^{-1/4} \, A^{1/2} \, \pi^{1/4} & \text{for } Pr < 3 * 10^{-4} \\
Nu = & \sqrt{2} \, a \, Nu^{1/2} \, Pr^{-0.1785+0.011\log(Pr)} & \text{for } 3 * 10^{-4} \leq Pr \leq 1 \\
& = \sqrt{2} \, a \, Nu^{1/2} \, Pr^{0.3215+0.011\log(Pr)} & \text{for } 1 \leq Pr \leq 3 \\
& = \sqrt{2} \, a \, Nu^{1/2} \, Pr^{1/3} \, E^{1/2} & \text{for } Pr > 3
\end{aligned} \tag{35}$$

$$\begin{aligned}
& = \sqrt{2} \, a \, Nu^{1/2} \, Pr^{-3/4} \, A^{3/2} \, \pi^{3/4} & \text{for } Pr < 3 * 10^{-4} \\
N_{th} = & \sqrt{2} \, a \, Nu^{1/2} \, Pr^{-0.5355+0.033\log(Pr)} & \text{for } 3 * 10^{-4} \leq Pr \leq 3 \\
& = \sqrt{2} \, a \, Nu^{1/2} \, Pr^{-0.0355+0.033\log(Pr)} & \text{for } 1 \leq Pr \leq 3 \\
& = \sqrt{2} \, a \, Nu^{1/2} \, E^{3/2} & \text{for } Pr > 3
\end{aligned} \tag{36}$$

3. Then we also need to estimate the bulk grid width minimal requirement. The natural convection we study is turbulent. As explained in the book of Pope [33], turbulence can be considered as composed of eddies of different sizes characterised by a size l , a velocity $u(l)$ and a timescale $\tau(l) = l/u(l)$. The kinetic energy enters the turbulence at the largest scale l_0 (comparable to the overall flow characteristic which is H in our natural convection case) and break up transferring their energy to smaller eddies, those smaller eddies undergo a similar break-up process to yet smaller eddies until dissipation by viscous action of the kinetic energy occurs at the smallest scales called Kolmogorov scales. This process is called the energy cascade. Each eddy has a Reynold number $Re(l) = \frac{u(l)l}{\nu}$ that will decrease during the energy cascade until viscosity is effective. The rate of dissipation ϵ is determinated by the first process's transfer of energy from the largest eddies l_0 . These eddies have kinetic energy of order u_0^2 and timescale of order $\tau_0 = u_0/l_0$ so the rate of transfer of energy ϵ can be supposed to scale as $\sim u_0^2/\tau_0 = u_0^3/l_0$ and this transfert of energy is nearly constant through the energy cascade. So for a given eddy size l we can estimate the velocity scales as $u(l) \sim (\epsilon l)^{1/3} \sim u_0(l/l_0)^{1/3}$ and $\tau(l) \sim (l^2/\epsilon) \sim \tau_0(l/l_0)^{2/3}$. We can thus observe that $u(l)$ and $\tau(l)$ decrease as l decreases confirming that $Re(l)$ decreases as the eddies become smaller. The $Re(l)$ of the eddy will decrease until the viscosity effect is no longer negligible, the lengthscale l_{DI} separates the inertial subrange where viscous effects are negligible and the dissipation range (see Figure 17). The production $\mathcal{P}$ appear explicitly mathematically with a negative sign in the the

mean-kinetic-energy equation. The action of the mean velocity gradients working against the Reynolds stresses removes kinetic energy from the mean flow ($\mathcal{P}$ appear as a negative term) and transfers it to the fluctuating velocity field. Full derivations is done in chapter 5 of the book of Pope [33].

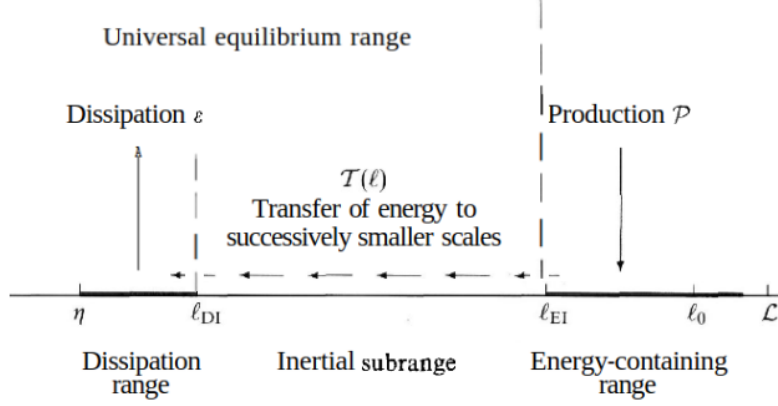


Figure 17: schematic diagram of the energy cascade [33]

As ν is an important parameter of the viscous dissipation, Kolmogorov suggested [34] that the smallest scales of turbulence are universal (similar for each turbulent flow) and that they depend only on ν and ϵ , this idea and dimensional analysis provide an expression for the smallest eddies, the Kolmogorov scales η :

$$\begin{aligned} l_\eta &= (\nu^3/\epsilon)^{1/4} \\ u_\eta &= (\epsilon\nu)^{1/4} \\ \tau_\eta &= (\nu/\epsilon)^{1/2} \end{aligned} \tag{37}$$

We can observe that $Re_\eta = 1$ confirms the viscous effects presence. Similarly temperature turbulence fluctuation presents also microscales called Batchelor scales η_θ [35]. If $Pr > 1$ $\eta_\theta < \eta$ and if $Pr < 1$ $\eta_\theta > \eta$. In order to simulate accurately all the scale of motions using Navier-Stokes equations, the method used is Direct Numerical Simulation (DNS) which resolves all the eddies regardless of their size, the mesh maximum bulk size l must thus be smaller than the smallest between the Kolmogorov scales and Batchelor scales, an estimation of this maximum grid size in the bulk can be computed using Pr, Ra and Nu [36]:

$$\begin{aligned} l_{scale} &= \pi H \left(\frac{Pr^2}{Ra Nu} \right)^{1/4} \quad \text{for } Pr \leq 1 \\ l_{scale} &= \pi H \left(\frac{1}{Pr Ra Nu} \right)^{1/4} \quad \text{for } Pr > 1 \end{aligned} \tag{38}$$

This DNS approach is computationally very expensive. In this work we use the large eddies simulation (LES) approach which resolves the large scales and the smaller scales are modeled.

The computational grid is designed to have sufficient resolution to capture the large turbulent eddies explicitly but it is limited in size and cannot resolve all turbulent structures down to the smallest scales (subgrid-scale eddies). Instead, they are modeled using subgrid-scale models. More discussion about the LES method is provided in section 4.7. As LES can have a lower resolution we can multiply the required length l by a factor of 4 as in [45] where comparison of DNS and LES with a less precise mesh has been done. Thus we require 4 times l as minimal width for a cell in the bulk. An alternative LES resolution requirement is to match the filtering cutoff width to the Taylor microscale, which for isotropic turbulence is defined as $\eta_l = (15\nu u^2/\epsilon)^{1/2}$ (from [35] which also explains that this microscale is also associated with the zero abscissa crossing of the Taylor series approximation of order 2 at zero of the auto correlation), where u is representative of the velocity in the bulk. With [32] and [37] the following relation can be used:

$$\frac{\eta_l}{2} = \frac{\sqrt{15}u^*}{[Ra(Nu - 1)]^{1/2}} \quad (39)$$

with

$$u^* = \sqrt{0.068Ra^{0.91} + 0.012Ra^{0.96}}$$

Overall as we follow the same procedure as in [32] we take for minimum mesh size in the bulk:

$$l_{bulk} = \text{minimum}(4l_{scale}, \frac{\eta_l}{2}) \quad (40)$$

4. We can then have a first approximation of the number of cells required:

$$N = \text{round}(\frac{H - 2 * \max(\delta_u, \delta_{th})}{l_{bulk}} + 2 * \max(N_u, N_{th})) \quad (41)$$

Once we have N , as $l_u = \frac{\delta_u}{N_u}$ and $l_{th} = \frac{\delta_{th}}{N_{th}}$ are more restrictive than l_{bulk} we increase β starting from $\beta = 1$ up to $\beta = 3$, if at some point the requirements of minimal number of points of both N_u and N_{th} in the boundary layers are fulfilled we stop to increase β and check if the bulk cell width is fulfilled. If either β increases up to 3 without fulfilling N_u and N_{th} or we cannot fulfill the bulk requirement we increase N by 2 and put β back to 1 before increasing it again.

The number of cells obtained by applying this procedure give the nubmer of cells in the vertical. For the number of cells along the axis x for example, if $W \geq H$ the number of cells in multiplied by $\frac{W}{H}$ in this direction but if $W \leq H$ the number of cells is kept the same as along the vertical.

4.6 Numerical Algorithm

The objective of the numerical algorithm will be to solve (19), (20) and (21) to obtain for each cell grid noted as index i, j, k (see Figure 18) the values $T_{i,j,k}$, $u_{i,j,k}$, $v_{i,j,k}$, $w_{i,j,k}$, P^0 and $P_{i,j,k}^1$.

The low Mach number approximation equations represent 5 equations and also μ , ρ , c_p , k will vary with the temperature using equation of interpolation from section 4.3. We thus have in total 9 equations for 10 unknowns, we close the equations by setting $P^0 = 1$ atm as our domain is open. The equations of the low Mach number

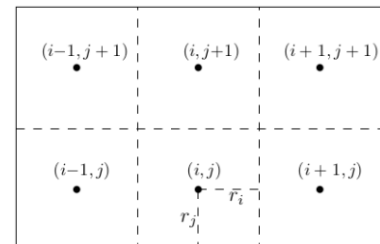


Figure 18: Schematic of the grid indices for a two dimensional grid

approximation (19), (20) and (21) need to be spatially and temporally discretized in order to solve them on the grid with linear algebra. The discretization is similar as in [46], for the spatial discretization we will use the following interpolation operator for the center on in-between cell surface:

$$\overline{f_{i\pm 1/2,j,k}}^x = \frac{f_{i\pm 1,j,k}ri_{i,j,k} + f_{i,j,k}ri_{i\pm 1,j,k}}{ri_{i,j,k} + ri_{i\pm 1,j,k}} \quad (42)$$

Where ri , rj and rk are respectively the half length width along each direction x, y and z (see Figure 18), as explained in section 4.1 we assume a rectilinear grid so the size of the cells in each of the three directions varies only along the respective direction ($ri_{i,j,k} = ri(i)$, $rj_{i,j,k} = rj(j)$ and $rk_{i,j,k} = rk(k)$). For the interpolation on faces along y axis and z axis, we just replace x by y,z and i by j,k. For the interpolations of the derivatives at the center of the cells and at the center of in-between surface we introduce the following operators:

$$\left. \frac{\delta f}{\delta x} \right|_{i,j,k} = \frac{\overline{f_{i+1/2,j,k}}^x - \overline{f_{i-1/2,j,k}}^x}{2ri_{i,j,k}} \quad (43)$$

$$\left. \frac{\delta f}{\delta x} \right|_{i\pm 1/2,j,k} = \pm \frac{f_{i\pm 1,j,k} - f_{i,j,k}}{ri_{i\pm 1,j,k} + ri_{i,j,k}} \quad (44)$$

$\frac{\delta f}{\delta y}$ and $\frac{\delta f}{\delta z}$ are similarly obtained. Now that we know how to spatially discretize the equation we can present the algorithm to solve them. The objective is, knowing the variable ϕ (which can be T, u, v, w) at each cell N at time t^n so ϕ^n , to calculate them at time t^{n+1} so to have ϕ^{n+1} by constructing a linear system:

$$\begin{pmatrix} A_{11}^n & A_{12}^n & \dots & \dots & A_{1N}^n \\ A_{21}^n & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & A_{\frac{N}{2}\frac{N}{2}}^n & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & A_{NN}^n \end{pmatrix} \begin{pmatrix} \phi_1^{n+1} \\ \phi_2^{n+1} \\ \dots \\ \phi_{\frac{N}{2}}^{n+1} \\ \dots \\ \phi_N^{n+1} \end{pmatrix} = \begin{pmatrix} B_1^n \\ B_1^n \\ \dots \\ B_{\frac{N}{2}}^n \\ \dots \\ B_N^n \end{pmatrix} \quad (45)$$

The process from going to ϕ^n to ϕ^{n+1} is done in two steps. We first obtain the fields variables at a predictor step, predicted variables are noted by ϕ^* and then they are recalculated to update them at the corrector step noted by ϕ^{n+1} .

4.6.1 Predictor Step

We will first calculate T^* using equation (21) reminded below, (we don't use the subscripts $()^0$ for simplicity):

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p \underline{v} \cdot \nabla T = \frac{1}{PrRe} \nabla \cdot (k \nabla T) \quad (46)$$

So the above equation will be discretized in order to create the linear system of linear equation system (45) by creating the matrix A^n , an unknown vector $\begin{pmatrix} T_1^* \\ \dots \\ T_N^* \end{pmatrix}$ and a right hand side vector

B $\begin{pmatrix} B_1^n \\ \dots \\ B_N^n \end{pmatrix}$. To obtain this, we discretize spatially and temporally equation (46). Regarding the

temporal discretization needed for the convection term $\hat{\rho}\hat{c}_p\mathbf{v} \cdot \nabla \hat{T}$ and the diffusion $\nabla \cdot (k \nabla \hat{T})$ we can either use explicit or implicit scheme to express them. However, using only implicit terms would lead to a matrix A with a lot of elements on each row (each unknown T^* depends on a lot of adjacent cells and consequently other unknowns, meaning each row of A has a lot of non-zero values) and thus this would lead to too much computation requirement, the code uses thus only implicit scheme along vertical derivative while the terms with gradients along the x axis and z axis are treated explicitly. The choice of the vertical axis to treat implicitly is because of the alignment with the vertical buoyancy effect. So the part of the equation that will be treated explicitly and put on the right hand side is:

$$Res_T = -\rho c_p \mathbf{v} \cdot \nabla T + \frac{1}{PrRe} \left(\frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) \right) \quad (47)$$

The term Res_T is treated explicitly with the two-step Adams-Bashforth method [48], which means to solve for T^* we need the values at n and $n-1$. We quickly remind the two step method, when we have a differential equation such as: $y' = f(t, y)$, when we know the value of f and y at t_n and look for the value at t_{n+1} we integrate the equation from t_n to t_{n+1} to obtain $y_{n+1} - y_n$ on the left hand side, and on the right hand side, we approximate the expression using Lagrange polynomial of order r , if $r = 0$ we just use the value at t_n on the right hand side, approximating it as a constant and thus by integration we find back the Euler method: $y_{n+1} - y_n = \underbrace{(t_{n+1} - t_n)}_{\Delta t} f(t_n, y_n)$. In the

code used for this work we use an approximation of order $r=1$, so the approximation is interpolated using the values at t_n and t_{n-1} :

$$f(t, y) \approx \sum_{r=0}^{r=1} \prod_{0 \leq k \leq 1; k \neq r} \frac{t - t_{n-k}}{t_{n-r} - t_{n-k}} f(t_{n-r}, y_{n-r}) \quad (48)$$

by integrating from t_n to t_{n+1} and with Δt constant (which is not strictly constant, see section 4.6.3, but a robust approximation verified in practise) so $\Delta t = t_n - t_{n-1} = t_{n+1} - t_n$ we obtain:

$$\int_{t_n}^{t_{n+1}} f(t, y) \approx \int_{t_n}^{t_{n+1}} \frac{t - t_{n-1}}{t_n - t_{n-1}} f(t_n, y_n) + \frac{t - t_n}{t_{n-1} - t_n} f(t_{n-1}, y_{n-1}) = \frac{3}{2} \Delta t f(t_n, y_n) - \frac{1}{2} \Delta t f(t_{n-1}, y_{n-1}) \quad (49)$$

So by using this result we will have $\frac{3}{2} \Delta t Res_T^n - \frac{1}{2} \Delta t Res_T^{n-1}$ and by using the interpolations equations (42), (43) and (44) we obtain a spatial and temporal discretization of Res_T but the convective term $\hat{\rho}\hat{c}_p\mathbf{v} \cdot \nabla \hat{T}$ used at a cell of coordinate ijk is not directly calculated using the values of ρ_{ijk} , $c_{p_{ijk}}$ and $\mathbf{v}_{ijk}$, as this term is originating from the conservative form with a divergence operator it make more sense to use the flux values interpolated at the inter face cells, so $\hat{\rho}\hat{c}_p\mathbf{v} \cdot \nabla \hat{T}$ will be interpolated using the values at the centre of the faces of the cells as follows from [47]:

$$\begin{aligned}
(\rho c_p \underline{v} \cdot \nabla T) \Big|_{ijk} \approx & \frac{\overline{(\rho c_p \underline{v})}_{i+\frac{1}{2},j,k}^x \frac{\delta T}{\delta x} \Big|_{i+\frac{1}{2},j,k} + \overline{(\rho c_p \underline{v})}_{i-\frac{1}{2},j,k}^x \frac{\delta T}{\delta x} \Big|_{i-\frac{1}{2},j,k}}{2} + \\
& \frac{\overline{(\rho c_p \underline{v})}_{i,j+\frac{1}{2},k}^y \frac{\delta T}{\delta x} \Big|_{i,j+\frac{1}{2},k} + \overline{(\rho c_p \underline{v})}_{i,j-\frac{1}{2},k}^y \frac{\delta T}{\delta x} \Big|_{i,j-\frac{1}{2},k}}{2} + \\
& \frac{\overline{(\rho c_p \underline{v})}_{i,j,k+\frac{1}{2}}^z \frac{\delta T}{\delta x} \Big|_{i,j,k+\frac{1}{2}} + \overline{(\rho c_p \underline{v})}_{i,j,k-\frac{1}{2}}^z \frac{\delta T}{\delta x} \Big|_{i,j,k-\frac{1}{2}}}{2}
\end{aligned} \tag{50}$$

The diffusion terms are discretized by applying the divergence theorem on the cell we obtain the discretization by using equation (43), as an example the discretization of the diffusive term along axis x is given:

$$\begin{aligned}
\frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) \Big|_{ijk} \approx & \frac{\overline{k}_{i+\frac{1}{2},j,k}^x \frac{\delta T}{\delta x} \Big|_{i+\frac{1}{2},j,k} - \overline{k}_{i-\frac{1}{2},j,k}^x \frac{\delta T}{\delta x} \Big|_{i-\frac{1}{2},j,k}}{2r_{i,j,k}} \\
\approx & \frac{\frac{(k_{i+1,j,k} r_{i,j,k} + k_{i,j,k} r_{i+1,j,k})}{r_{i,j,k} + r_{i+1,j,k}} \frac{(T_{i+1,j,k} - T_{i,j,k})}{r_{i,j,k} + r_{i+1,j,k}} - \frac{(k_{i,j,k} r_{i-1,j,k} + k_{i-1,j,k} r_{i,j,k})}{r_{i-1,j,k} + r_{i,j,k}} \frac{(T_{i,j,k} - T_{i-1,j,k})}{r_{i-1,j,k} + r_{i,j,k}}}{2r_{i,j,k}}
\end{aligned} \tag{51}$$

The diffusive term along y is treated implicitly using the Crank-Nicholson method, the temporal discretization is as follow:

$$\int_{t_n}^{t_*} \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) \Big|_{i,j,k} \approx \frac{1}{2} \Delta t \frac{\partial}{\partial y} \left(k^n \frac{\partial T^{(n)}}{\partial y} + k^n \frac{\partial T^{(*)}}{\partial y} \right) \Big|_{i,j,k} \tag{52}$$

The spatial discretization of the two diffusive terms at time t_n and t_* of (52) will be the same as for equation (51) and by developing the discretization of $\frac{1}{2} \Delta t \frac{\partial}{\partial y} (k^n \frac{\partial T^{(*)}}{\partial y})$ the terms $T_{i,j,k}^{(*)}$, $T_{i,j-1,k}^{(*)}$ and $T_{i,j+1,k}^{(*)}$ will appear and the coefficients in front of these terms will go in the matrix A as it is implicit.

Thus from the equation of energy (46) we end up with the following temporal discretized equation with the implicit terms on the left hand side and explicit on the right:

$$\begin{aligned}
\rho^n c_p^n T_{i,j,k}^* - \frac{1}{RePr} \frac{1}{2} \Delta t \frac{\partial}{\partial y} \left(k^n \frac{\partial T^{(*)}}{\partial y} \right) \Big|_{i,j,k} = \\
\rho^n c_p^n T_{i,j,k}^n + \frac{3}{2} \Delta t Res_{T-i,j,k}^n - \frac{1}{2} \Delta t Res_{T-i,j,k}^{n-1} + \frac{1}{RePr} \frac{1}{2} \Delta t \frac{\partial}{\partial y} \left(k^n \frac{\partial T^{(n)}}{\partial y} \right) \Big|_{i,j,k}
\end{aligned} \tag{53}$$

As a synthesis: once the equation (53) is also spatially discretized, we end up with the following linear system for the ijk cell:

$$\begin{aligned}
& \begin{pmatrix} \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \frac{-\Delta t \cdot \overline{k_{i,j-1/2,k}^n}^y}{(rj_{i,j-1,k} + rj_{i,j,k})} & \rho_{ijk}^n c_{p-ijk}^n + \frac{\Delta t \cdot (\frac{\overline{k_{i,j-1,k}^n}^y}{(rj_{i,j-1,k} + rj_{i,j,k})} + \frac{\overline{k_{i,j+1,k}^n}^y}{(rj_{i,j+1,k} + rj_{i,j,k})})}{2RePr2rj_{i,j,k}} & \frac{-\Delta t \cdot \overline{k_{i,j+1/2,k}^n}^y}{(rj_{i,j+1,k} + rj_{i,j,k})} & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} \dots \\ T_{i,j-1,k}^* \\ T_{i,j,k}^* \\ T_{i,j+1,k}^* \\ \dots \end{pmatrix} \\
& = \begin{pmatrix} \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \rho_{ijk}^n c_{p-ijk}^n T_{ijk}^n + \Delta t \cdot (\frac{3}{2} Res_{T-i,j,k}^n - \frac{1}{2} Res_{T-i,j,k}^{n-1}) + \frac{\Delta t}{RePr} \frac{1}{2} \frac{\overline{k_{i,j+1/2,k}^n}^y \frac{\delta T^n}{\delta y} \Big|_{i,j+\frac{1}{2},k} - \overline{k_{i,j-1/2,k}^n}^y \frac{\delta T^n}{\delta y} \Big|_{i,j-\frac{1}{2},k}}{2rj_{i,j,k}} & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} \dots \\ T_{i,j-1,k}^* \\ T_{i,j,k}^* \\ T_{i,j+1,k}^* \\ \dots \end{pmatrix} \quad (54)
\end{aligned}$$

We can thus see that we end up with a tri-diagonal matrix which is easy to solve using Thomas algorithm [49] and which is not very computational expensive. After the evaluation of T^* , the predicted value of the fluid density ρ^* , c_p^* , k^* and μ^* are obtained by the equations of states in function of T^* from section 4.2.

Then the code proceeds to calculate $\underline{v}^*$ and $\underline{p}^*$. This is done in two steps, first calculating an intermediate velocity $\tilde{v}$ by solving the momentum equation (20) without the pressure gradient term and the body force $\underline{\rho g}$:

$$\frac{\partial(\rho \underline{v})}{\partial t} + \nabla \cdot (\rho \underline{v} \underline{v}) = \nabla \cdot (\mu(\nabla \underline{v} + \nabla \underline{v}^T - \frac{2}{3} \nabla \cdot \underline{v})) \quad (55)$$

The above equation represents three equations, one for each u,v and w velocity dimension of $\tilde{v}$. For each one, we create again a linear system, similarly as before, when we solve for each velocity dimension, the derivatives along the vertical y of the unknown are treated implicitly and the rest of the diffusion terms and the convective terms as explicit in a similar way as for the temperature, we obtain the following right hand side as follows:

$$\begin{aligned}
Res_u &= -\nabla \cdot (\rho \underline{v} u) + \frac{1}{Re} [\frac{\partial}{\partial x} (\mu(2\frac{\partial u}{\partial x} - \frac{2}{3} \nabla \cdot \underline{v})) + \frac{\partial}{\partial y} (\mu \frac{\partial v}{\partial x}) + \frac{\partial}{\partial z} (\mu(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}))] \\
Res_v &= -\nabla \cdot (\rho \underline{v} v) + \frac{1}{Re} [\frac{\partial}{\partial x} (\mu(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x})) - \frac{2}{3} \frac{\partial}{\partial y} (\mu(\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z})) + \frac{\partial}{\partial z} (\mu(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}))] \\
Res_w &= -\nabla \cdot (\rho \underline{v} w) + \frac{1}{Re} [\frac{\partial}{\partial x} (\mu(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x})) + \frac{\partial}{\partial y} (\mu \frac{\partial v}{\partial z}) + \frac{\partial}{\partial z} (\mu(2\frac{\partial w}{\partial z} - \frac{2}{3} \nabla \cdot \underline{v}))]
\end{aligned} \quad (56)$$

As we can see in the above equation for each Res the terms of double derivatives along y ($\frac{\partial}{\partial y} (\mu \frac{\partial}{\partial y} \dots)$) do not appear because they are treated implicitly. Similarly as for the energy equation, we end up with the following equation to solve:

$$\begin{aligned}
\frac{\rho^* \underline{\tilde{v}} - \rho^n \underline{v}^n}{\Delta t} \Big|_{i,j,k} &= \frac{3}{2} Res_{\underline{v}}^{(n)} \Big|_{i,j,k} - \frac{1}{2} Res_{\underline{v}}^{(n-1)} \Big|_{i,j,k} \\
&+ \frac{1}{2} \frac{\mu^n}{Re} \frac{\partial}{\partial y} \left(\frac{\partial u^n}{\partial y} \underline{e}_x + \frac{4}{3} \frac{\partial v^n}{\partial y} \underline{e}_y + \frac{\partial w^n}{\partial y} \underline{e}_w \right) \Big|_{i,j,k} \\
&+ \frac{1}{2} \frac{\mu^*}{Re} \frac{\partial}{\partial y} \left(\frac{\partial u^*}{\partial y} \underline{e}_x + \frac{4}{3} \frac{\partial v^*}{\partial y} \underline{e}_y + \frac{\partial w^*}{\partial y} \underline{e}_w \right) \Big|_{i,j,k}
\end{aligned} \tag{57}$$

The spatial discretization to obtain the linear system follows the same logic as the energy equation.

For the discretization of the convective term $\nabla \cdot (\rho^n \underline{v}^n \underline{v}^n)$ in $Res_{\underline{v}}^n$, interpolation of $(\rho^n u^n) \Big|_{i \pm \frac{1}{2}, j, k}$, $(\rho^n v^n) \Big|_{i, j \pm \frac{1}{2}, k}$ and $(\rho^n w^n) \Big|_{i, j, k \pm \frac{1}{2}}$ are needed but the code won't straight use $\overline{(\rho^n u^n)}_{i \pm \frac{1}{2}, j, k}^x$, $\overline{(\rho^n v^n)}_{i, j \pm \frac{1}{2}, k}^y$ and $\overline{(\rho^n w^n)}_{i, j, k \pm \frac{1}{2}}^z$ from equation (42). Indeed, contrary to staggered grid, collocated grid arrangement can produce spurious oscillations of the pressure field called checker-board oscillation or odd-even decoupling. This problem can be remedied with an alternative flux interpolation method for the convective flux, first introduced by Rhie & Chow [40]. Applied to this work, the code will use the following auxiliary flux:

$$\begin{aligned}
F_u^n \Big|_{i \pm \frac{1}{2}, j, k} &= (\rho^n u^n) \Big|_{i \pm \frac{1}{2}, j, k} = \overline{(\rho^n \tilde{u}^{n-1})}_{i \pm \frac{1}{2}, j, k}^x - \frac{\delta P'^n}{\delta x} \Big|_{i \pm \frac{1}{2}, j, k} \Delta t + Ri \ y_j \ \frac{\delta \rho^n}{\delta x} \Big|_{i \pm \frac{1}{2}, j, k} \Delta t \\
F_v^n \Big|_{i, j \pm \frac{1}{2}, k} &= (\rho^n v^n) \Big|_{i, j \pm \frac{1}{2}, k} = \overline{(\rho^n \tilde{v}^{n-1})}_{i, j \pm \frac{1}{2}, k}^y - \frac{\delta P'^n}{\delta y} \Big|_{i, j \pm \frac{1}{2}, k} \Delta t + Ri \ \overline{y}_{j \pm \frac{1}{2}} \ \frac{\delta \rho^n}{\delta y} \Big|_{i, j \pm \frac{1}{2}, k} \Delta t \\
F_w^n \Big|_{i, j, k \pm \frac{1}{2}} &= (\rho^n w^n) \Big|_{i, j, k \pm \frac{1}{2}} = \overline{(\rho^n \tilde{w}^{n-1})}_{i, j, k \pm \frac{1}{2}}^z - \frac{\delta P'^n}{\delta z} \Big|_{i, j, k \pm \frac{1}{2}} \Delta t + Ri \ y_j \ \frac{\delta \rho^n}{\delta z} \Big|_{i, j, k \pm \frac{1}{2}} \Delta t
\end{aligned} \tag{58}$$

The term $\tilde{u}$ is the provisional velocity calculated during the corrector step (see below), the subscript $n-1$ means it is the velocity calculated during the corrector step of the previous iteration (the iteration going from $n-1$ to n). With the use of equations (58) the convective term in $Res_{\underline{v}-ijk}$ is discretized as follows:

$$\begin{aligned}
\nabla \cdot (\rho \underline{v} \underline{v}) \Big|_{i,j,k} &= \frac{F_u \Big|_{i+\frac{1}{2}, j, k} \overline{\underline{v}}_{i+\frac{1}{2}, j, k}^x - F_u \Big|_{i-\frac{1}{2}, j, k} \overline{\underline{v}}_{i-\frac{1}{2}, j, k}^x}{2ri_{i,j,k}} + \frac{F_v \Big|_{i, j+\frac{1}{2}, k} \overline{\underline{v}}_{i, j+\frac{1}{2}, k}^y - F_v \Big|_{i, j-\frac{1}{2}, k} \overline{\underline{v}}_{i, j-\frac{1}{2}, k}^y}{2rj_{i,j,k}} \\
&+ \frac{F_w \Big|_{i, j, k+\frac{1}{2}} \overline{\underline{v}}_{i, j, k+\frac{1}{2}}^z - F_w \Big|_{i, j, k-\frac{1}{2}} \overline{\underline{v}}_{i, j, k-\frac{1}{2}}^z}{2rk_{i,j,k}}
\end{aligned} \tag{59}$$

Some more explanations about the pressure oscillation and justifications of the use of this alternative interpolation method is provided in section 4.6.5.

Once we have the value of $\tilde{v}$, we calculate the value $\underline{v}^*$ using the momentum equation with the pressure and the buoyancy force:

$$\frac{\rho^* \underline{v}^* - \rho^* \underline{\tilde{v}}}{\Delta t} = -\nabla P^{(*)} - \rho^* Ri \ \underline{e}_y \quad \text{with} \quad (Ri = \frac{l_{ref}|g|}{v_{ref}^2}) \tag{60}$$

As mentioned in [39] sometimes the Navier–Stokes equations are written in terms of the piezo-metric pressure, $P' = P + \rho|g|y$, in near-zero Froude number $Fr = \frac{v}{\sqrt{gH}}$ the body forces are large and can overwhelm the other terms, so writing the pressure in this form eliminates them from the governing equations. This operation is done by substituting $P' = P + \rho R i y$ and:

$$\rho \text{Ri } \underline{e}_y = \nabla(\rho R i y) - R i y \nabla \rho \quad (61)$$

Applying (61) to (60) and applying the divergence, we obtain:

$$\nabla \cdot \nabla(P'^*) = \frac{1}{\Delta t} \nabla \cdot (\rho^* \underline{\tilde{v}}) + \frac{3\rho^* - 4\rho^n + \rho^{n-1}}{2\Delta t^2} + R i \nabla \cdot (y \nabla(\rho)) \quad (62)$$

The term $\frac{3\rho^* - 4\rho^n + \rho^{n-1}}{2\Delta t^2}$ is obtained by using the continuity equation (19), we replace $-\frac{1}{\Delta t} \nabla \cdot (\rho^* \underline{v}^*)$ with $\frac{1}{\Delta t} \frac{\partial \rho}{\partial t} \Big|_{t=t_*}$ and a implicit backward scheme time discretization is used [51] so $\frac{\partial \rho}{\partial t} \Big|_{t=t_*}$ is approximated using a lagrange interpolation polynomial of the function $\rho(t)$ of order 2 at points t_* , $t_n (= t_{*-1})$ and $t_{n-1} (= t_{*-2})$ and taking the derivative at point t_* :

$$\frac{\partial \rho}{\partial t} \Big|_{t=t_*} \approx \frac{\partial}{\partial t} \Big|_{t=t_*} \left(\sum_{r=0}^{r=2} \prod_{0 \leq k \leq 2; k \neq r} \frac{t - t_{*-k}}{t_{*-r} - t_{*-k}} \rho(t_{*-r}) \right) = \frac{3\rho(t_*) - 4\rho(t_n) + \rho(t_{n-1})}{2\Delta t} \quad (63)$$

This Poisson's equation is solved using Petsc library [50] and gives the solution for P'^* . We then use equation (60) to obtain $\underline{v}^*$.

4.6.2 Corrector Step

In the corrector step, the variables are updated to t_{n+1} , the procedure is very similar to the corrector step, but the explicit terms are treated using the trapezoidal rule using the predicted values, so the energy equation is solved with:

$$c_p^* \rho^* \frac{T^{n+1} - T^n}{\Delta t} \Big|_{i,j,k} = \frac{1}{2} \text{Res}_{T-i,j,k}^n + \frac{1}{2} \text{Res}_{T-i,j,k}^{*} + \frac{1}{\text{RePr}} \frac{1}{2} \frac{\partial}{\partial y} \left(k^* \frac{\partial T^{(n)}}{\partial y} + k^* \frac{\partial T^{(n+1)}}{\partial y} \right) \Big|_{i,j,k} \quad (64)$$

After the evaluation of T^{n+1} , the predicted value of the fluid density ρ^{n+1} , c_p^{n+1} , k^{n+1} and μ^{n+1} are obtained by the equations of states. Then, we calculate the provisional velocity for the corrector step $\underline{\tilde{v}}$ using:

$$\begin{aligned} \frac{\rho^{n+1} \underline{\tilde{v}} - \rho^n \underline{v}^n}{\Delta t} \Big|_{i,j,k} &= \frac{1}{2} \text{Res}_{\underline{v}}^{(n)} \Big|_{i,j,k} + \frac{1}{2} \text{Res}_{\underline{v}}^{(*)} \Big|_{i,j,k} \\ &+ \frac{1}{2} \frac{\mu^n}{\text{Re}} \frac{\partial}{\partial y} \left(\frac{\partial u^n}{\partial y} \underline{e}_x + \frac{4}{3} \frac{\partial v^n}{\partial y} \underline{e}_y + \frac{\partial w^n}{\partial y} \underline{e}_w \right) \Big|_{i,j,k} \\ &+ \frac{1}{2} \frac{\mu^{n+1}}{\text{Re}} \frac{\partial}{\partial y} \left(\frac{\partial u^{n+1}}{\partial y} \underline{e}_x + \frac{4}{3} \frac{\partial v^{n+1}}{\partial y} \underline{e}_y + \frac{\partial w^{n+1}}{\partial y} \underline{e}_w \right) \Big|_{i,j,k} \end{aligned} \quad (65)$$

Once again for the discretization of the convective term in $\text{Res}_{\underline{v}}$ we use a slightly different interpolation $F_{\underline{v}}^*$ similar as in equation 58 but replacing $\underline{\tilde{v}}^{n-1}$ by the current $\underline{v}^*$ and ρ^n , P'^n by ρ^* and P'^* . Next, we consider the fluid momentum equation written in terms of $\underline{\tilde{v}}$:

$$\frac{\rho^{n+1} \underline{\tilde{v}}^{n+1}}{\Delta t} = \frac{\rho^{n+1} \underline{\tilde{v}}}{\Delta t} - \nabla P'^{(n+1)} + \text{Ri } y \nabla \rho^{n+1} \quad (66)$$

Similarly as in the predictor step, we apply the divergence and solve the Poisson's equation:

$$\nabla \cdot (\nabla P^{(n+1)}) = \frac{1}{\Delta t} \nabla \cdot (\rho^{(n+1)} \underline{v}) + \frac{3\rho^{(n+1)} - 4\rho^{(n)} + \rho^{(n-1)}}{2\Delta t^2} + \text{Ri} \nabla \cdot (y \nabla \rho^{(n+1)}). \quad (67)$$

Once $p^{(n+1)}$ is obtained, $\underline{v}^{n+1}$ is directly calculated using (66). A last, temperature computation is done with updated scalar elements (using $\rho^{n+1}, \mu^{n+1}, c_p^{n+1}$ and k^{n+1}) and $Res_{T-i,j,k}^{n+1}$ instead of $Res_{T-i,j,k}^*$

$$c_p^{n+1} \rho^{n+1} \frac{T^{n+1} - T^n}{\Delta t} \Big|_{i,j,k} = \frac{1}{2} Res_{T-i,j,k}^n + \frac{1}{2} Res_{T-i,j,k}^{n+1} + \frac{1}{RePr} \frac{1}{2} \frac{\partial}{\partial y} (k^{n+1} \frac{\partial T^{(n)}}{\partial y} + k^{n+1} \frac{\partial T^{(n+1)}}{\partial y}) \Big|_{i,j,k} \quad (68)$$

This last update of T^{n+1} is recommended by [47], numerical experiments performed by the authors therein show a reduction of energy conservation errors that may arise in flows subjected to strong thermal gradients.

4.6.3 Time increment

At each step, the time increment Δt is calculated based on the definition of the Courant number, $C = \frac{U \Delta t}{\Delta X}$ [53]. It can be interpreted as the distance that the fluid contained in a cell will move, towards another cell distant of a distance ΔX , due to its velocity U , during a time step of length Δt . The mesh is known, so we know each value of ΔX , and the velocity U is known from the previous time step. The only unknown, that we aim to determine, is the time increment Δt .

The whole idea is that the fluid contained in a cell may not end up further than the adjacent cell, at the end of a single time step of length Δt_i . The figure below (1 dimension) explains that, if the non-dimensional number C is bigger than 1, the fluid will make big gaps, more than one cell at a time. It can be avoided if $C < 1$. Big gaps will induce a loss of precision and stability in our simulation.

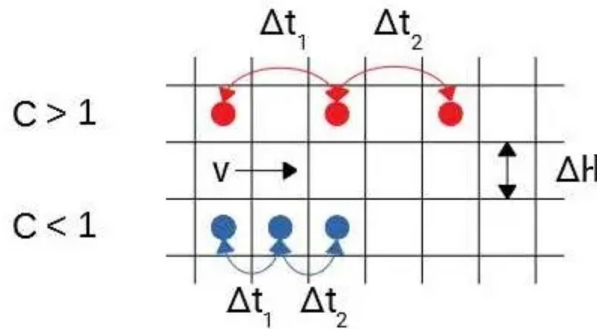


Figure 19: Fluid displacement after one and two time steps, as a function of C

In practice, we wanted to make sure that, nowhere in the grid, the value of C exceeds 0,5. At each time step of the simulation, we have selected, for each direction (x, y, z), the smallest value of t : $\min(\frac{\Delta x}{u}, \frac{\Delta y}{v}, \frac{\Delta z}{w})$, of which we take the minimum among the grid.

Then, we recall our criterion :

$$C = \frac{\Delta t \cdot v_i}{\Delta x_i} \leq 0,5 = CFL_{max}$$

We re-write this equation to find the biggest time increment Δt that we may chose :

$$\Delta t = \frac{0,5}{\min_i(\frac{v_i}{\Delta x_i})} = 0,5 \cdot \max_i(\frac{\Delta x_i}{v_i})$$

In practise instead of $CFL_{max} = 0.5$ we take lower value to be more precise, in this work the value is taken between 0.1 and 0.3. The time increment also has to respect the Von Neumann stability analysis [38] for transport equation 26, Δt has to respect $\Delta t \leq 0.5 \frac{\Delta^2 x}{\omega}$ with $\omega = \frac{\mu}{\rho}$ if considering the momentum equation or $\omega = \frac{k}{\rho c_p}$ if considering the energy equation, in our case for the momentum equation is a higher constraint . Overall the minimum value of all those constraints has to be respected.

4.6.4 Boundary conditions

The algorithm implements two possible types of boundary conditions : the Dirichlet conditions (the property of the fluid, against the boundary, are dictated by a given value), and the Neumann conditions (the gradient of a property, in the direction of the boundary and evaluated against the boundary, is dictated by a given value). For instance, in work, the Neumann condition is the adiabatic condition. Thus, the gradient of temperature is equal to zero in the direction of the wall.

As we have explained, the mesh is composed of blue cells, and a layer of red virtual cells around. The latter are useful for the boundary conditions. In the figure below, we show the situation close to the boundary.

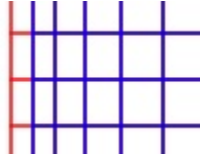


Figure 20: Boundary cells (blue) adjacent to the red virtual cells outside the boundary

We use the red virtual cells in the following way :

- For the Dirichlet conditions, the value of the red virtual cells (i.e. the cells at the boundary) is set such that the interpolated value between the red and the adjacent blue cell is equal to the given value, so for example for a Dirichlet boundary equal zero the red value is just the negative of the adjacent blue.
- For the Neumann conditions, in our situation we only have zero Neumann conditions so we make sure that the gradient of the field at the wall (boundary between the red and blue) is equal to zero. The quantity inside the red virtual cell is set at the same value as the blue cell adjacent to it to achieve that.

4.6.5 Checkerboard oscillation and auxiliaries flux interpolation

In this section we briefly explain the phenomena of checkerboard oscillation and a justification of the utilisation of the auxiliary fluxes interpolation methods of equation (58).

The construction of the Poisson's equation to solve the scalar Pressure P can be seen as a combination of the continuity equation and the momentum equation. Indeed, we can also start from the continuity to obtain the same Poisson's equation. We start from:

$$\nabla \cdot (\rho^n \underline{v}^n) = -\frac{\partial \rho}{\partial t} \Big|_{t=t^n} \quad (69)$$

We insert the momentum equation $\rho^n \underline{v}^n = -\nabla P^{(n)} \Delta t + \rho^n \check{\underline{v}}^{n-1}$ (we don't use the piezometric pressure here for simplicity and to be clear, we remind that $\check{\underline{v}}^{n-1}$ is the provisional velocity obtained during the corrector step of the iteration going from $n-1$ to n):

$$\nabla \cdot (-\nabla P^{(n)} \Delta t + \rho^n \check{\underline{v}}^{n-1}) = -\frac{\partial \rho}{\partial t} \Big|_{t=t^n} \quad (70)$$

And we obtain back :

$$\nabla \cdot \nabla (P^{(n)}) = \frac{1}{\Delta t} \frac{\partial \rho}{\partial t} \Big|_{t=t^n} + \frac{1}{\Delta t} \nabla \cdot (\rho^n \check{\underline{v}}^{n-1}) \quad (71)$$

It is important to keep in mind that the Laplacian operator applying on P is the product of the divergence operator originating from the continuity equation and the gradient operator that comes from the momentum equations. As pointed out in the book [26] it is essential that the consistency of these operators are maintained and the outer and inner derivatives may be discretized using different schemes, they have to be the same than the discretization used in the continuity and momentum equations. In order to maintain this consistency for the approximations used to discretize the double derivative on P , it is better to derive the equation for the pressure from the discretized continuity and momentum equations rather than by approximating the double derivative directly. Indeed to illustrate this we develop the left hand side of equation (69) :

$$\begin{aligned} \nabla \cdot (\rho^n \underline{v}^n)_{i,j,k} \approx & \frac{(\rho^n u^n)_{i+\frac{1}{2},j,k} - (\rho^n u^n)_{i-\frac{1}{2},j,k}}{2r i_{i,j,k}} + \frac{(\rho^n v^n)_{i,j+\frac{1}{2},k} - (\rho^n v^n)_{i,j-\frac{1}{2},k}}{2r j_{i,j,k}} \\ & + \frac{(\rho^n w^n)_{i,j,k+\frac{1}{2}} - (\rho^n w^n)_{i,j,k-\frac{1}{2}}}{2r k_{i,j,k}} \end{aligned} \quad (72)$$

For a collocated grid, we need to interpolate $\rho^n \underline{v}^n$ at inter cell points $i + \frac{1}{2}, j, k$ etc A candidate (but we will explain why it causes the oscillation) is to use equation 42 i.e $(\rho^n \underline{v}^n)_{i \pm \frac{1}{2}, j, k} \approx \overline{(\rho^n \underline{v}^n)_{i \pm 1/2, j, k}}^x = \frac{(\rho^n \underline{v}^n)_{i \pm 1, j, k} r i_{i,j,k} + (\rho^n \underline{v}^n)_{i, j, k} r i_{i \pm 1, j, k}}{r i_{i,j,k} + r i_{i \pm 1, j, k}}$.

So, as said previously, in order to maintain the consistency if $\overline{(\rho^n \underline{v}^n)_{i \pm 1/2, j, k}}^x$ is chosen, the Laplacian operator on P needs to be discretized as follows:

$$\begin{aligned} (\nabla \cdot \nabla P)_{i,j,k} \approx & \frac{\overline{(\frac{\delta P}{\delta x})_{i+\frac{1}{2},j,k}}^x - \overline{(\frac{\delta P}{\delta x})_{i-\frac{1}{2},j,k}}^x}{2r i_{i,j,k}} + \frac{\overline{(\frac{\delta P}{\delta x})_{i,j+\frac{1}{2},k}}^y - \overline{(\frac{\delta P}{\delta x})_{i,j-\frac{1}{2},k}}^y}{2r j_{i,j,k}} \\ & + \frac{\overline{(\frac{\delta P}{\delta x})_{i,j,k+\frac{1}{2}}}^z - \overline{(\frac{\delta P}{\delta x})_{i,j,k-\frac{1}{2}}}^z}{2r k_{i,j,k}} \end{aligned} \quad (73)$$

Another way to understand this above equation is applying the momentum equation once the continuity equation is already discretized in 72 and interpolated with $\overline{(\rho^n \underline{v}^n)_{i \pm 1/2, j, k}}^x$ so the momentum equation is applied to replace each value under the over bared terms.

But $\overline{(\frac{\delta P}{\delta x})_{i+\frac{1}{2},j,k}}^x \neq \frac{\delta P}{\delta x} \Big|_{i+\frac{1}{2},j,k} (= \frac{P_{i+1,j,k} - P_{i-1,j,k}}{r i_{i,j,k} + r i_{i+1,j,k}})$, instead it is an interpolation using $\frac{\delta P}{\delta x} \Big|_{i,j,k}$ and

$\frac{\delta P}{\delta x} \Big|_{i+1,j,k}$. Furthermore, an important element is that for a uniform equidistant mesh of width $\Delta x = 2ri_{j,k} = 2ri_{\pm 1,j,k}$, $\frac{\delta P}{\delta x} \Big|_{i,j,k}$ doesn't depend on the value of $P_{i,j,k}$:

$$\frac{\delta P}{\delta x} \Big|_{i,j,k} = \frac{\overline{P_{i+\frac{1}{2},j,k}}^x (= \frac{P_{i+1,j,k} + P_{i,j,k}}{2}) - \overline{P_{i-\frac{1}{2},j,k}}^x (= \frac{P_{i-1,j,k} + P_{i,j,k}}{2})}{\Delta x} = \frac{P_{i+1,j,k} - P_{i-1,j,k}}{2\Delta x} \quad (74)$$

So by further developping equation (73) for a uniform equidistant mesh along each dimension axis :

$$\begin{aligned} (\nabla \cdot \nabla P)_{i,j,k} &\approx \frac{\frac{\delta P}{\delta x} \Big|_{i,j,k} + \frac{\delta P}{\delta x} \Big|_{i+1,j,k}}{2} - \frac{\frac{\delta P}{\delta x} \Big|_{i,j,k} + \frac{\delta P}{\delta x} \Big|_{i-1,j,k}}{2} + \frac{\frac{\delta P}{\delta y} \Big|_{i,j,k} + \frac{\delta P}{\delta y} \Big|_{i,j+1,k}}{2} - \frac{\frac{\delta P}{\delta y} \Big|_{i,j,k} + \frac{\delta P}{\delta y} \Big|_{i,j-1,k}}{2} \\ &\quad - \frac{\frac{\delta P}{\delta z} \Big|_{i,j,k} + \frac{\delta P}{\delta z} \Big|_{i,j,k+1}}{2} + \frac{\frac{\delta P}{\delta z} \Big|_{i,j,k} + \frac{\delta P}{\delta z} \Big|_{i,j,k-1}}{2} \\ &\approx \frac{P_{i+2,j,k} - 2P_{i,j,k} + P_{i-2,j,k}}{2\Delta x} + \frac{P_{i,j+2,k} - 2P_{i,j,k} + P_{i,j-2,k}}{2\Delta y} \\ &\quad + \frac{P_{i,j,k+2} - 2P_{i,j,k} + P_{i,j,k-2}}{2\Delta z} \end{aligned} \quad (75)$$

We can observe that, on the above equation, the pressure equation at a cell i, j, k doesn't depend on the pressure values of the adjacent cells $(i \pm 1, j, k)$, $(i, j \pm 1, k)$ and $(i, j, k \pm 1)$. So, for a collocated equidistant mesh grid, we have seen that using the interpolation $(\rho^n \underline{v}^n)_{i \pm 1/2, j, k}^x$ and keeping the consistency of the operator $\nabla \cdot \nabla$ in the Poisson's equation lead to an uncoupling between the odd and even index cell's pressures. So we can have a different solution for each combination of odd-even i, j, k , so 2 solutions for a 1D grid to 8 for a 3D grid. The pressure will oscillate from cell to cell between each solution. A 1D illustration is provided on figure 21 and on 2D a superimposition of four uniform pressure fields that could arise in a normally physical uniform pressure but numerically resulting by 4 uniform fields of dynamic pressure like in figure 22.

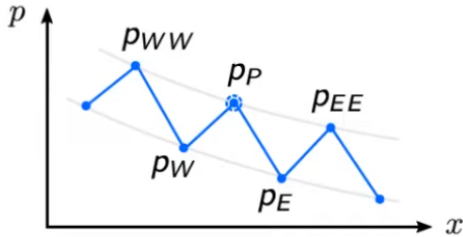


Figure 21: 1D example of cell to cell pressure oscillation between 2 solutions. [41]

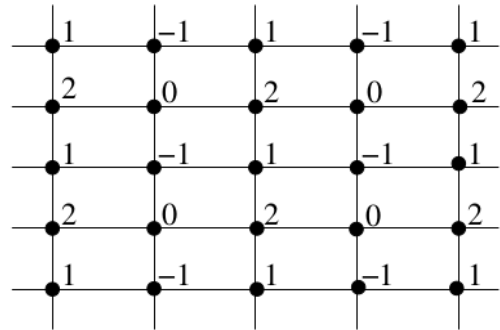


Figure 22: Example of checkerboard pressure field distribution, of four superimposed uniform fields on a 2D-spacing grid [26]

In a staggered grid, the velocities are stored directly at the inter face cells. So there is no need to interpolate at equation (72) and the momentum equation can be applied on equation (72) without

over bar interpolation thus directly using $\frac{\delta P}{\delta x}\Big|_{i+\frac{1}{2},j,k}$ ($= \frac{P_{i+1,j,k}-P_{i-1,j,k}}{\Delta x}$) instead of $\overline{(\frac{\delta P}{\delta x})_{i+\frac{1}{2},j,k}}^x$. This would lead to equation 75 having the result :

$$(\nabla \cdot \nabla P)_{i,j,k} \approx \frac{P_{i+1,j,k} - 2P_{i,j,k} + P_{i-1,j,k}}{2\Delta x} + \frac{P_{i,j+1,k} - 2P_{i,j,k} + P_{i,j-1,k}}{2\Delta y} + \frac{P_{i,j,k+1} - 2P_{i,j,k} + P_{i,j,k-1}}{2\Delta z} \quad (76)$$

And, as a result, having the adjacent cells pressure coupled. For a collocated grid a possible solution is to use a different interpolation for the interface center values like $(\rho^n \underline{u}^n)_{i+\frac{1}{2},j,k}$ etc. The idea is to use:

$$(\rho^n u^n)_{i+\frac{1}{2},j,k} \approx \overline{(\rho^n u^n)_{i\pm 1/2,j,k}}^x - \left(\frac{\delta P}{\delta x}\Big|_{i+\frac{1}{2},j,k} - \overline{(\frac{\delta P}{\delta x})_{i+\frac{1}{2},j,k}}^x \right) \quad (77)$$

By using this interpolation in equation (72) and applying the momentum equation for $\overline{(\rho^n u^n)_{i\pm 1/2,j,k}}^x$ the appearing $\overline{(\frac{\delta P}{\delta x})_{i+\frac{1}{2},j,k}}^x$ will be removed and replaced by $\frac{\delta P}{\delta x}\Big|_{i+\frac{1}{2},j,k}$ by the added corrective term $-(\frac{\delta P}{\delta x}\Big|_{i+\frac{1}{2},j,k} - \overline{(\frac{\delta P}{\delta x})_{i+\frac{1}{2},j,k}}^x)$. This modified interpolation makes sense and can be derived if you consider a control volume centered on the center face $i + \frac{1}{2}, j, k$ as done in [42] and [43]. Furthermore, we remind on the one hand that $P = P' - \rho Ri y$ so :

$$-\left(\frac{\delta P}{\delta x}\Big|_{i+\frac{1}{2},j,k} - \overline{(\frac{\delta P}{\delta x})_{i+\frac{1}{2},j,k}}^x \right) = -\left[\frac{\delta P'}{\delta x}\Big|_{i+\frac{1}{2},j,k} - \overline{(\frac{\delta P'}{\delta x})_{i+\frac{1}{2},j,k}}^x \right] + \left[Ri y_j \frac{\delta \rho}{\delta x}\Big|_{i+\frac{1}{2},j,k} - Ri \overline{(y \frac{\delta \rho}{\delta x})_{i+\frac{1}{2},j,k}}^x \right] \quad (78)$$

(we briefly comment that in the case of derivation along y that $\frac{\partial(P' - \rho Ri y)}{\partial y} = \frac{\partial P'}{\partial y} - Ri y \frac{\partial \rho}{\partial y} - \rho Ri$, but by applying this to the two terms on the left in equation (78) the two added terms ρRi will cancel each other. We just have to add a precision on the right side of (78) by replacing y by $\overline{y}_{j+\frac{1}{2}}^y$ like in the expression of F_u^n in equation (58)).

Finally, by reminding that $(\rho^n u^n)_{i,j,k} = -\frac{\delta P'^{(n)}}{\delta x}\Big|_{i,j,k} \Delta t + \rho^n \check{u}^{n-1} + Ri y_j \frac{\delta \rho}{\delta x}\Big|_{i,j,k}$ and applying it to equation (77) to develop the term $\overline{(\rho^n u^n)_{i\pm 1/2,j,k}}^x$ and using (78), we find back $F_u^n\Big|_{i+\frac{1}{2},j,k}$ as in 58:

$$(\rho^n u^n)_{i+\frac{1}{2},j,k} \approx \overline{(\rho^n \check{u}^{n-1})_{i+\frac{1}{2},j,k}}^x - \frac{\delta P'^n}{\delta x}\Big|_{i+\frac{1}{2},j,k} \Delta t + Ri y_j \frac{\delta \rho^n}{\delta x}\Big|_{i+\frac{1}{2},j,k} \Delta t \quad (79)$$

As a final comment, the important argument mentioned above that $\frac{\delta P}{\delta x}\Big|_{i,j,k}$ doesn't depend on $P_{i,j,k}$ illustrated by equation (74) leading to the uncoupling of adjacent cell's pressure (equation 75), this doesn't strictly hold in a case of an non-equidistant mesh where $\frac{\delta P}{\delta x}\Big|_{i,j,k}$ does actually depend on $P_{i,j,k}$, however if $ri_{i-1,j,k}$, $ri_{i,j,k}$ and $ri_{i+1,j,k}$ are not too much different, the coefficients multiplying $P_{i-1,j,k}$ and $P_{i+1,j,k}$ that would appear once the equation 75 is developed are lower than those multiplying $P_{i-2,j,k}$, $P_{i,j,k}$ and $P_{i+2,j,k}$ thus presenting a low coupling between adjacent cells. It would be interesting to further investigate in the literature the effect of non-equidistant meshes on the pressure oscillation, the article [42] showed that on a non-equidistant mesh (it took one with a strong variation of $ri_{i-1,j,k}$, $ri_{i,j,k}$ and $ri_{i+1,j,k}$) the auxiliary method still filters out the oscillation but didn't mention in details the effect of the grid on the occurring oscillations themselves.

4.7 Turbulence Modelling with LES Lagrangian Dynamic Model

The natural convection occurring in the pool is turbulent in this work, which means there is an unsteady velocity field. As explained in section 4.5 turbulent flows may be viewed as a hierarchy of eddies over a range of lengthscales to the smallest scales where they dissipate : the Kolmogorov scales. Direct Numerical Simulation resolves all the eddies, regardless of their size, the mesh size must thus be smaller and thus is very computational expensive. In order to simulate at high Rayleigh number, we use a LES method which is less computational expensive than a DNS method. In LES, the dynamics of the larger-scale motions are computed explicitly and the influence of the smaller scales than the grid (sub-grid scales SGS) are modelled. The cut off between the structures of a turbulent flow that are resolved and the ones which are modelled is done by applying a spatial filter to the governing equations. This procedure is done by the convolution of a quantity of interest ϕ with a low-pass filter function G (larger scales have a lower wavenumber). The equations are solved for those filtered quantities, mathematically the filtered velocity is for example $\bar{v}(\underline{x}, t)$:

$$\bar{v}(\underline{x}, t) = \int_{\Omega} G(\underline{r}, \underline{x}) v(\underline{x} - \underline{r}, t) d\underline{r} \quad (80)$$

where integration is over the entire flow domain Ω and the specified filter function G satisfies the normalised condition:

$$\int_{\Omega} G(\underline{r}, \underline{x}) d\underline{r} = 1 \quad (81)$$

In the simplest case, the filter function is independent of $\underline{x}$ so $G(\underline{r}, \underline{x}) = G(\underline{r})$ which allows the commutation of the filter with spatial derivative. Figure 23 shows some typical filters in 1D. More theoretical background about the filters and spectral analysis in wavenumber space using Fourier transform is provided in chapter 13 of the book of Pope [33].

Name	Filter function	Transfer function
General	$G(r)$	$\hat{G}(\kappa) \equiv \int_{-\infty}^{\infty} e^{i\kappa r} G(r) dr$
Box	$\frac{1}{\Delta} H(\frac{1}{2}\Delta - r)$	$\frac{\sin(\frac{1}{2}\kappa\Delta)}{\frac{1}{2}\kappa\Delta}$
Gaussian	$\left(\frac{6}{\pi\Delta^2}\right)^{1/2} \exp\left(-\frac{6r^2}{\Delta^2}\right)$	$\exp\left(-\frac{\kappa^2\Delta^2}{24}\right)$
Sharp spectral	$\frac{\sin(\pi r/\Delta)}{\pi r}$	$H(\kappa_c - \kappa),$ $\kappa_c \equiv \pi/\Delta$
Cauchy	$\frac{a}{\pi\Delta[(r/\Delta)^2 + a^2]}, \quad a = \frac{\pi}{24}$	$\exp(-a\Delta \kappa)$
Pao		$\exp\left(-\frac{\pi^{2/3}}{24}(\Delta \kappa)^{4/3}\right)$

Figure 23: Filter functions and transfer functions for one-dimensional filters [33]

The velocity is decomposed $v(\underline{x}, r) = \overline{v(\underline{x}, r)} + v'(\underline{x}, r)$. $v'(\underline{x}, r)$ is the residual field representing structures smaller than the filter width. As we are dealing with variable density flows, to avoid

having to model the sub-filter scale term of the mass conservation equation, we use a density-weighted filtering operation proposed by Favre [52], defined for an arbitrary quantity ϕ as:

$$\check{\phi} = \frac{\overline{\rho\phi}}{\bar{\rho}} \quad (82)$$

So, similarly, the velocity $\underline{v}(\underline{x}, t)$ is then decomposed into a slightly modified decomposition $\underline{v}(\underline{x}, t) = \underline{v}(\underline{x}, t) + \underline{v}''(\underline{x}, t)$. Applying the filter operation to the low Mach number approximation equations (19), (20) and (21), they become the filtered equations (we don't use the subscripts $()^0$ for simplicity) :

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \underline{\check{v}}) = 0 \quad (83)$$

$$\frac{\partial \bar{\rho} \underline{\check{v}}}{\partial t} + \nabla \cdot (\bar{\rho} \underline{\check{v}} \underline{\check{v}}) = -\nabla \cdot (\bar{P} - \frac{1}{3} \tau_{kk}^R) + \nabla \cdot \underline{\check{\tau}} + \bar{\rho} \underline{g} + \nabla \cdot (\underline{\tau}^r) \quad (84)$$

$$\frac{\partial \bar{\rho} \underline{\check{h}}}{\partial t} + \nabla \cdot (\bar{\rho} \underline{\check{h}} \underline{\check{v}}) = \frac{1}{PrRe} \nabla \cdot (k \nabla \bar{T}) - \nabla \cdot (\underline{q}^R) \quad (85)$$

Two terms appear, the sub-grid scale stress tensor $\underline{\tau}^R = -\bar{\rho}(\underline{\check{v}}\underline{\check{v}} - \underline{\check{v}}\underline{\check{v}})$ with it's anisotropic part $\underline{\tau}^r = \underline{\tau}^R - \frac{1}{3} \tau_{kk}^R \underline{I}$ and the sub-grid scale heat flux vector $\underline{q}^R = \bar{\rho}(\underline{\check{v}}\bar{T} - \bar{T}\underline{\check{v}})$. Also the term $\bar{P} - \frac{1}{3} \tau_{kk}^R$ is called the effective pressure and it is this value that is actually solved by the Poisson's equation in the algorithm. In order to close the equations for the filtered velocity, a model for the anisotropic sub-grid scale stress tensor is needed. The filtering operation in large eddy simulation can be implicit or explicit. The implicit filtering simply writes down the filtered above equations together with a model for the subgrid-scale stresses and then applies the desired solving algorithm as explained in 4.6 to this implicitly filtered system. In this way, the grid or the numerical discretization scheme can be assumed to be the low-pass filter (a simple example illustrating this concept for an equivalence between a finite difference operator and the exact derivative of a filtered variable is done at equation (4) of [54]). In this work, implicit filtering is used, it is often difficult to determine the shape of the implicit LES filter effectively applied. The papers [55] and [56] give some insight about the implicit filtering when using a finite volume method, volume-averaging can be interpreted as a top-hat spatial filtering (similar as the Box filter in figure 23) operation that smooths out the small-scale components. In the explicitly filtered approach, the filter is defined unambiguously and the convolution of equation (80) is done explicitly during the computation. So the terms "filtered" and "residual/subfiltered scales" are more appropriate terms used in explicit filtering than "resolved" and "subgrid scales" which are more appropriate for the implicit filtering. The filter cut off wavenumber is lower than the grid cut off wavenumber filtering effect, so that the scales filtered and kept by the explicit filter are larger than those resolved by the grid. So, for a same final cut off wavenumber target, explicit filtering needs a finer mesh leading to higher computational cost.

The purpose of subgrid (or subfilter for the explicit filtering procedure) scale modelling is to provide closure for the terms that were added in the governing equations by the filtering operation. The aim of the model is to withdraw energy from the filtered turbulent structures in order to imitate the forward energy cascade (see section 4.5) in the unresolved part. A common way to model the subgrid (or subfilter) scales is based on an artificial eddy viscosity approach. This can be accomplished by introducing an artificial turbulent viscosity, μ_t and considering:

$$\underline{\tau}^r \approx 2\mu_t \underline{\check{S}}^d \quad (86)$$

Several models of LES exist to give a way to calculate μ_t and can be quiet complex. In this work, the code uses the Lagrangian dynamic model procedure. It involves the application of an explicit second filter noted $\tilde{\phi}$ on top of the first filtering presented before (for simplicity and purpose of explanation, we consider constant density in the following paragraph and thus we don't use the Favre's filter notation $\check{\phi}$ but just keep the generic $\bar{\phi}$ notation for the first applied filter which can either be implicit or explicit, the reasoning is the same). The second filter, always explicit, called test filter has filter width $\tilde{\Delta}$, which is typically taken to be twice the one of the first filter $\bar{\Delta}$ (the width Δ mentioned are in the physical space, not the wavenumber space). So we obtain a filtered simple velocity vector $\bar{v}$ and a double filtered velocity vector $\tilde{v}$. The application of the first filter followed by the application of the second filter can be seen as the application of a unique filter $\tilde{\phi}$ which is a combination of the two filters with a width $\tilde{\Delta}$. The eddies are thus in three categories: the unknown eddies of lenghtscales going from the Kolmogorov lenghtscales η up to $\bar{\Delta}$, the known eddies of lenghtscale going from $\bar{\Delta}$ to $\tilde{\Delta}$ and finally the eddies of lenghtscale above $\tilde{\Delta}$ also known. The essential ingredient in the dynamic procedure is the assumption that the same model with the same value of the parameters coefficients to calculate μ_t can be applied to both the actual first filter $\bar{\phi}$ and the combined double filter $\tilde{\phi}$. It will use the known scales between $\bar{\Delta}$ and $\tilde{\Delta}$ to tune the parameter modelling the sub double filtered scales using in order to match closely the already know scales going from $\bar{\Delta}$ to $\tilde{\Delta}$. In a single filtered application, if $\underline{\tau}^R = -\rho(\bar{v}\bar{v} - \bar{v}\bar{v})$ is the stress tensor formed by turbulent motions of intermediate scale between η and $\bar{\Delta}$ applied to the scales with a lenghtscale above $\bar{\Delta}$, then, by analogy, the tensor:

$$\underline{\underline{T}} = -\rho(\tilde{v}\tilde{v} - \tilde{v}\tilde{v}) \quad (87)$$

is the stress tensor formed by turbulent motions of intermediate scale between η and $\tilde{\Delta}$ and applied to the scales with a lenghtscale above $\tilde{\Delta}$. Also, by the same analogy, the tensor:

$$\underline{\underline{L}} = -\rho(\bar{v}\tilde{v} - \tilde{v}\bar{v}) \quad (88)$$

is the stress tensor formed by turbulent motions of intermediate scale between $\bar{\Delta}$ and $\tilde{\Delta}$ and applied to the scales with a lenghtscale above $\tilde{\Delta}$. So the difference $\underline{\underline{T}} - \underline{\underline{L}}$ is the stress formed by turbulent motions of intermediate scale between η and $\bar{\Delta}$ applied to the scales with a lenghtscale above $\tilde{\Delta}$ and by developing:

$$\underline{\underline{T}} - \underline{\underline{L}} = -\rho(\tilde{v}\tilde{v} - \bar{v}\bar{v}) = \underline{\underline{\tau}}^R \quad (89)$$

which is equivalent to the Germano's identity [33]:

$$\underline{\underline{L}} = \underline{\underline{T}} - \underline{\underline{\tau}}^R \quad (90)$$

In the above equation, $\underline{\underline{L}}$ is called the resolved stress because we know everything to compute it exactly at each iteration. $\underline{\underline{\tau}}^R$ and $\underline{\underline{T}}$ are called the residual stresses based on the single and double filtering operations respectively, they can only be approximated by a model. As said before, an important assumption is that the same model with the same constant parameter values can be applied to both. The dynamic process is a procedure rather than a model as any subfilter-scale model can be used as a basis for it. For example, if we use the Smagorinsky model [33]:

$$\underline{\underline{\tau}}^r = \underline{\underline{\tau}}^R - \underbrace{\frac{1}{3}\tau_{kk}^R I}_{=\mu_t} \approx -2c_{S^d}\bar{\Delta}^2 \left| \overline{S^d} \right| \overline{\underline{\underline{S^d}}} \quad (91)$$

with $|\overline{S^d}| \equiv (2\bar{S}_{ij}^d \bar{S}_{ij}^d)^{1/2}$

The same model applied for $\underline{\underline{T}}$ with assuming the same constant parameter c_S :

$$\underline{\underline{T}}^d = \underline{\underline{T}} - \frac{1}{3} T_{kk} \underline{\underline{I}} \approx -2c_{S^d} \tilde{\Delta}^2 \widetilde{|\overline{S^d}|} \widetilde{\underline{\underline{S^d}}} \quad (92)$$

By using equations (90), (91) and (92), we get the approximation:

$$\underline{\underline{L}}^d = \underline{\underline{L}} - \frac{1}{3} L_{kk} \underline{\underline{I}} \approx 2c_S \bar{\Delta}^2 \widetilde{|\overline{S^d}|} \widetilde{\underline{\underline{S^d}}} - 2c_S \tilde{\Delta}^2 \widetilde{|\overline{S^d}|} \widetilde{\underline{\underline{S^d}}} \quad (93)$$

In the above equation, the only unknown is c_S , but this equation actually represents several equations due to the presence of tensors, so it is an overdetermined system and c_S cannot be chosen to satisfy exactly the equations, so the objective is to minimize the error :

$$\underline{\underline{e}} = \underline{\underline{L}}^d - \left(2c_S \bar{\Delta}^2 \widetilde{|\overline{S^d}|} \widetilde{\underline{\underline{S^d}}} - 2c_S \tilde{\Delta}^2 \widetilde{|\overline{S^d}|} \widetilde{\underline{\underline{S^d}}} \right) \quad (94)$$

This minimisation is usually done in a global least-square sense, the full derivations of the Lagrangian dynamic model is not given here as it is complex, we refer to [44] for the full derivation. The turbulent viscosity μ_t is computed at the end of the predictor and the corrector step of each iteration, it is also calculated for each grid point i, j, k and added to $\mu(T)$. So, in section 4.6, the μ used in the equations of the algorithm is in fact $\mu(T) + \mu_t$.

Then the sub-grid scale heat flux vector $\underline{q}^R$ is simply modelled by considering:

$$\underline{q}^R \approx -k_t \nabla \overline{T} \quad (95)$$

And k_t is linked with μ_t with a constant turbulent Prandtl number $Pr_t = \frac{c_p \mu_t}{k_t}$. In this work, Pr_t is set equal to 0.4 as in [32].

So, to be perfectly rigorous in section 4.6, the used and resolved variables should have been used with the subscripts $\bar{\phi}$ and $\hat{\phi}$. Finally, we have to keep in mind that those are spatial filtered values and do still vary with time due to the turbulence, they are not time averaged values $\langle \phi \rangle$. In the following sections, we will continue for simplicity not to use the spatial filtered subscripts.

5 Numerical results

5.1 General methodology

The objective of the simulations in this work is to analyse for different aspects ratios AR the emerging turbulent structures Large Scale Circulation (LSC) and turbulence statistics. The convention we use to specify an aspect ratio is $AR = \frac{W}{H} : 1 : \frac{L}{H}$, the vertical height H is kept constant at 0.045 m like in previous works [32] and is constant throughout the work. The reference temperature is kept at 330 K in order to have a coherent reference temperature with previous works [32],[45] and [57]. The difference temperature $\Delta T = T_{hot} - T_{cold}$ is thus calculated from the target Rayleigh number with equation 8. The simulations have been run during 500 T_f (see equation (25), to remove initial transient effect, the averaging over time starts after 200 T_f . The turbulent structure is analysed with the software Paraview [58], a visualisation software to plot the velocity fields and the temperature scalar. It is the time average quantities that are of interest in a turbulence simulation post-processing. As explained and analysed in [59] and [57], the LSC is not static, it undergoes non periodic re-orientations. So, when observing the LSC on Paraview, care is needed that the observed averaged structure is approximately steady, smaller averaging periods are first investigated step by

step on visualisation to detect such re-orientations. If they occur during 200-500 T_f averaging periods, it will be shown and discussed. A choice is often made of an averaging time interval where the structure is known to be stable to observe the main LSC and to present some insight full Paraview plots in this paper. However, the turbulence statistics analysis (see below) is always done on a full average over $300T_f$. The plots will mainly consist of streamline representation and slice cuts off to visualise inside the domain the LSC. Often, the LSC analysis will be illustrated for one of the two Rayleigh as the LSC is often very similar. When some differences occur, it will be a bit discussed.

About the turbulent statistics, they are displayed and analysed from bottom to top graphs along the vertical y . A quantity averaged over time is noted $\langle \phi \rangle_t$ (the averaging period is given as comment), we plot some of them along a chosen vertical line or we also average them both in time and on the horizontal plane noted $\langle \phi \rangle_{txz}$. The decomposition of a quantity is thus $\phi = \langle \phi \rangle_t + \phi'_t$ (ϕ' is a similar notation as in section 4.7 but not the same meaning). The temperature field is non-dimensional using (we remind that the hat ^ symbol means dimensional quantity):

$$\theta = \frac{\hat{T} - T_{ref}}{\Delta T} \quad (96)$$

Investigated statistics include the non-dimensional root mean square (rms) over time temperature:

$$\theta_{rms-t} = \sqrt{\langle \theta'_t \theta'_t \rangle_t} \quad (97)$$

and a variant of it, the root mean square (rms) over time and horizontal plane temperature:

$$\theta_{rms-txz} = \sqrt{\langle \theta'_{txz} \theta'_{txz} \rangle_{txz}} \quad (98)$$

The rms values tell us about the intensity of the turbulence effect (in laminar the rms over time is zero). The velocities u, v and w are also analysed, however, a horizontal rms is calculated combining u and w as follows:

$$u_{rms} = \sqrt{\langle u'u' \rangle + \langle w'w' \rangle} \quad (99)$$

(the rms can either be $t - rms$ or $txz - rms$ with the same logic).

The last statistic that we focus on is the the turbulent heat flux area-averaged $\langle \theta'_{txz} v'_{txz} \rangle_{txz}$. This value combines the temperature and vertical velocity, it provide some correlation between the two quantities.

Finally, we also investigate the non-dimensional mean heat transfer flux across the xz plane at height y measured by the local Nusselt number Nu_y . The non-dimensional is made by dividing the dimensional heat flux along y by $k_{ref} \frac{\Delta T}{H}$. So we have (we remind that the hat ^ symbol means dimensional quantity):

$$Nu_y = \left\langle \frac{\hat{q}_{convection} + \hat{q}_{conduction}}{k_{ref} \frac{\Delta T}{H}} \cdot e_y \right\rangle_{txz} = \left\langle \frac{\hat{\rho} \hat{v} \hat{c}_p (\hat{T} - T_{ref})}{k_{ref} \frac{\Delta T}{H}} + \frac{-\hat{k} \frac{\partial \hat{T}}{\partial y}}{k_{ref} \frac{\Delta T}{H}} \right\rangle_{txz} \quad (100)$$

By further developing using $v_{ref} = U_f$ from equation (24) and as the C++ code doesn't store $\hat{c}_p$ at each time step and each cell, we make the approximation $\hat{c}_p = c_{p-ref}$, we end up with:

$$Nu_y = \underbrace{\sqrt{PrRa} \langle \rho v \theta \rangle_{txz}}_{=Nu_{conv-y}} + \underbrace{\langle -k \frac{\partial \theta}{\partial y} \rangle_{txz}}_{=Nu_{diff-y}} \quad (101)$$

And the global Nusselt number Nu_G is obtained by averaging over the whole volume:

$$Nu_G = \sqrt{PrRa} \langle \rho v \theta \rangle_{txyz} + \langle -k \frac{\partial \theta}{\partial y} \rangle_{txyz} \quad (102)$$

Computing those Nusselt numbers will allow us to compare the heat transfer among the aspect ratios.

All those statistics have been obtained by post processing the data delivered by the code in C++, using Python language.

5.2 Standard case, aspect ratio AR=1:1:1

We have first started this work by running a standard case of aspect ratio AR=1:1:1 to test our manipulation of the C++ code and the post processing by comparing it with same cube aspect ratio case of [57] and [59]. In the other sections below, the large scale circulations will be compared with those of the standard case.

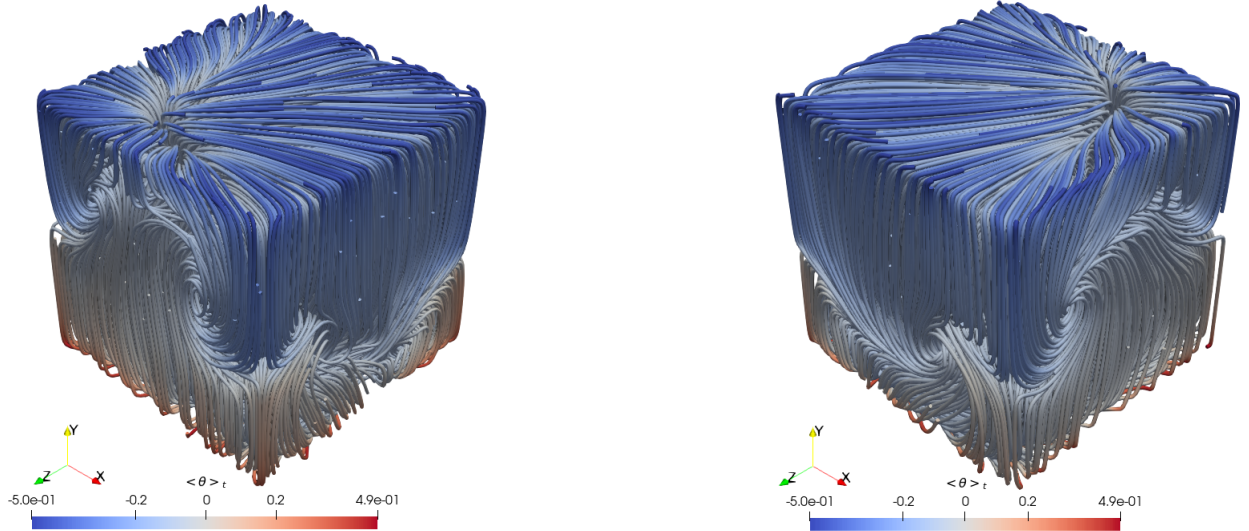


Figure 24: Streamlines plots with $\langle \theta \rangle_t$ of Rayleigh 10^7 (left) and Rayleigh $5 \cdot 10^7$ (left)

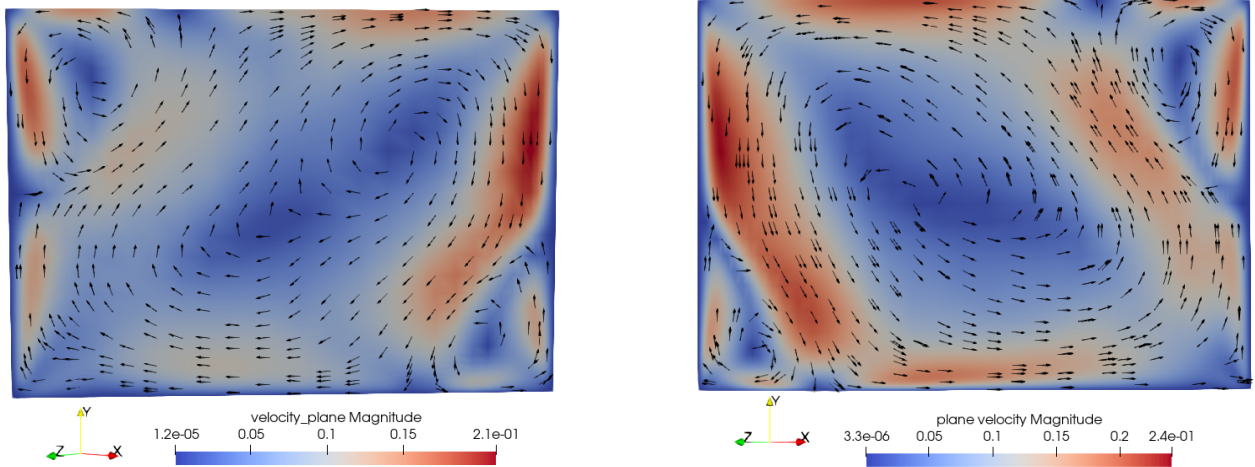


Figure 25: Diagonal slice along the LSC plane for Rayleigh 10^7 (left) and Rayleigh 5.10^7 (left), the plane velocity is the magnitude of the velocity vector in the plane (the normal component has been removed)

In this standard case, the flow topology is characterized by a large-scale circulation (LSC) occurring in a plane containing one of the diagonals of the cube, while we observe on the orthogonal diagonal two counter-rotating vortices. The impingement zone is concentrated and can be well observed near a corner of the top plate and in the opposite corner of the bottom plate. Near the impingement zone, the LSC plane also contains re-circulations than can be observed on the top left or bottom right of the figure 25, this observation is coherent with the streamlines of figure 24.

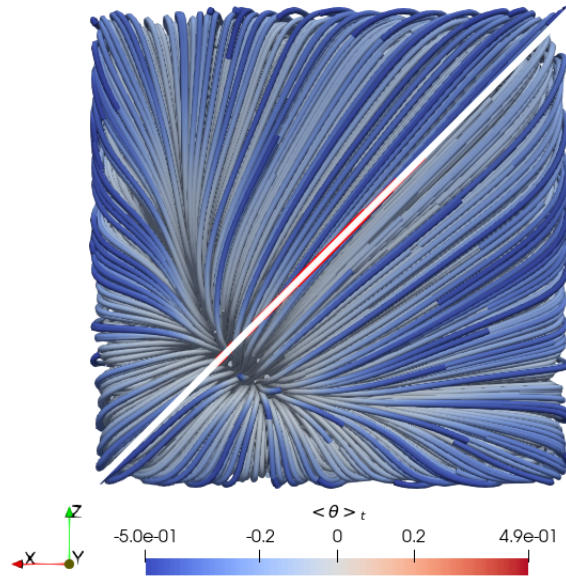


Figure 26: Schematic of the cut off plane along the diagonal done in the figure above

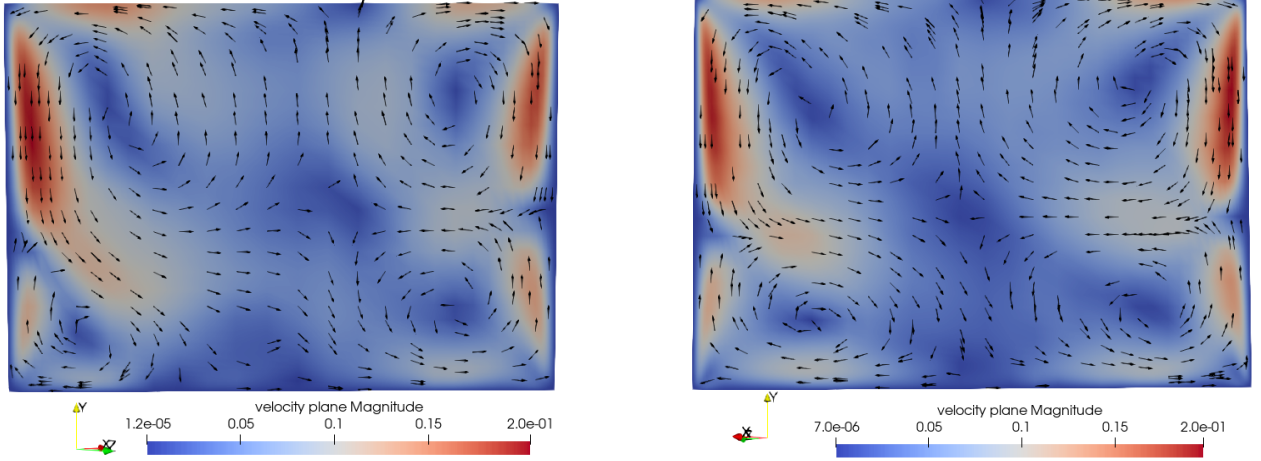


Figure 27: Orthogonal plane plotting the plane velocity (normal component of the velocity vector has been removed), at $Ra = 10^7$ on the left and $5 \cdot 10^7$ on the right

The above figures are the orthogonal planes, we can clearly observe the counter-rotating vortices, the ones above are slightly bigger than the ones below. During the simulations, we have also observed a reorientation of the diagonal flow, the LSC main diagonal flow remains the same at the beginning and at the end by changing its direction of circulation and the impingement zone went to the opposite corner as illustrated below:

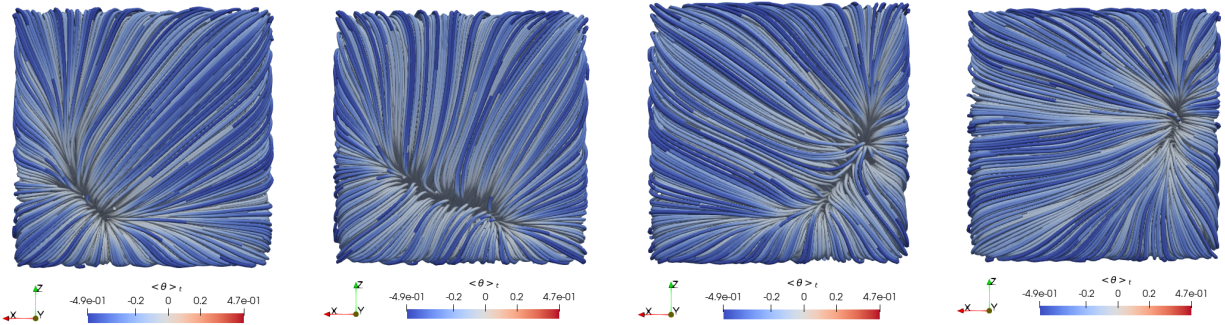


Figure 28: Example of reorientation sequence in an $AR=1:1:1$ with $Rayleigh = 5 \cdot 10^7$, average pictures taking from left to right at $100 - 150 T_f$, $150 - 200 T_f$, $200 - 250 T_f$ and $250 - 300 T_f$

This section was a remind of the cuboid with free slip at the upper boundary.

5.3 Aspect ratio from $AR=1:1:1$ to $AR=4:1:1$

In this section, the aspect ratio will vary by changing the width W and keeping H and L constant. First, we will get some insight of the emerging circulation structure for each aspect ratio, and then, at the end, the turbulence statistics will be compared altogether graphically.

5.3.1 Aspect ratio $AR=2:1:1$

We first observe the case where $\frac{W}{H} = 2$: the streamlines are similar for the two Rayleigh numbers, we observe one impingement point at the top in the middle along a side and two at the bottom on

the opposite corners.

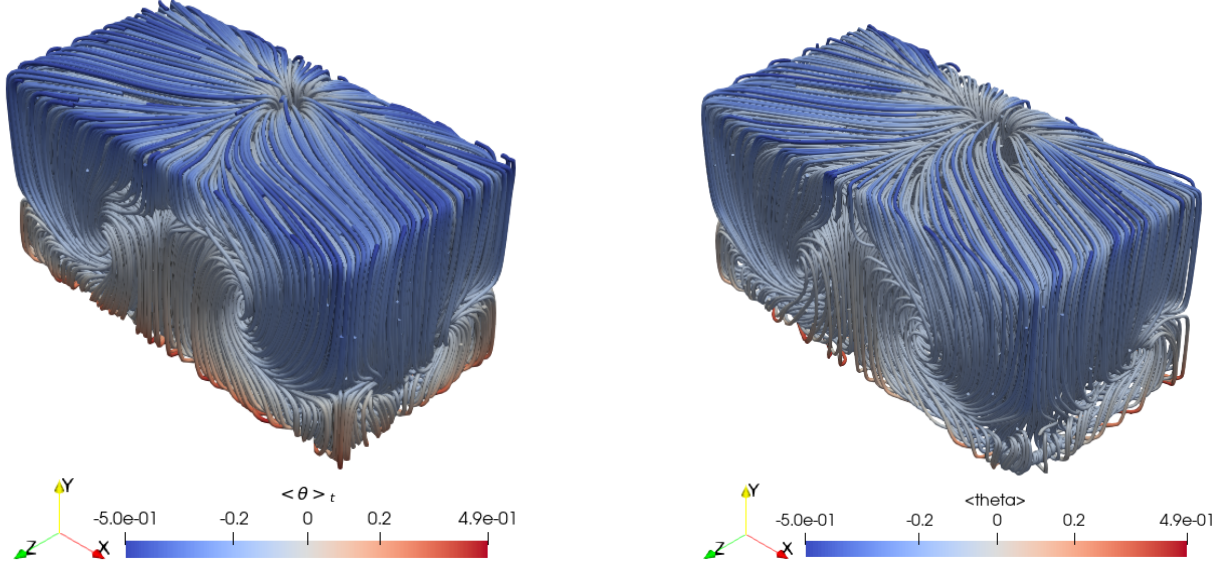


Figure 29: Plots of streamlines, average θ for $Ra = 10^7$ on the left and $Ra = 5 \cdot 10^7$ on the right

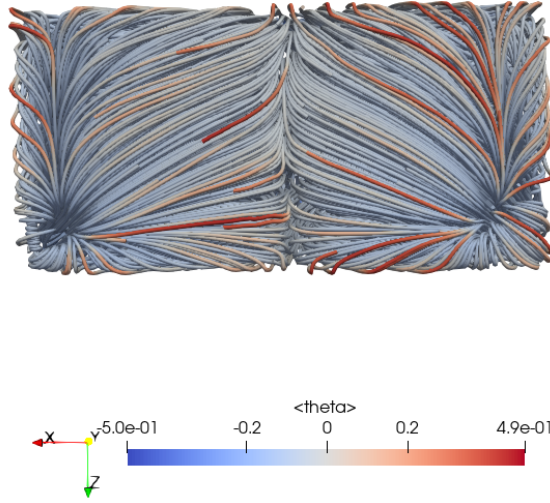


Figure 30: Streamlines from the bottom at $Ra = 5 \cdot 10^7$

One may think by looking at those above streamlines that the structure is just the double duplication as the standard case. However, by looking at the circulation in the planes joining the impingement points, we indeed observe some similarities with the standard case as seen on the upper left image of figure 31) but the orthogonal plane doesn't show the two counter-rotating vortices.

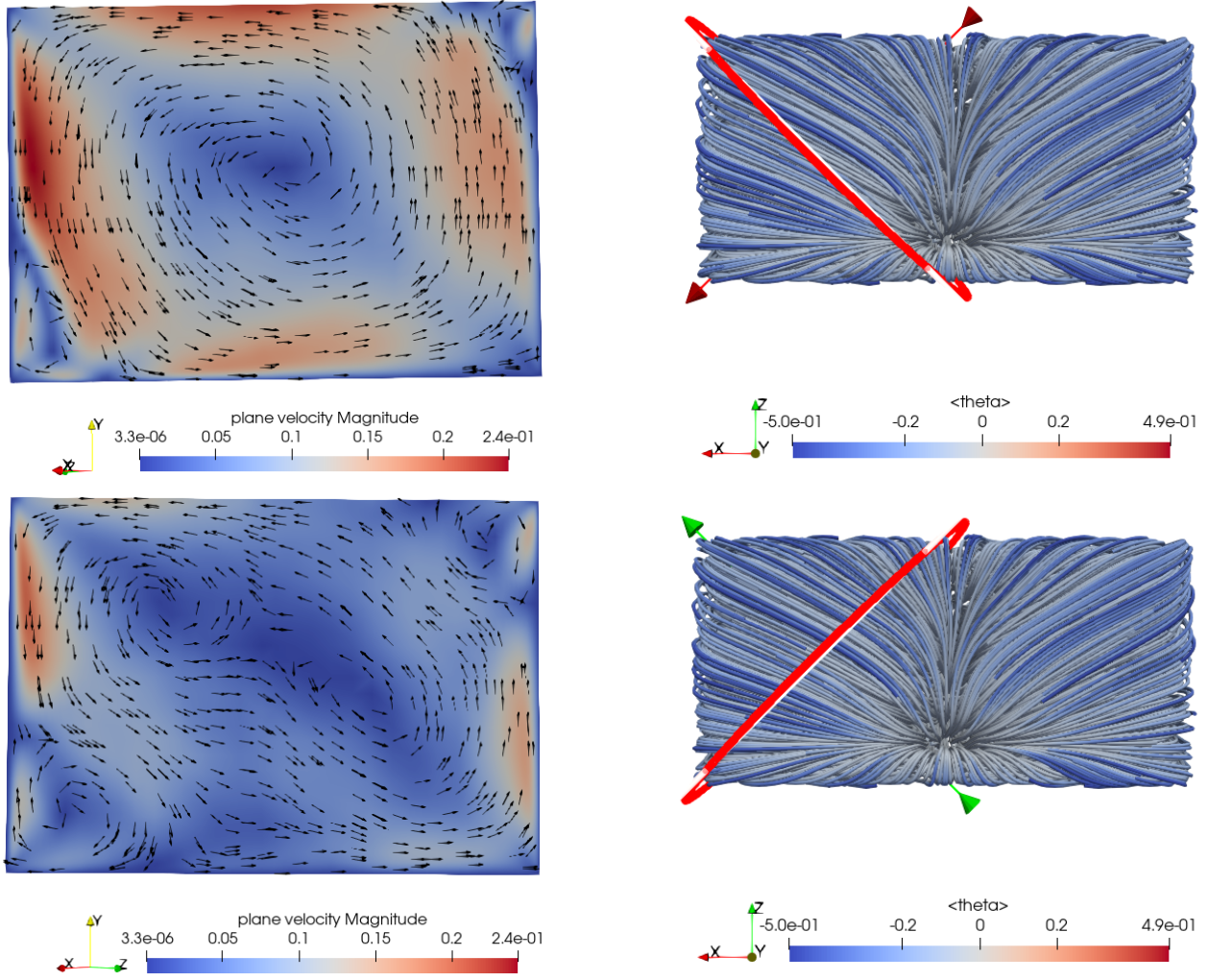


Figure 31: Plane velocity plots on the left, both at $Ra = 5 \cdot 10^7$, with the corresponding slice seen from above on the respective right image

To understand more clearly the structure underlying, we made some clips from the 3D streamlines structures as shown on figure ??.

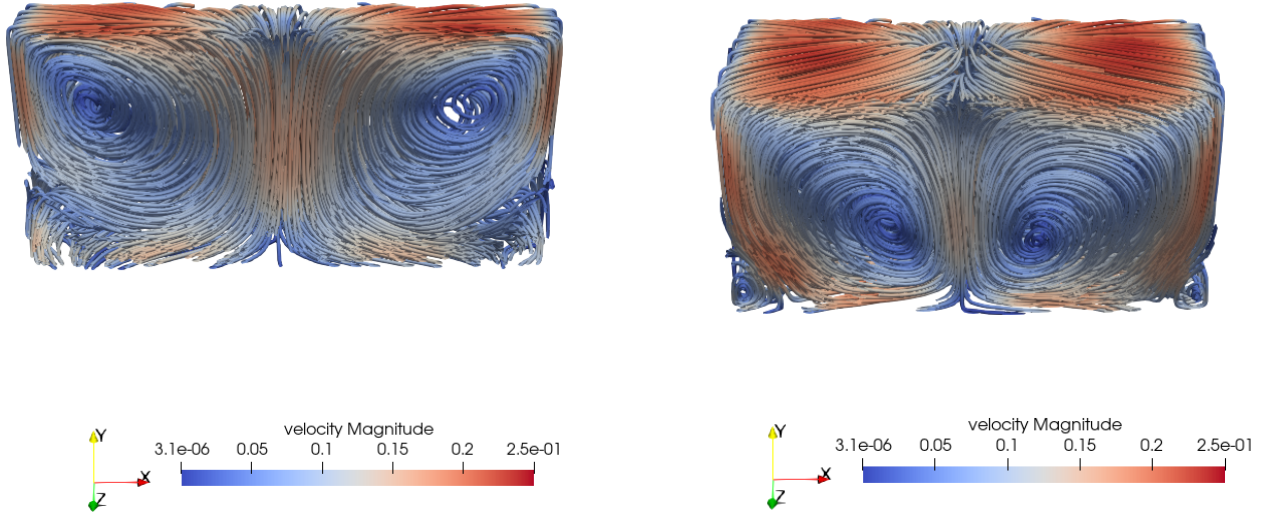


Figure 32: Doubles rolls observation for $Ra=5 \cdot 10^7$ for $AR=2:1:1$

One clip is at the level of the impingement point (on the left image of figure 32), we observe two convection roll structures, the axis of the rolls isn't exactly perpendicular to the xy axis. Indeed, by doing a parallel clip further away, we can remark that the centre axis of the rolls went closer to the middle and lower. Furthermore, we observed one movement of the impingement point, it changed side as shown on figure 33 but the rolls structure didn't change his circulation direction like a reorientation in the standard case. Indeed, the roll's axis changed a bit and present a reverse situation, the extremity closest from the center and lowest goes further and higher and vice versa.

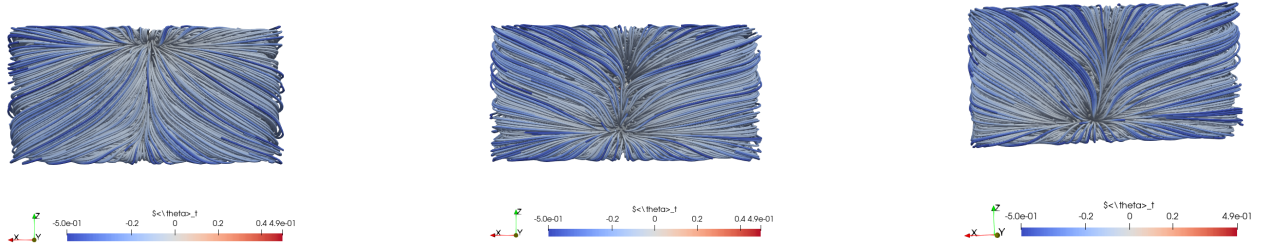


Figure 33: Movement of the impingement point sequence in an $AR=2:1:1$ with $Rayleigh = 5 \cdot 10^7$, averaging pictures taking from left to right at $50 - 100 T_f$, $100 - 150 T_f$ and $150 - 200 T_f$

5.3.2 Aspect ratio $AR=3:1:1$ and Aspect ratio $AR=4:1:1$

The aspects ratios $\frac{W}{H} = 3$ and $\frac{W}{H} = 4$ are very similar as shown on figure 34 comparing two different Rayleigh numbers and two different aspect ratios. Similarly, there is a double roll convection cell, the axis is more centred and horizontal than in the previous case and the impingement point is centred and doesn't move significantly.

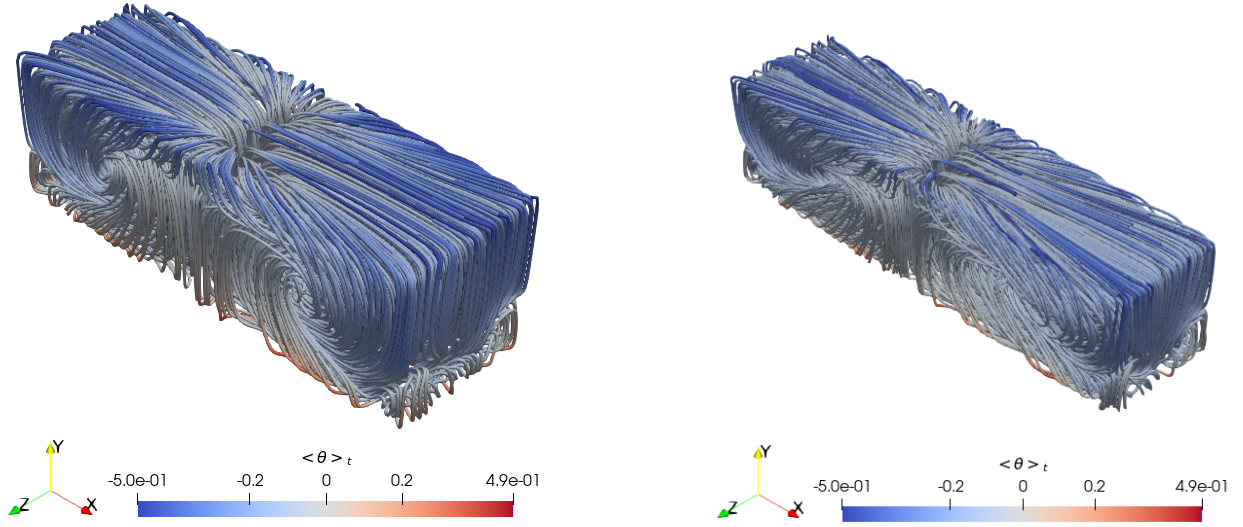


Figure 34: Streamlines at $Ra = 10^7$ with $\frac{W}{H} = 3$ on the left and Streamlines at $Ra = 5 \cdot 10^7$ with $\frac{W}{H} = 4$ on the right

The convection cells are very clean and stable, we can observe a small re-circulation on the cut of the plan $z = 0.5$ at the bottom, towards the external. This re-circulation is more important at the planes get closer to the faces $z = 0$ and $z = 1$ (see figure 35).

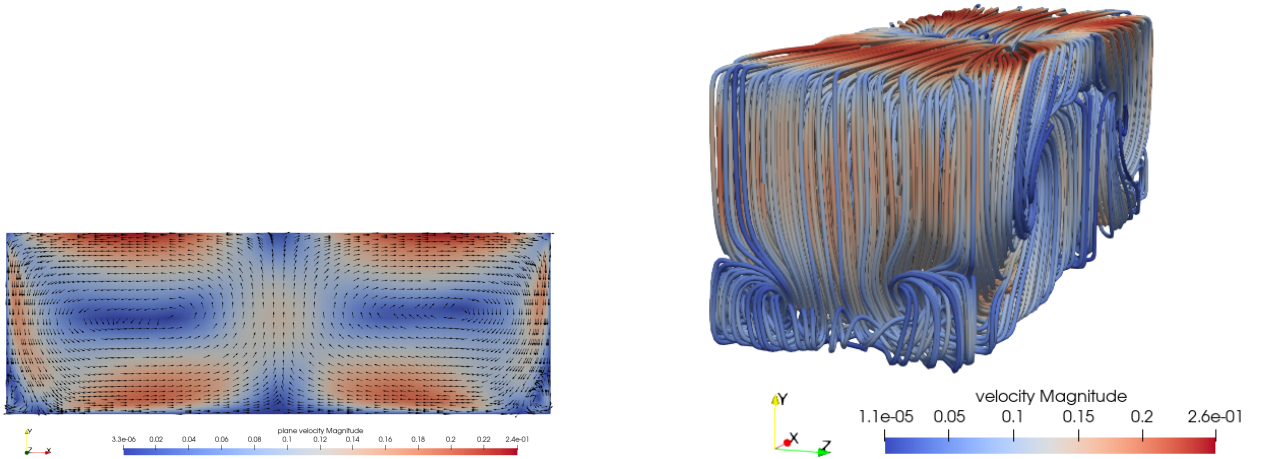


Figure 35: Plane cut at $z = 0.5$ (left) for $\frac{W}{H} = 3$ and $Ra = 10^7$ and streamlines seen from the side

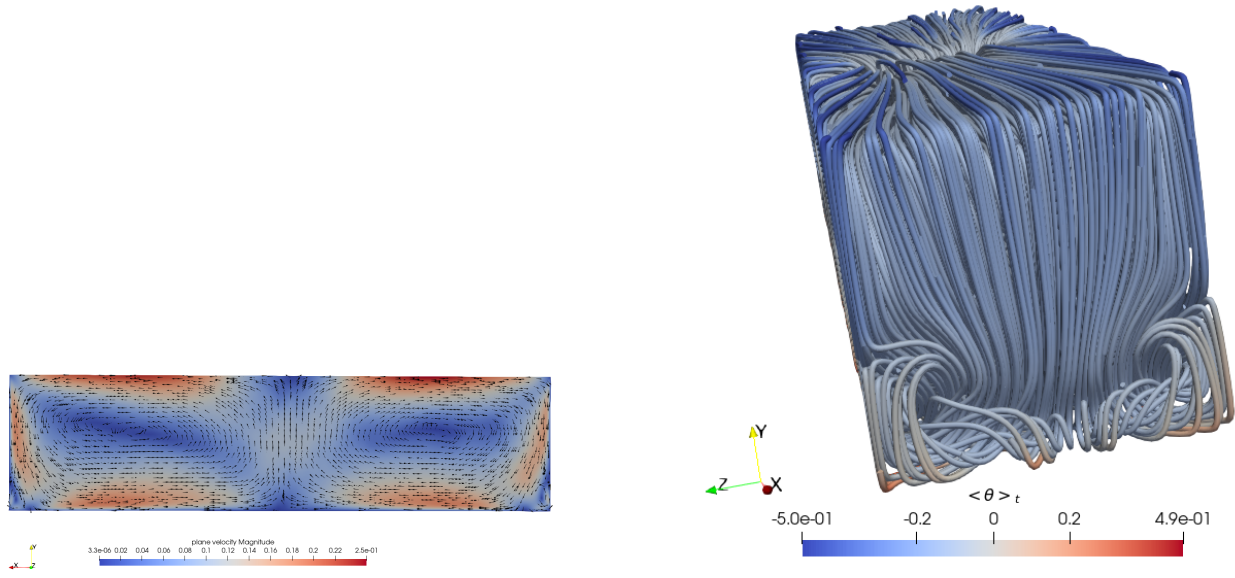


Figure 36: Plane cut at $z = 0.5$ (left) for $\frac{W}{H} = 4$ and $Ra = 5 \cdot 10^7$ and streamlines seen from the side

5.4 Turbulence statistics for Aspect ratio from AR=1:1:1 to AR=4:1:1

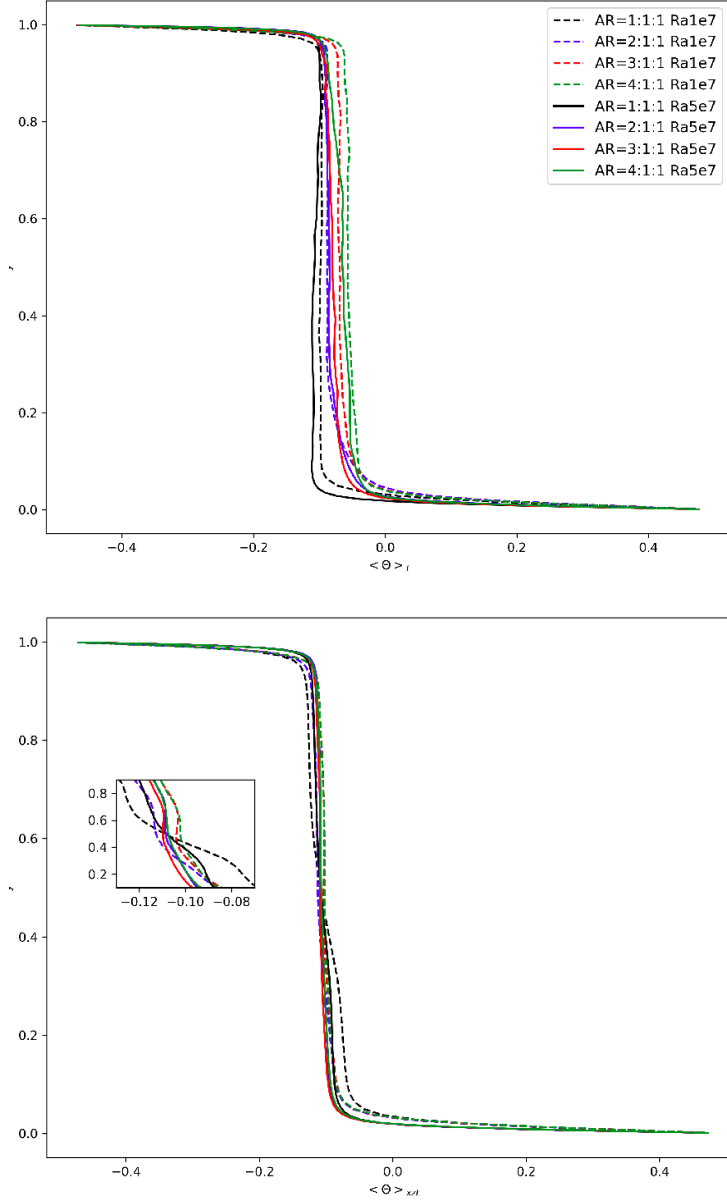


Figure 37: On the top, $\langle \theta \rangle_t$ plotted along the vertical centre line and on the bottom $\langle \theta \rangle_t$ xz the temperature area averaged along the vertical

The temperature profiles plotted on Figure 37 are coherent from previous studies [45]. Near the bottom wall, the temperature changes approximately linearly along the vertical. In this thin thermal boundary layer conduction of heat is the main heat transfer. Then, after a transition phase, the temperature reaches a constant value in the bulk of the domain where convection is the main heat transfer (see below the graph of the convection Nusselt and conduction Nusselt as a complement). In this bulk zone, the temperature isn't equal to T_{ref} but lower (shifted to the left) due to the free slip upper boundary compare to the upper fixed wall as analysed by [57]. Regarding the influence of the AR on figure 37, at both Rayleigh numbers investigated, the center line is shifted back

toward the middle in presence of higher AR, this effect is less visible however for the area averaged temperature.

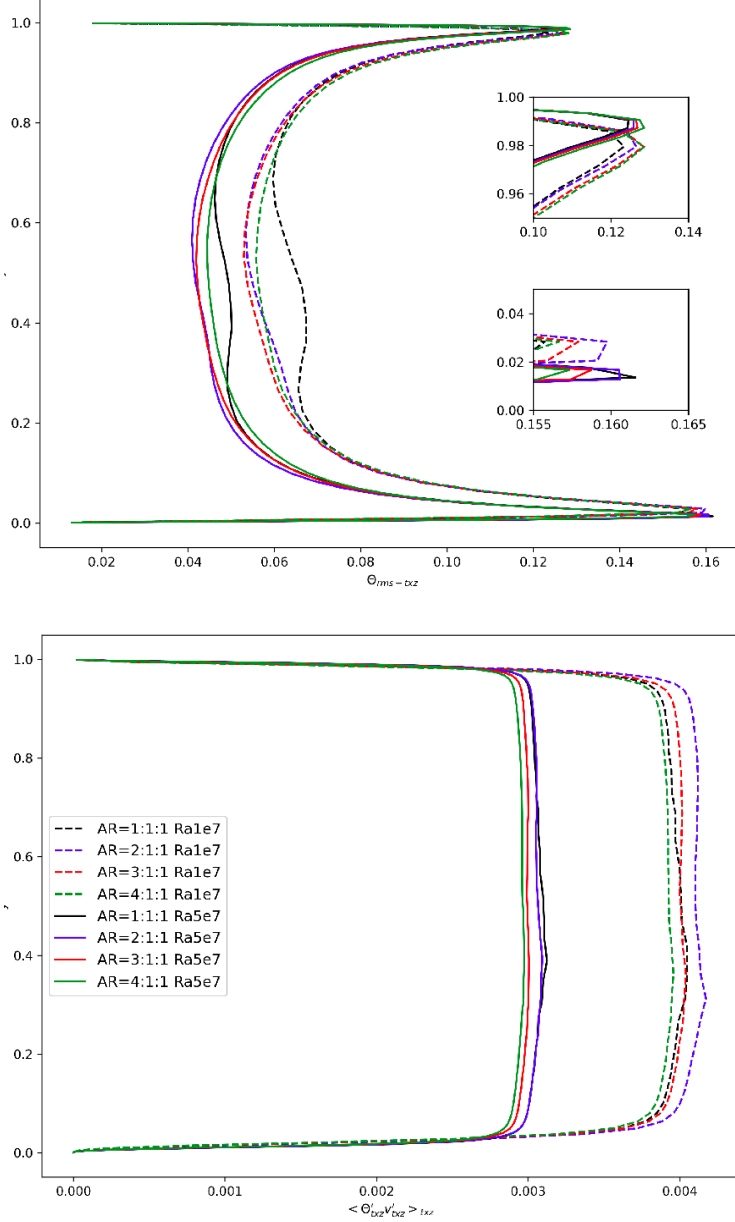


Figure 38: On the top, $\theta_{rms-txz}$ along the vertical and on the bottom $\langle \theta'_{txz} v'_{txz} \rangle_{txz}$ along the vertical

Regarding the rms (over time and area) (on the of figure 38) several observation can be done. The bulk values of the $\theta_{rms-txz}$ are lower for higher Rayleigh which is coherent with other observations studies [57]. The peaks in the thermal boundary layers occur closer to the wall for higher Rayleigh numbers and a higher aspect ratio has the tendency to increase that peak value except for the bottom peak values of the Rayleigh values equal to $5 \cdot 10^7$. Regarding the turbulent heat flux $\langle \theta'_{txz} v'_{txz} \rangle_{txz}$, the aspect ratio seems to decrease it.

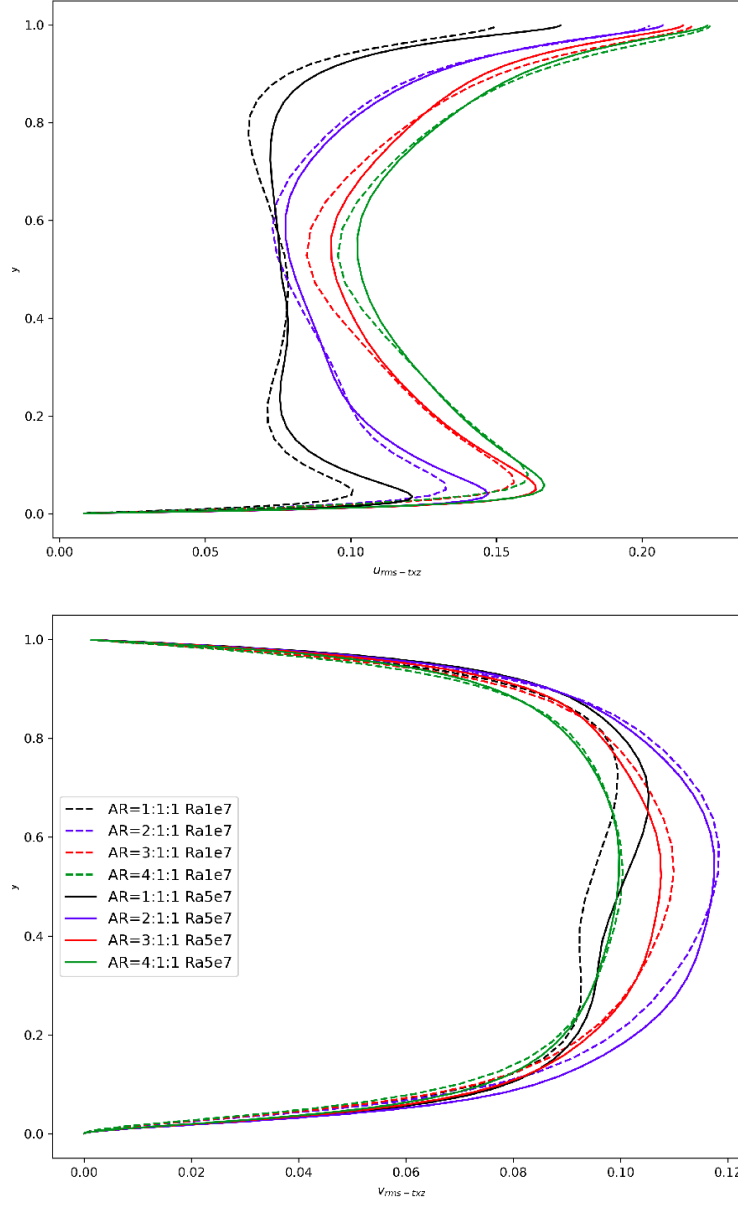


Figure 39: On the top, $u_{rms-txz}$ along the vertical and on the bottom, $v_{rms-txz}$ along the vertical

About the rms velocities, the aspect ratio increases the turbulence intensities of horizontal velocities whereas it is the contrary for $v_{rms-txz}$.

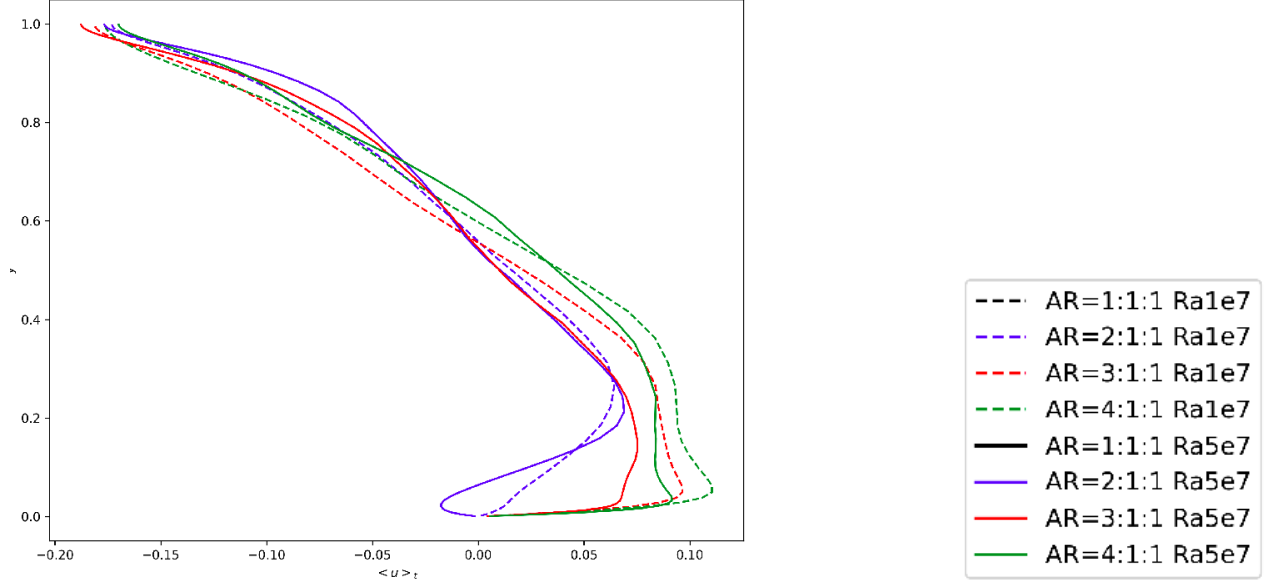


Figure 40: On the left, $\langle u \rangle_t$ along the vertical for $\hat{x} = \frac{1}{4}W$ and $\hat{z} = \frac{1}{2}L$

One interesting velocity statistic to plot is the horizontal velocity $\langle u \rangle_t$ at the vertical center line of the first half (at $\hat{x} = \frac{1}{4}$ and at $\hat{z} = \frac{1}{2}L$). The three aspect ratios from 2 to 4 present some similar dual rolls, so plotting that horizontal velocity along the vertical allows to compare the speeds in the rolls where the velocity is mainly horizontal. Both at the upper circulation and lower circulation, the aspect ratio increases the centre u speed, however this increase is less significant at the free slip boundary side.

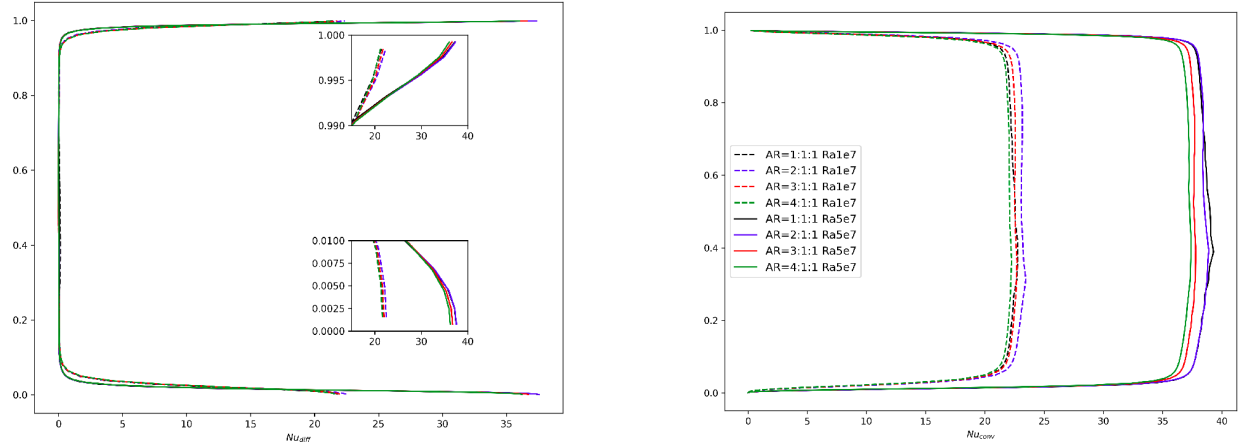


Figure 41: On the left the Nu convection along the vertical and on the right the Nu convection

Finally, we can have a look on the Nusselt numbers, we can observe that the increase of the aspect ratio has negligible effect on the diffusion Nusselt, but mostly has the effect to decrease the convection Nusselt in the bulk. This is quite coherent with the total averaging of the Nusselt G as displayed in the table below, the reduction of Nu_G with AR is especially visible for the higher Rayleigh case:

Ar & Ra	Nu_G
AR=1:1:1 Ra 1e7	22.359
AR=2:1:1 Ra 1e7	23.082
AR=3:1:1 Ra 1e7	22.489
AR=4:1:1 Ra 1e7	22.008
AR=1:1:1 Ra 5e7	38.476
AR=2:1:1 Ra 5e7	38.370
AR=3:1:1 Ra 5e7	37.524
AR=4:1:1 Ra 5e7	37.054

Table 1: Nu_G for each case of study

5.5 Aspect ratio from AR=1:1:1 to AR= $\frac{1}{4}$:1: $\frac{1}{4}$

In this section, we will quickly analyse the effect of varying the aspect ratio $\frac{W}{H} = \frac{L}{H}$ from 1 to $\frac{1}{4}$, we keep thus at the base $W = L$. Unfortunately, one simulation ($Ar = \frac{1}{3}$ at $Ra = 5 \cdot 10^7$) was wrongly parameterised and one simulation has clear numerical errors ($Ar = \frac{1}{4}$ at $Ra = 10^7$), which might be due to unbalanced sizes of the cells in the mesh.

5.5.1 Aspect ratio AR= $\frac{1}{2}$

We first start with an aspect ratio of $\frac{1}{2}$, the result of the emerging structure is similar for both investigated Rayleigh numbers.

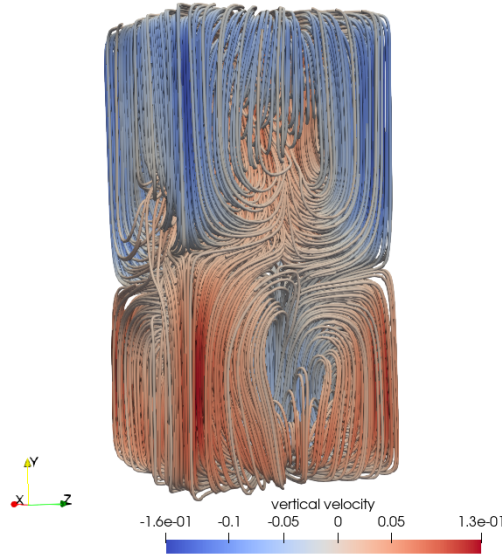


Figure 42: Streamlines at $Ra = 5 \cdot 10^7$ for an aspect ratio AR=1: $\frac{1}{2}$: $\frac{1}{2}$

[32] investigated a similar aspect ratio but for a higher Rayleigh and observed similar but elongated circulation than the standard case. In our case, at lower Rayleigh, we observe 8 rolls in total: 4 on the above part and 4 on the under half approximately with an impingement point located in the middle. These rolls are located along the vertical corners, as can be seen on figure 43, but they are not homogeneous, as can be seen by comparing the middle plane cut and the right

one on figure 43. Some above rolls are longer and have downward streamlines that join the lower rolls. The middle plane clearly shows the difference between upper right and upper left rolls. The location of those slightly different rolls can change over time, switching to another diagonal.

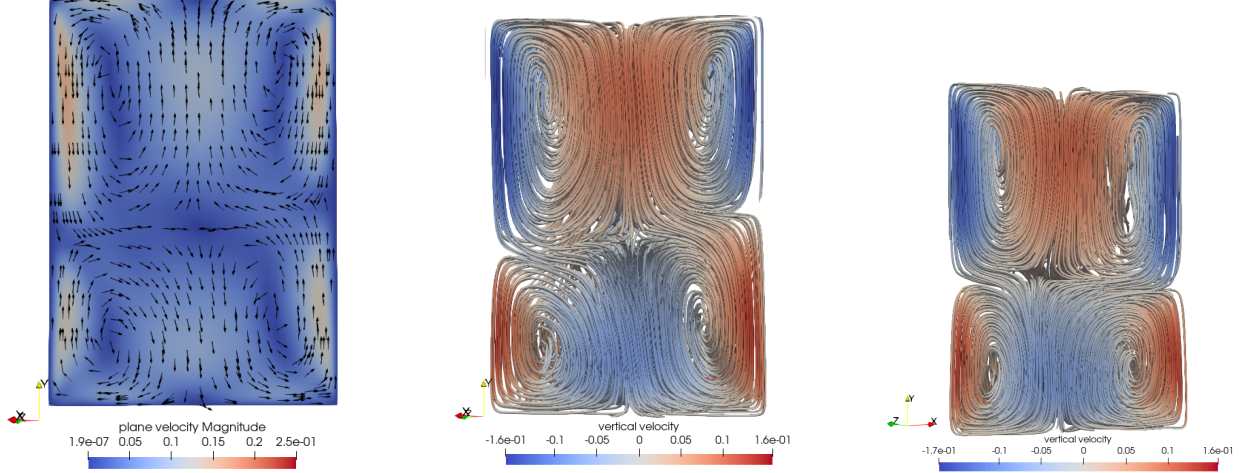


Figure 43: Sections of figure 42: the middle and the left represent the same plane, the one on the right represents the perpendicular plane

5.5.2 Aspect ratio $AR=\frac{1}{4}$

The pattern at higher aspect ratio remains the same at those observed above, the streamline connections and in-homogeneity between the rolls become more apparent, the rolls at the lower half are now longer than those above (figure 44).

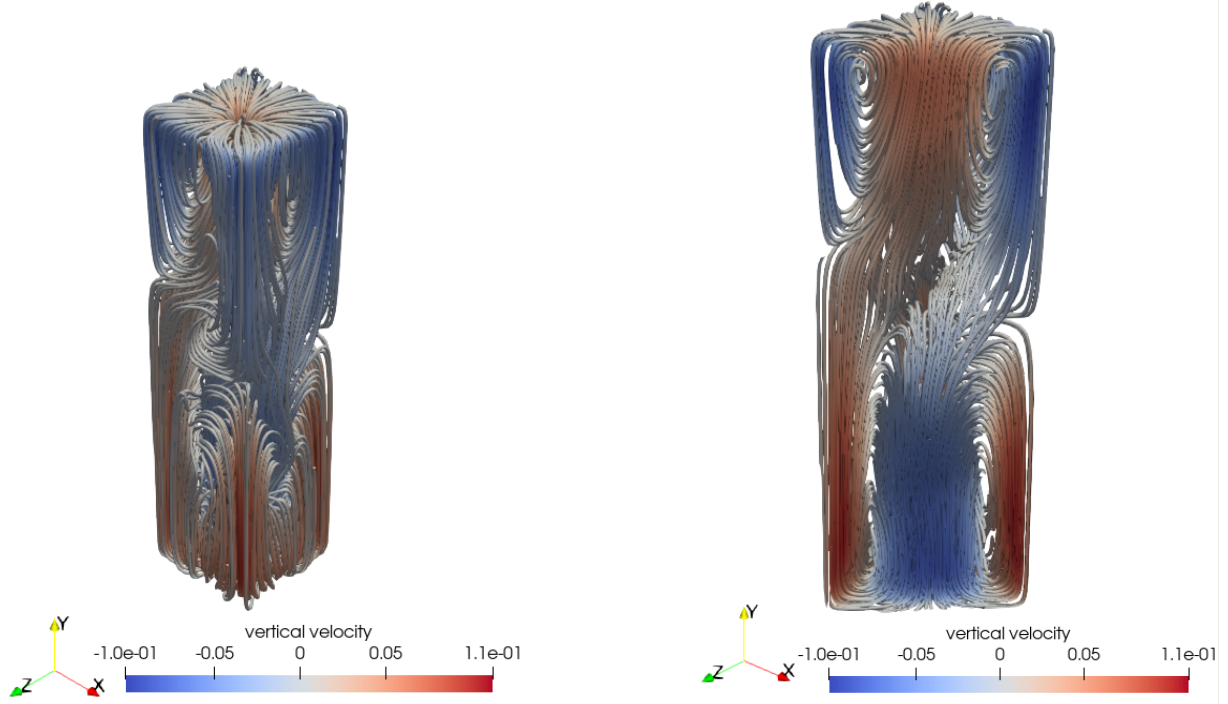


Figure 44: Streamlines plot and section for an aspect ratio of 4 at $Ra = 5 \cdot 10^7$

5.5.3 Turbulence statistics from $AR=1:1:1$ to $AR=\frac{1}{4}:1:\frac{1}{4}$

In this section, we will follow the same procedure as the previous observation of turbulence statistics.

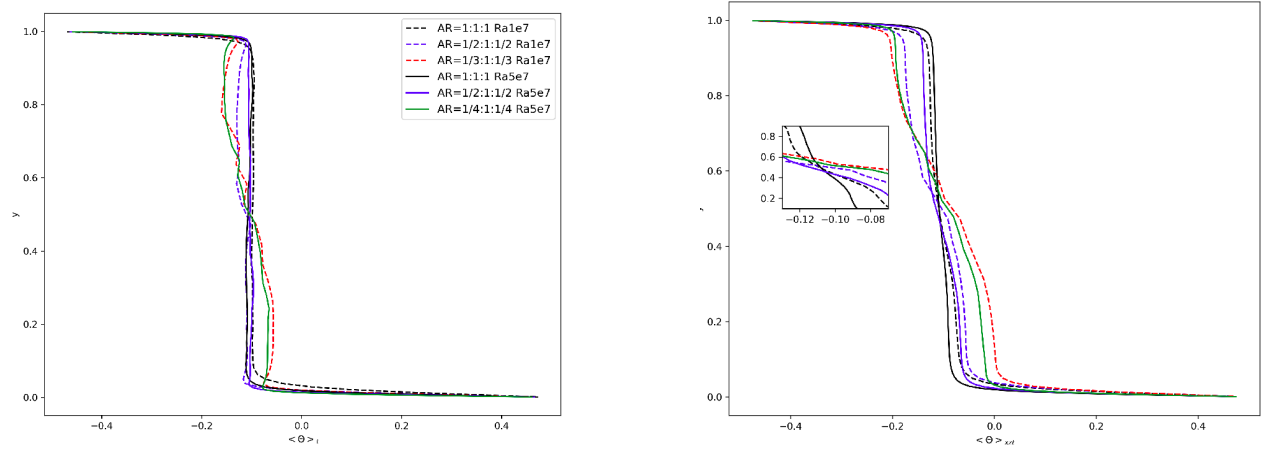


Figure 45: On the left, $\langle \theta \rangle_t$ plotted along the vertical centre line and on the right $\langle \theta \rangle_t$ the temperature area averaged along the vertical

On figure 45, we can clearly observe that, in this case, the temperature isn't constant in the bulk, there is an asymmetry at mid-height, the higher the aspect ratio will be, the higher this effect takes place and even more at lower Rayleigh number. We can presume that this is due to opposite circulation of the rolls in the middle and the clear asymmetry at half-height at the interface of the

rolls.

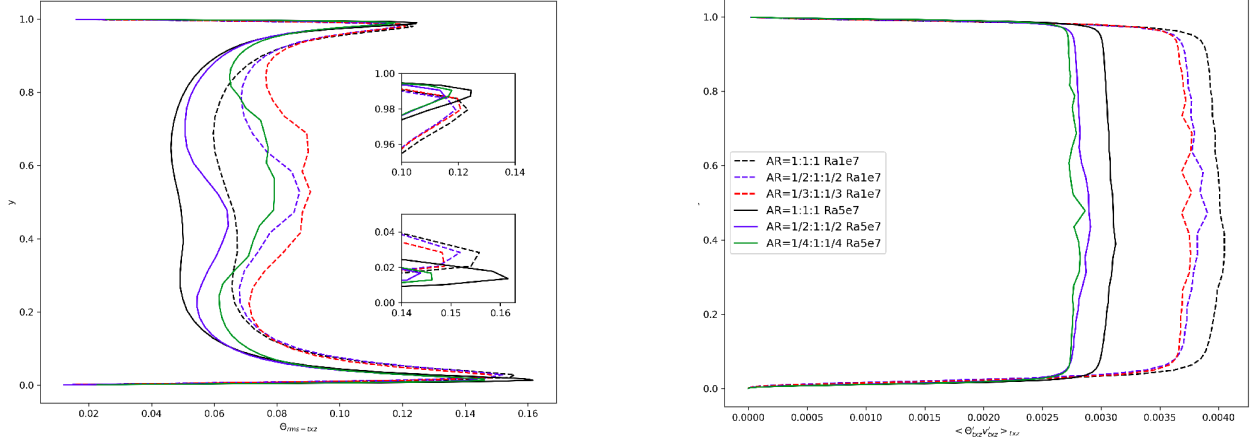


Figure 46: On the left, $\theta_{rms-txz}$ along the vertical and on the right $\langle \theta'_{txz} v'_{txz} \rangle_{txz}$ along the vertical

We still have higher Rayleigh who has a lower $\theta_{rms-txz}$ but, in this case, the aspect ratio has the contrary effect by increasing the bulk rms. Regarding the turbulent heat flux $\langle \theta'_{txz} \rangle_{txz}$, the patterns are similar than in previous turbulence analysis.

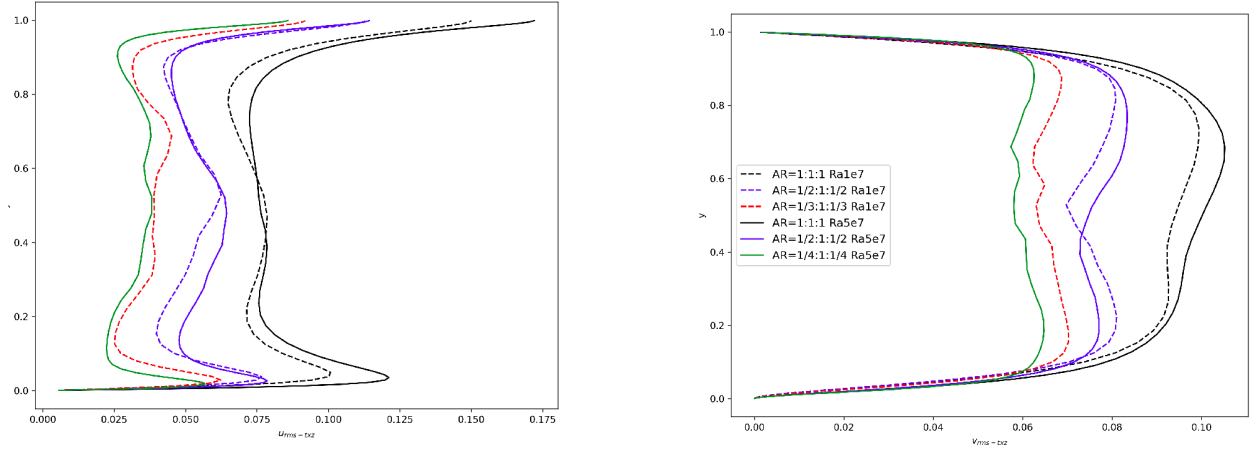


Figure 47: On the left, $u_{rms-txz}$ along the vertical and on the right $u_{rms-txz}$ along the vertical

We have the opposite result of what we had before for the u_{rms} : the aspect ratio seems to reduce this turbulence intensity instead of increasing it.

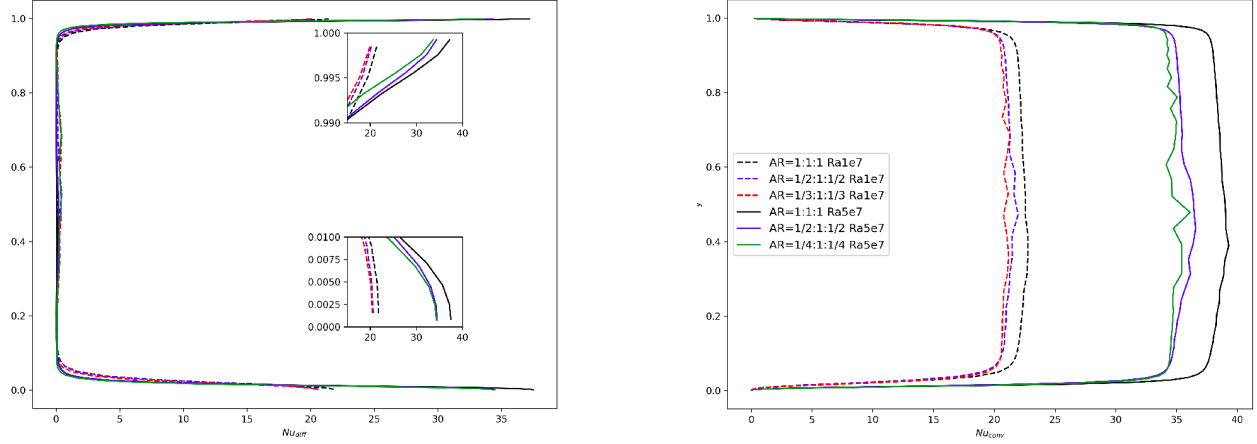


Figure 48: Nu conduction on the left and Nu convection on the right

The Nusselt number trends are quite similar than the other aspect ratio, the convection Nusselt seems to reduce in response of an increase of the aspect ratio. In this case, the Nu_G is fully coherent with this observation.

Table 2: Table of Nu_G values

Paramètres	Valeur
AR=1:1:1 Ra1e7	22.359
AR= $\frac{1}{2}$:1:1/2 Ra1e7	21.313
AR= $\frac{1}{3}$:1:1/3 Ra1e7	21.040
AR=1:1:1 Ra5e7	38.476
AR= $\frac{1}{2}$:1:1/2 Ra5e7	35.553
AR= $\frac{1}{4}$:1:1/4 Ra5e7	34.916

5.6 Aspect ratio AR=2:1:2

A simulation modelling a flat pool has also been simulated at the two Rayleigh numbers. It can eventually give some information of a pool half evaporated. Some major differences have been observed between the two Rayleigh numbers. First, at $Ra = 5 \cdot 10^7$, we observe a similar circulation as the standard case, of course it is more "flat" but the structure is the same: a main circulation along a diagonal joining a top and a bottom impingement and counter rotating vortices on the diagonals (see Figures 49 and 50). The structure is also very stable, no significant movement has been observed.

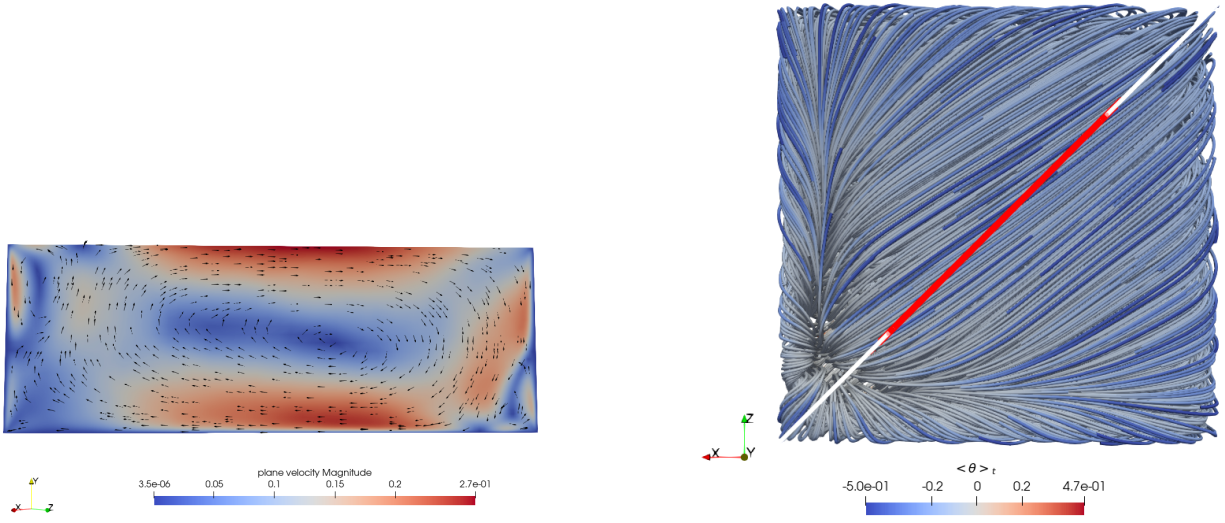


Figure 49: Main diagonal cut, for the case of $\text{Rayleigh} = 5 \cdot 10^7$

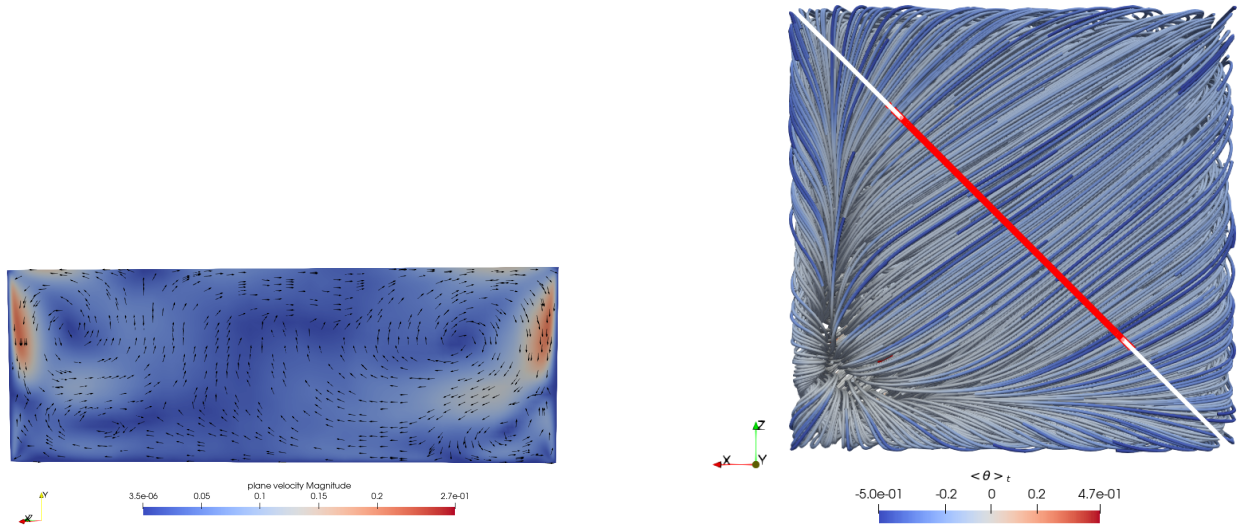


Figure 50: Orthogonal diagonal cut, for the case of $\text{Rayleigh} = 5 \cdot 10^7$

For the case of $\text{Ra} = 10^7$, at the beginning of the simulation, we can see two impingement points at the top and at the bottom (see figure 51).

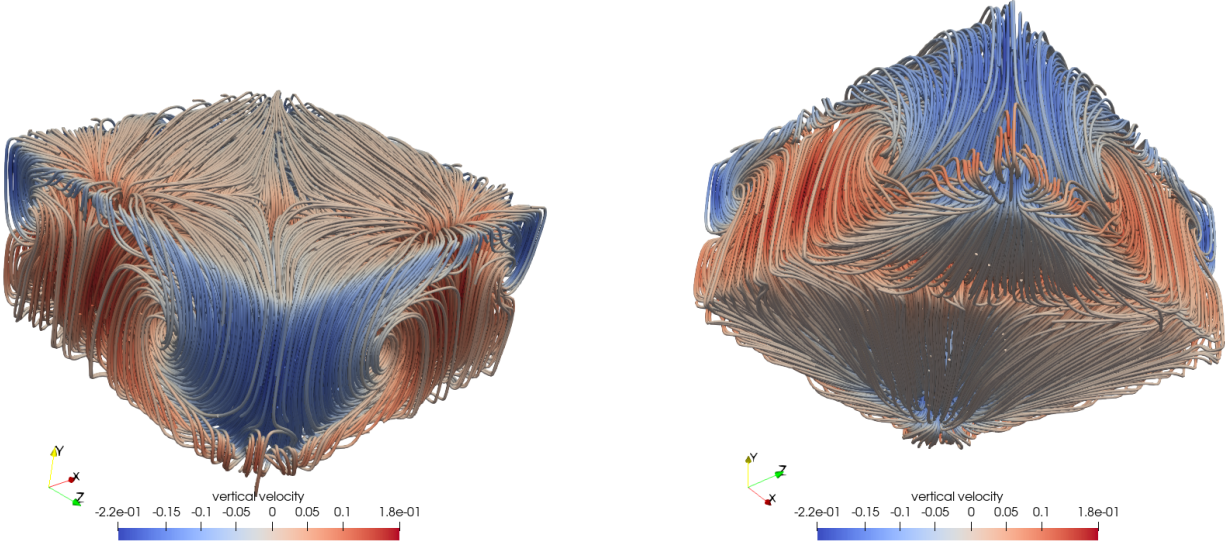


Figure 51: Streamlines seen from above and bottom for $Ra = 10^7$

To get some insight of the flow we sliced below, the line between the two impingement points is an area of upward flow who transversely go the rest of the domain (see figure 52).

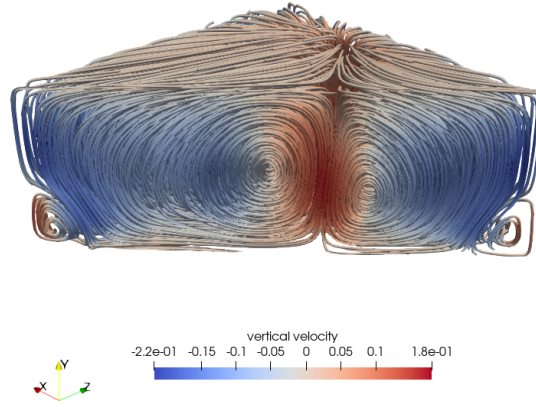


Figure 52: Slice at $Ra = 10^7$

Halfway through the simulation, the pattern started to move and the impingements joined each other to create a pattern close to the $Ra = 5 \cdot 10^7$ case (see figure 53).

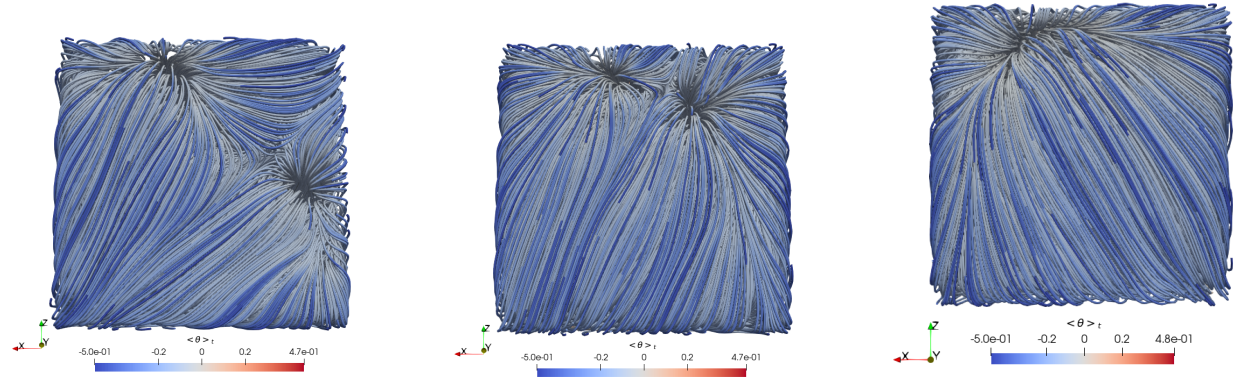


Figure 53: Sequence of reorientation for $Ra = 10^7$

The turbulence statistics are provided, as there is not enough data to really try to find some conclusions, they are just given as indicative below, we can just remark that they seem to be close to the observations for aspect ratios obtained by increasing W :

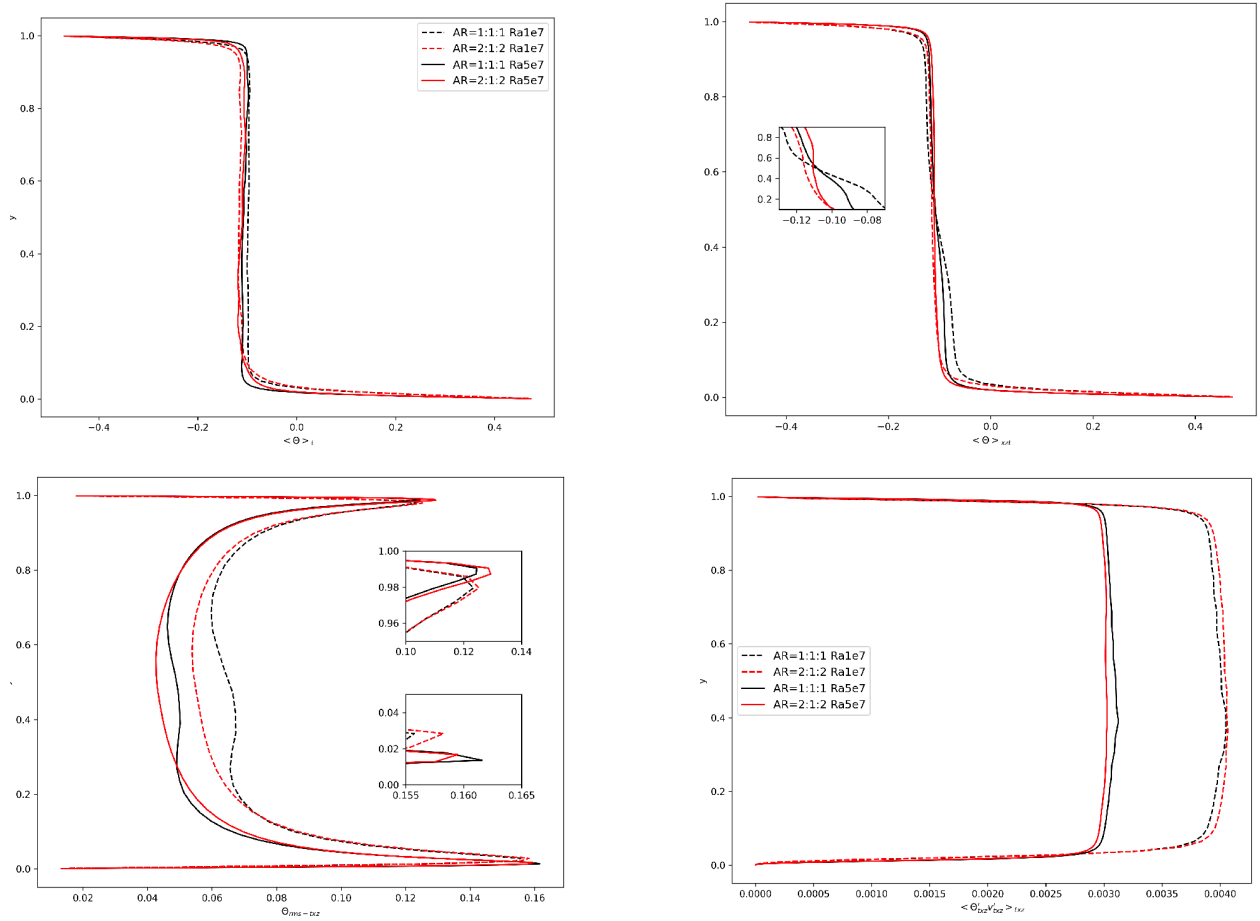


Figure 54: Turbulence statistics for an aspect ratio AR=2:1:2, part 1

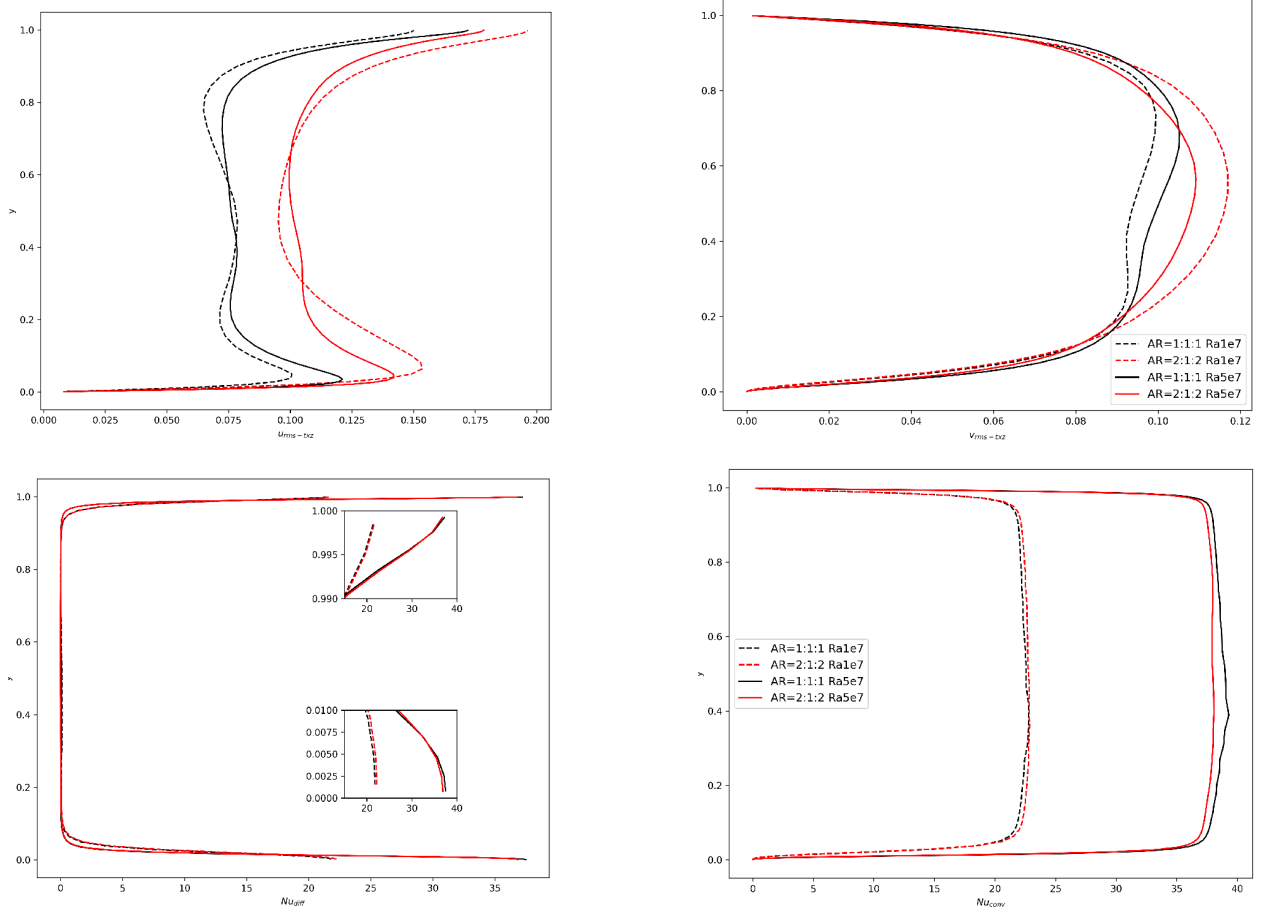


Figure 55: Turbulence statistics for an aspect ratio AR=2:1:2, part 2

5.7 Aspect ratio from AR=1:1:1 to AR= $\frac{1}{4}$:1:1

In this section we will briefly give some information on what happens if we decrease W but keeping L constant, at W divided by $(AR=\frac{1}{2} : 1 : 1)$ we still observe one big circulation contrary to the case $AR=\frac{1}{2}:1:\frac{1}{2}$, but contrary to the standard case the impingement point is not in a corner and the main circulation pattern is not in a diagonal but mainly in a plane with constant $\hat{x}=0.5 W$, see figure 56

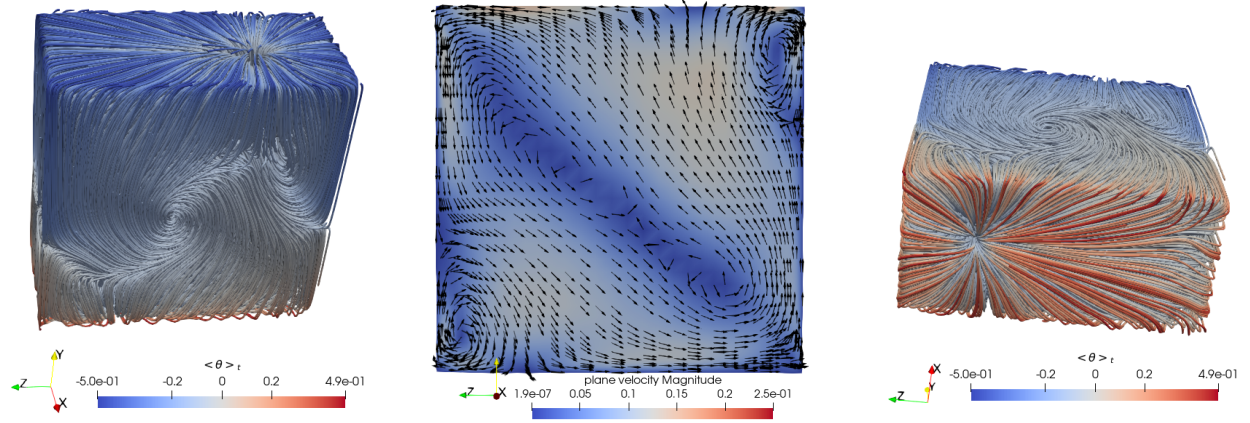


Figure 56: Plots at $Ra=5 \cdot 10^7$, the upper left shows the streamlines from above and the bottom image from below, the image on the right shows a section showing the main flow pattern

By further increasing the aspect ratio we then also observe dual rolls from bottom to left appearing but we only have 4 in total instead of 8 see figure 57

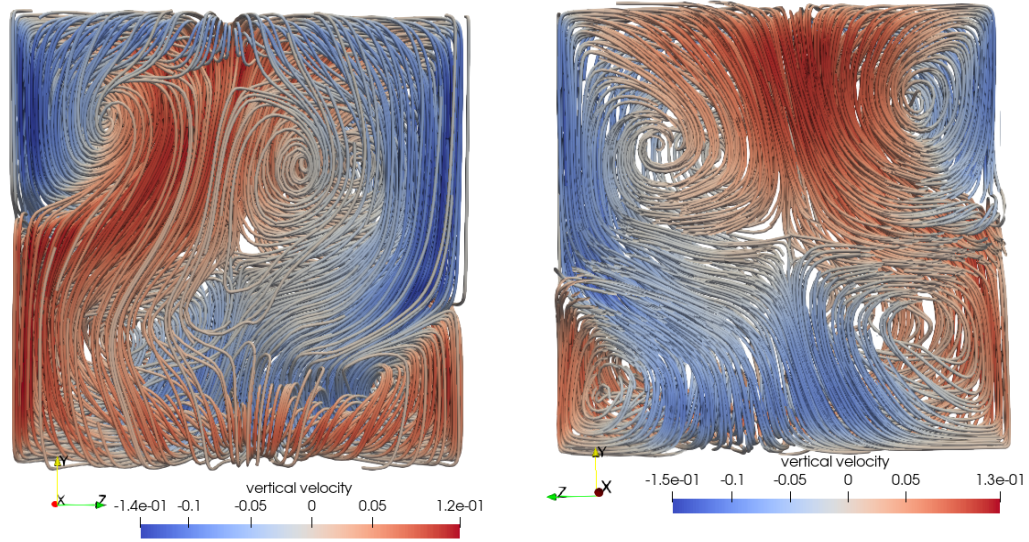


Figure 57: On the left streamlines at $AR=\frac{1}{4}:1:1$, on the right a section along the plane $\hat{x}=0.5$ W

Like the previous section we add the turbulence statistics for indicative, they seems to be coherent with the observations done for the aspect ratios $AR=1:1:1 - \frac{1}{4}:1:\frac{1}{4}$:

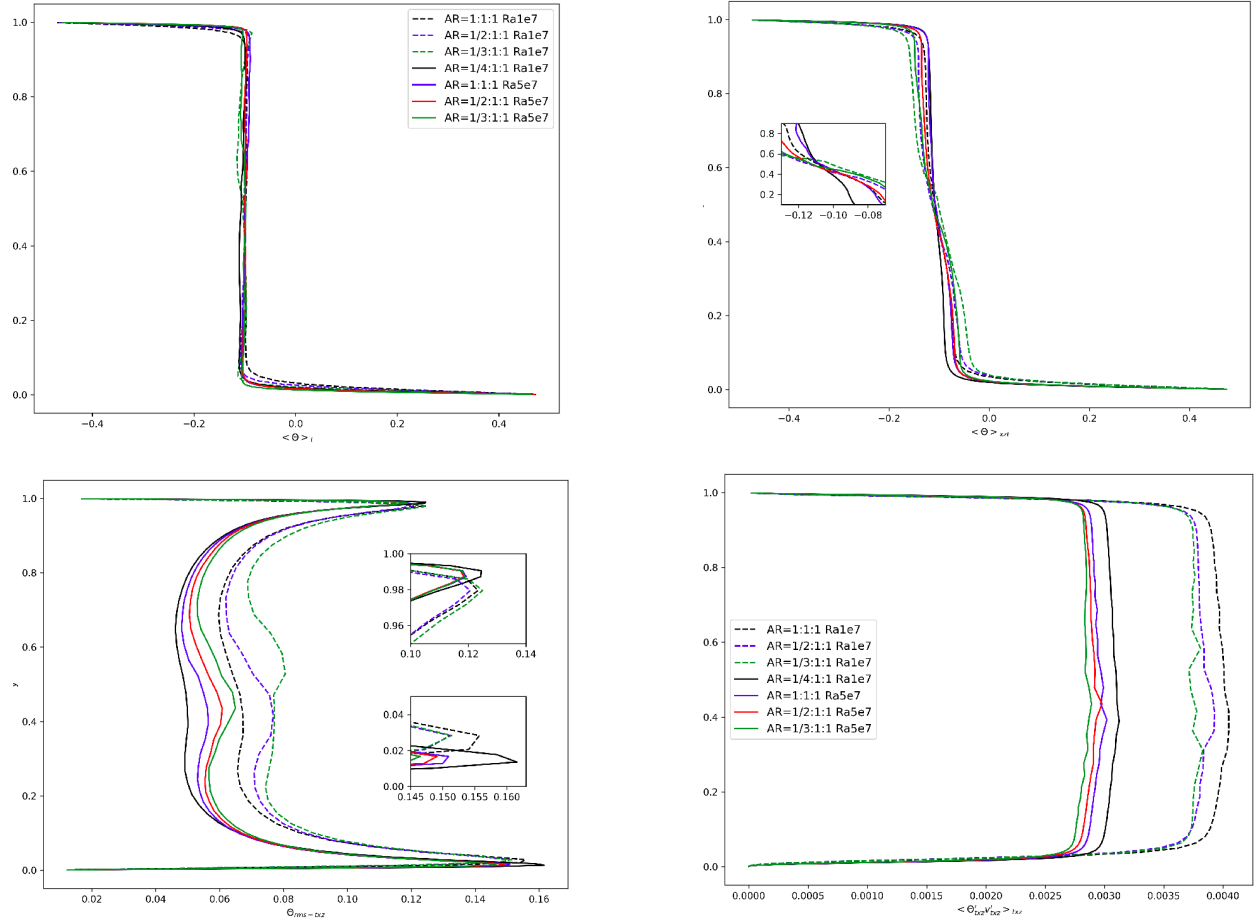


Figure 58: Turbulence statistics for an aspect ratio $AR = \frac{1}{4}:1:1$, part 1

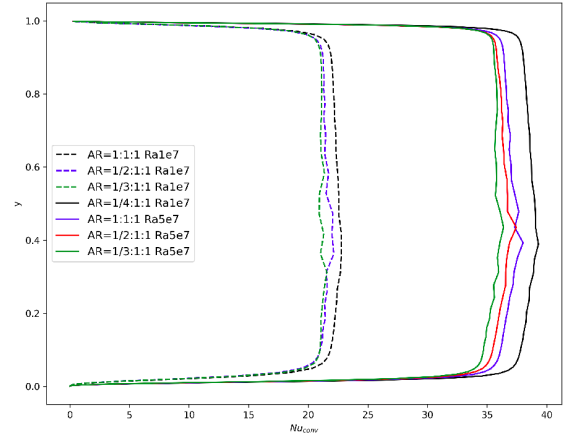
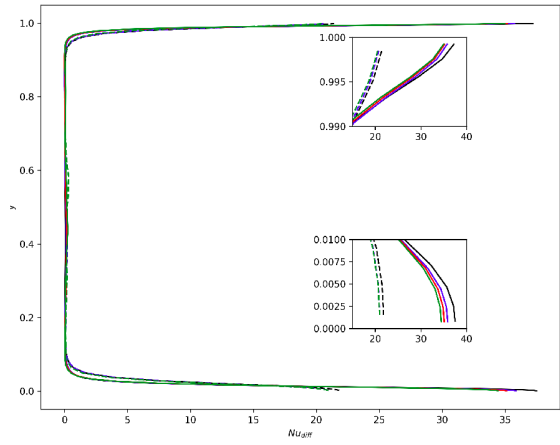
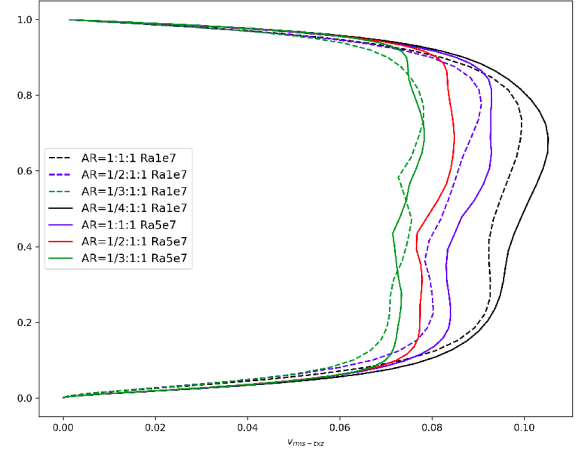
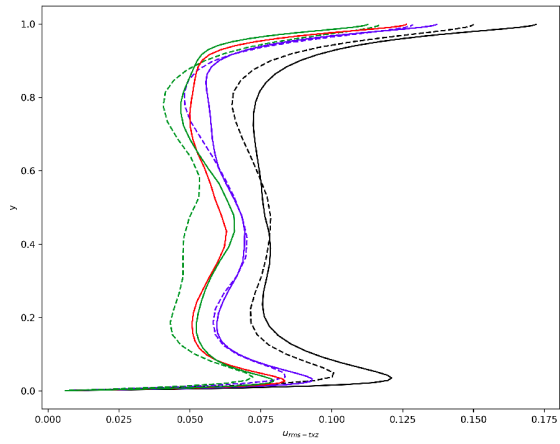


Figure 59: Turbulence statistics for an aspect ratio $AR=\frac{1}{4}:1:1$, part 2

5.8 Conclusion

This paper has investigated the natural convection of water for a simplified model of a nuclear spent fuel pools by means of numerical study. Different aspect ratios were analysed in order to visualise the cell convection pattern structure and to observe the effect of the aspect ratio on some important turbulence statistics.

As a general remark, increasing the aspect ratio, whether in the horizontal or vertical direction, led to the apparition of more natural convection cells compared to the standard case. Some reorientation of the flow patterns were detected for some aspect ratios. These deserve longer simulation time investigation using more precise, well placed, numerical probes to visualise graphically the frequency of reorientation. An increase in the horizontal direction sometimes has an opposite effect on the turbulence statistics, compared to an increase in the vertical direction, for example for $u_{rms-txz}$. While increasing the width, we have an increase of $u_{rms-txz}$ while increasing the height, however, we have a decrease for example.

The project fits within a broader framework of simulation of loss of cooling accident state of the art. Some assumptions like the boundaries conditions could have been more complex to get closer to the reality of a spent fuel pool. Also for instance, we have assumed that level of water stays the same. In the reality, quick evaporation can occur.

The field of nuclear energy has future, and I am glad to have done some research of which it is the subject.

References

- [1] IEA . *World gross electricity production by source*, 2019
<https://www.statista.com/statistics/269811/world-electricity-production-by-energy-source/>, IEA. Licence: CC BY 4.0 (consulted may 17, 2023)
- [2] J.-M. Jancovici . *Cours Mines Paris Tech*, juin 2019
<https://jancovici.com/publications-et-co/cours-mines-paristech-2019/cours-mines-paris-tech-juin-2019/> (consulted may 17, 2023)
- [3] A. Paleja . *With 24 units under construction, China leads the world in building nuclear power plants*, 2023, interestingengineering
<https://interestingengineering.com/culture/china-leads-building-nuclear-power-plants> (consulted apr 27, 2023)
- [4] IPCC Working Group III *Mitigation of Climate Change*, 2023
<https://www.ipcc.ch/working-group/wg3/> (consulted may 17, 2023)
- [5] tech-faq . *How do nuclear power plants works*
<https://www.tech-faq.com/how-do-nuclear-power-plants-work.html> (consulted may 24, 2023)
- [6] Wikipedia . *Neutron activation*
https://en.wikipedia.org/wiki/Neutron_activation (consulted may 24,2023)
- [7] World Nuclear Association . *Radioactive Waste Management*, 2022 WorldNuclear
<https://world-nuclear.org/information-library/nuclear-fuel-cycle/nuclear-wastes/radioactive-waste-management.aspx> (consulted jun 25, 2023)
- [8] Wikipedia . *Neutron capture*
https://en.wikipedia.org/wiki/Neutron_capture (consulted july 4,2023)
- [9] World Nuclear Association . *What is nuclear waste, and what do we do with it?*, WorldNuclear
<https://www.world-nuclear.org/nuclear-essentials/what-is-nuclear-waste-and-what-do-we-do-with-it.aspx> (consulted jun 25, 2023)
- [10] World Nuclear Association . *How is used nuclear fuel managed ?*, WorldNuclear
<https://www.world-nuclear.org/our-association/publications/technical-positions/how-is-used-nuclear-fuel-managed.aspx>(consulted jun 25, 2023)
- [11] EDF Energy . *Managing Spent Fuel at Hinkley Point C*
<https://www.edfenergy.com/energy/nuclear-new-build-projects/hinkley-point-c/about/managing-spent-fuel-hinkley-point-c> (consulted july 10, 2023)
- [12] SKODA JS . *Spent fuel storage in spent fuel pools at nuclear power plants*, 2021
<https://www.skoda-js.cz/reference/spent-fuel-storage-in-spent-fuel-pools-at-nuclear-power-plants/> (consulted july 10, 2023)
- [13] J. Daković, D. Grgić . "Analysis of spent fuel pool loss of coolant inventory accident progression", *Journal of Energy*, vol. 66 Number 1–4 Special Issue, 2017. DOI: 10.37798/2017661-498

- [14] Nuclear and Radiation Studies Board . *Lessons Learned from the Fukushima Nuclear Accident for Improving Safety and Security of U.S. Nuclear Plant*
Washington, DC, The National Academies Press, 2016. DOI: 10.17226/21874.
- [15] Committee on the Safety of Nuclear Installations (CSNI) . *Phenomena Identification and Ranking Table*, 2018, Nuclear Energy Agency (NEA)
- [16] V. Ramshesh . "Safety aspect concerning radiolytic gas generation in reactors"
Science Progress, vol. 84(1), 2001, p69-85.
- [17] Committee on the Safety of Nuclear Installations . *Status Report on Spent Fuel Pools under Loss-of-Cooling and Loss-of-Coolant Accident Conditions*, 2015, Nuclear Energy Agency (NEA)
- [18] International Atomic Energy Agency . "IAEA nuclear safety and security glossary"
IAEA, 2022. ISBN: 78-92-0-141122-8 (pdf)
- [19] SPF LOCA . *Overview and objectives*
<https://sites.google.com/view/sfp-loca/overview-objectives> (consulted 12 july 2023)
- [20] SITN . *Nuclear chemistry: Lessons from the Fukushima Daiichi disaster*
<https://sitn.hms.harvard.edu/flash/2011/nuclear-chemistry-lessons-from-the-fukushima-daiichi-disaster/>(consulted august 10, 2023)
- [21] F. Incropera et al . *Fundamentals of Heat and Mass Transfer, 6th Edition*
John Wiley Sons, Ltd., 2007. ISBN: 9780471761150.
- [22] V. Legat, G. Winckelmans . *Mécanique des fluides et transferts I*
Course notes, 2019-2020
- [23] H. Bénard . "Étude expérimentale des courants de convection dans une nappe liquide Régime permanent : tourbillons cellulaires"
Journal de Physique Théorique et Appliquée, vol. 9, 1900, p513-524. DOI: 10.1051/jphysap:019000090051300
- [24] H. Mhina and S. Souley Hassane, "A numerical investigation of Rayleigh-Bénard convection with an obstruction"
SIAM, SIURO, vol. 15, 2022. DOI: arXiv:2110.11470v1
- [25] P. Wahlgren . "Overview and Literature Survey of Natural and Forced Convection in Attic Insulation"
Journal of Building Physics, vol. 30(4), 2007, p351-370. DOI:10.1177/1744259106075947
- [26] M. Peric, J. H. Ferziger . *Computational Methods for Fluid Dynamics*
Springer, 2002
- [27] D. D. Gray; A. Giorgini . "The validity of the boussinesq approximation for liquids and gases."
International Journal of Heat and Mass Transfer, vol. 19, 1976, p545-551. DOI:10.1016/0017-9310(76)90168-x
- [28] M. V. Papalexandris. *Combustion and Fuels*
PUL Presses universitaires de Louvain, 2020. ISBN: 978-2-87558-980-4

- [29] Léa Boittin, Marie-Odile Bristeau, François Bouchut, Anne Mangeney, Jacques Sainte-Marie, et al. "Low-Mach type approximation of the Navier-Stokes system with temperature and salinity for free surface flows." *Communications in Mathematical Sciences*, 2023, 21 (1), pp.151-172. 10.4310/CMS.2023.v21.n1.a7. hal-02510711v3
- [30] M. Holmgren . *X Steam, Thermodynamic properties of water and steam*, 2020
<https://pypi.org/project/pyXSteam/> (consulted feb 1, 2023)
- [31] O. Shishkina et al . "Boundary layer structure in turbulent thermal convection and its consequences for the required numerical resolution"
New Journal of Physics, vol. 12, 2010. DOI: 10.1088/1367-2630/12/7/075022.
- [32] W. A. Hay, J. Martin, B. Migot, M. V. Papalexandris . "Turbulent thermal convection driven by free-surface evaporation in cuboidal domains of different aspect ratios"
Physics of Fluids, vol. 33(1), 2021. DOI:10.1063/5.0035277
- [33] S. B. Pope *Turbulent Flows*
Cambridge University Press, 2000. ISBN 1139643355, 9781139643351
- [34] A. N. Kolmogorov . "Local structure of turbulence in an incompressible fluid at very high Reynolds numbers"
Doklady Akademii Nauk SSSR, vol.30, 1941 p.301-305. ADS: 1941DoSSR..30..301K
- [35] H. Tennekes, J. L. Lumley . *A First Course in Turbulence*
The MIT Press, 1972. ISBN: 9780262310901
- [36] G. Grotzbach . "Spatial resolution requirements for direct numerical simulation of the Rayleigh-Bénard convection"
Journal of Computational Physics, vol. 49(2), 1983, p. 241–264. DOI:10.1016/0021-9991(83)90125-
- [37] S.-H. Peng, K. Hanjalic, L. Davidson . "Large-eddy simulation and deduced scaling analysis of Rayleigh–Bénard convection up to $Ra = 10^9$ "
Journal of Turbulence, vol. 7, 2006. DOI:10.1080/14685240600953462
- [38] Wikipedia . *Von Neumann stability analysis*
https://en.wikipedia.org/wiki/Von_Neumann_stability_analysis (consulted may 24, 2023)
- [39] W. Hong, D. Walker . "Reynolds-averaged equations for free-surface flows with application to high-Froude-number jet spreading"
Journal of Fluid Mechanics, 417, 2000, p. 183-209. DOI:10.1017/S0022112000008892
- [40] C. M. Rhie, W. L. Chow . "Numerical study of the turbulent flow past an airfoil with trailing edge separation"
AIAA Journal, 21(11), 1983, p. 1525–1532. DOI:10.2514/3.8284
- [41] Aidan Wimshurst [CFD] *Rhie & Chow Interpolation (Part 1): Chequerboard Oscillations*, 2021
https://www.youtube.com/watch?v=yqZ59Xn_aF8 (consulted aug 8, 2023)
- [42] P. Bartholomew, F. Denner, M. H. Abdol-Azis, A. Marquis, B. G. M. van Wachem . "Unified formulation of the momentum-weighted interpolation for collocated variable arrangements"
Journal of Computational Physics, 375, 177–208, 2018. doi:10.1016/j.jcp.2018.08.030

- [43] A. Wimshurst [CFD] *Rhie & Chow Interpolation (Part 3): Deriving the Correction!*, 2021
<https://www.youtube.com/watch?v=PmEUiUB8ETk&t=1101s> (consulted aug 8, 2023)
- [44] C. Meneveau, T. S. Lund, W. H. Cabot . "A Lagrangian dynamic subgrid-scale model of turbulence"
Journal of Fluid Mechanics, vol. 319, 353-385, 1996. DOI:
<https://doi.org/10.1017/S0022112096007379>
- [45] W. A. Hay, M. V. Papalexandris . "Numerical simulations of turbulent thermal convection with a free-slip upper boundary"
The Royal Society, vol. 475, 2019. DOI.org/10.1098/rspa.2019.0601
- [46] Phd Antoniadis . *Modeling and numerical simulation of transient flows in superposed porous and pure-fluid layers*
 UCLouvain, dial.pr, 2015
- [47] B. Lessani, M. V. Papalexandris . "Time-accurate calculation of variable density flows with strong temperature gradients and combustion"
Journal of Computational Physics, vol. 212, 2006, p. 218-246. DOI: 10.1016/j.jcp.2005.07.001
- [48] J.-P. Demailly . "Analyse numérique et équations différentielles"
Les Ulis, EDP Sciences, coll. Grenoble Sciences, 2006 ISBN: 2-86883-891-X
- [49] P. Niyogi, S. K. Chakrabartty, M. K. Laha . *Introduction to Computational Fluid Dynamics*
 Pearson Education India, 2006, p. 76. ISBN 978-81-7758-764-7.
- [50] PETSC . *Portable, Extensible Toolkit for Scientific Computation*
<https://petsc.org/release/> (consulted apr 16, 2023)
- [51] OpenFoam . *Backward time scheme*
<https://www.openfoam.com/documentation/guides/latest/doc/guide-schemes-time-backward.html> (Consulted apr 16, 2023)
- [52] A. Favre. *Statistical equations of turbulent gases*. In Problems of hydro-dynamics and continuum mechanics, pages 231–266. SIAM, Philadelphia, 1969
- [53] IdealSimulations. *Courant number*
<https://www.idealsimulations.com/resources/courant-number-cfd/> (consulted apr 22, 2023)
- [54] Lund, Thomas. (2003). "The Use of Explicit Filters in Large Eddy Simulation." *Computers & Mathematics with Applications*. 46. 603-616. DOI: 10.1016/S0898-1221(03)90019-8.
- [55] Denaro, F. M. (2011). "What does Finite Volume-based implicit filtering really resolve in Large-Eddy Simulations ?" *Journal of Computational Physics*, 230(10), 3849–3883. doi:10.1016/j.jcp.2011.02.011
- [56] Denaro, F. M., & De Stefano, G. (2010). "A new development of the dynamic procedure in large-eddy simulation based on a Finite Volume integral approach. Application to stratified turbulence." *Theoretical and Computational Fluid Dynamics*, 25(5), 315–355. doi:10.1007/s00162-010-0202-x

- [57] Master thesis, Marichal, Joauma. *Numerical study of natural convection of water in a nuclear spent fuel pool*
Ecole polytechnique de Louvain, Université catholique de Louvain, 2020. Prom. : Militadis Papalexandris.
<http://hdl.handle.net/2078.1/thesis:25153> (consulted may 2023)
- [58] Paraview .
<https://www.paraview.org/> (consulted apr 24, 2023)
- [59] Foroozani N, Niemela JJ, Armenio V, Sreenivasan KR. "Reorientations of the large-scale flow in turbulent convection in a cube"
Phys Rev E. 2017 Mar;95(3-1):033107. doi: 10.1103/PhysRevE.95.033107. Epub 2017 Mar 10. PMID: 28415317.

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