Design of a buoyancy-driven Pressurized Thermal Shock test case for nuclear energy application

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A.S.
Abstract

Introduction
The integrity assessment of the Reactor Pressure Vessel (RPV) is considered to be an important issue for lifetime extension of nuclear reactors. A severe transient that can threaten the integrity of the RPV is the existence of a Pressurized Thermal Shock (PTS). The term PTS encompasses all those events that involve the rapid cooling of the vessel internal wall, that may induce the criticality of existing or postulated flaws inside the vessel wall. The most dangerous accident has been identified in the Emergency Core Cooling (ECC) injection during a Loss Of Coolant Accident (LOCA)[13]: if the cooling system of the Nuclear Power Plant (NPP) somehow fails, the heat generated by the fission can damage the structure, therefore ECC water is injected to the reactor, the mixing of the emergency cold fluid and the hot working water generates the thermal shock on the walls of the vessel.

Even though RPVs are designed to resist under several critical conditions, and all the components are manufactured according to the highest safety standards, still ageing management programs check continuously safety margins, through In-Service Inspections (ISI), surveillance programs and dosimetry [5]. PTS evaluation is part of the ageing management programme of NPPs and is based on three analyses:

• **Probabilistic Safety Assessment** (PSA): based on the plant safety analysis report, a review of all possible transients is made and the more significant are selected.

• **Thermal Hydraulic analysis** (T-H): fluid temperature distribution in the RPV nozzles, and downcomer are evaluated, hence the corresponding heat transfer coefficient with the RPV inner surface is calculated.

• **Probabilistic Fracture Mechanics** (PFM): according to fabrication, examinations, and conventional measure the crack location, size and shape are defined.

Finally, with the analysis of the results a safety margin factor that indicates the failure probability of the reactor vessel is estimated.

The Thermal Hydraulic analysis plays an important role in the evaluation of PTS, since it investigates the overall response of the system to the transient, and determines, via the Downcomer Mixing Analysis, the complex three dimensional thermal mixing phenomena occurring in the downcomer. Historically, one-dimensional models failed to reliably predict such scenarios, while on the other hand Computational Fluid Dynamics (CFD) can bring real benefits in terms of more realistic and more predictive capabilities. However, an extensive validation programme is necessary, since numerical analysis for nuclear applications is not as common as in other engineering fields, and in absence of experimental data, Direct Numerical Simulation (DNS) can serve as
reference, because it is accurate enough to characterize completely all flow and heat transport phenomena involved. DNS, though, is also the most expensive approach, in terms of time, and usually it is not yet feasible to perform DNS for real life applications with the hardware resources currently available. Therefore a preliminary study is essential in order to simplify the real configuration, in order to make the problem reasonably simple for a DNS approach but, at the same time, remaining as realistic as possible to reproduce all the main features of the configuration considered.

That is why the purpose of the project ongoing at the Nuclear Research and Consultancy Group (NRG) is to provide a DNS database, for a simplified PTS configuration. This can be very helpful for the scientific community: to understand the complex flow and heat transport in detail, but more importantly, this case could serve as database for the validation of any other numerical methods studying PTS. In order to get to this simpler setup, we need a preliminary study, NRG already worked on this kind of calibration [17], the PTS event was studied at constant density (accounting only for the forced convection). The present work started from this experience, and created a benchmark for DNS calculation, of a single-phase buoyancy-driven PTS event, through a series of Reynolds Average Navier Stokes Simulations (RANS), much less time consuming and more flexible then DNS, several aspects of the PTS design have been calibrated and further optimized, the effect of all the geometric parameters and their respective influence on the overall flow topology was studied, and the imposed boundary conditions were calibrated to correctly reproduce the flow regimes and achieve a realistic case for the final DNS computation.

**CFD model**

**Boundary conditions**

The initial selection of the flow configuration is based on the ROCOM test facility. However, in the present work, the geometric design is simplified in order to facilitate the high fidelity DNS requirements. The selected simplified domain is shown in Fig.1 and consists of:

- **Square leg**: where the relatively cold fluid is injected (Inlet 1), and it is characterized by the hydraulic diameter $D_h$

- **Downcomer**: where the mixing takes place. In the upper-side the hot fluid is injected (Inlet 2), at the bottom the outlet is present

- **Shround and Vessel**: bounding walls enclosing the fluid

The mass flow rate imposed in the square leg is the same used in a ROCOM test case [8], the fluid is entering the domain at a bulk velocity of $U_1 = 0.018 \text{ m/s}$ and a relatively cold temperature of 293 K. At the Inlet 2 the flow is injected at 353 K and the velocity has been calibrated during the previous experience at NRG. At the outlet a gauge pressure equal to 0 is imposed. No-slip boundary conditions are imposed on the walls bounding the fluid domain in the span wise direction, while conjugate heat transfer is calculated at the solid-fluid interface, finally adiabatic conditions are applied at external boundaries of the solid. The details of the assigned geometric parameters and boundary conditions are given in Tab1.

**Fluid and material properties**
Parameter | Description | \( U_1 = 0.018 \, \text{m/s} \)  
| --- | --- | --- |
| Inlet 1 | Inlet with relatively cold water | \( T = 293 \, \text{K} \)  
| | | \( \rho = 997.16 \, \text{kg/m}^3 \)  
| Inlet 2 | Inlet with relatively hot water | \( U_2 = 0.0018 \, \text{m/s} \)  
| | | \( T = 353 \, \text{K} \)  
| | | \( \rho = 970.19 \, \text{kg/m}^3 \)  
| \( D_h \) | Diameter of the cold leg | \( D_h = 0.15 \, \text{m} \)  
| \( L \) | Cold leg length | \( L = 1 \, \text{m} \)  
| \( H_1 \) | Upper height | \( H_1 = 1 \, \text{m} \)  
| \( H_2 \) | Downcomer height | \( H_2 = 3.5 \, \text{m} \)  
| \( W \) | Width of the downcomer | \( W = 2 \, \text{m} \)  
| \( D_v \) | Thickness of the vessel | \( D_v = 0.05 \, \text{m} \)  
| \( D_s \) | Thickness of the shroud | \( D_s = 0.025 \, \text{m} \)  
| \( D_d \) | Thickness of the downcomer | \( D_d = 0.075 \, \text{m} \)  

Table 1: Initial setup of the PTS experiment

The working fluid is water, whose properties are considered to depend only on the temperature and here, in particular, are approximated with the following quadratic functions:

- Density: \( \rho = 777.214 + 1.7469 \, T - 0.0034 \, T^2 \, [\text{kg/m}^3] \)
- Dynamic viscosity: \( \mu = 0.019 - 1.06 \times 10^{-4} \, T + 1.48 \times 10^{-7} \, T^2 \, [\text{Pa} \cdot \text{s}] \)
- Thermal conductivity: \( k = -0.788 + 0.008 \, T - 1.361 \times 10^{-5} \, T^2 \, [\text{W/m/K}] \)
- Specific heat: \( C_p = 5186.439 - 6.443 \, T + 0.011 \, T^2 \, [\text{J/kg/K}] \)

The solid parts are made of 16MND5 steel, with constant properties at 323 K:

- Density: 7840 \, \text{kg/m}^3
- Thermal Conductivity: 45.98 \, \text{W/m/K}
- Specific heat: 476.50 \, \text{J/kg/K}

**Froude number**

In order to have an idea of the impact of the buoyancy forces on the mixing, based on the ROCOM’s experience [15], we chose the Froude number (\( Fr \)) as measure of the buoyancy effect:

\[
Fr = \frac{u_{in}}{\sqrt{gh \frac{\rho_1 - \rho_2}{\rho_1}}} \tag{1}
\]

The \( Fr \) number is a dimensionless parameter that can be seen as the ratio between inertia (\( u_{in} \)) and weight (\( \frac{\rho_1 - \rho_2}{\rho_1} \, g \)). In our formulation the Froude number depends on:

- \( u_{in} \): inlet velocity (\( U_1 \))
<table>
<thead>
<tr>
<th>Case</th>
<th>$U_1 [m/s]$</th>
<th>$U_2 [m/s]$</th>
<th>$\Delta T [K]$</th>
<th>Model</th>
<th>Domain</th>
<th>$\Delta \rho$</th>
<th>Fr</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>0.018</td>
<td>10%$U_1$</td>
<td>293 + 353</td>
<td>EBRSM</td>
<td></td>
<td>3%</td>
<td>0.018</td>
</tr>
<tr>
<td>1b</td>
<td>0.018</td>
<td>5%$U_1$</td>
<td>293 + 353</td>
<td>EBRSM</td>
<td></td>
<td>3%</td>
<td>0.018</td>
</tr>
<tr>
<td>1c</td>
<td>0.018</td>
<td>0</td>
<td>293 + 353</td>
<td>EBRSM</td>
<td></td>
<td>3%</td>
<td>0.018</td>
</tr>
<tr>
<td>2a</td>
<td>0.018</td>
<td>0</td>
<td>293 + 353</td>
<td>EBRSM</td>
<td>$H + 6D_h$</td>
<td>3%</td>
<td>0.016</td>
</tr>
<tr>
<td>2b</td>
<td>0.018</td>
<td>0</td>
<td>293 + 353</td>
<td>EBRSM</td>
<td>$H + 6D_h W + 6D_h$</td>
<td>3%</td>
<td>0.016</td>
</tr>
<tr>
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<td>EBRSM</td>
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<td>0.016</td>
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<tr>
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<td>0</td>
<td>293 + 353</td>
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<td>$H + 3D_h$</td>
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<td>0.017</td>
</tr>
<tr>
<td>3b</td>
<td>0.018</td>
<td>0</td>
<td>293 + 353</td>
<td>EBRSM</td>
<td>$H + 3D_h W + 6D_h$</td>
<td>3%</td>
<td>0.017</td>
</tr>
<tr>
<td>4a</td>
<td>0.018</td>
<td>0</td>
<td>303 + 343</td>
<td>EBRSM</td>
<td>$H + 3D_h W + 6D_h$</td>
<td>2%</td>
<td>0.020</td>
</tr>
<tr>
<td>4b</td>
<td>0.018</td>
<td>0</td>
<td>278 + 368</td>
<td>EBRSM</td>
<td>$H + 3D_h W + 6D_h$</td>
<td>4%</td>
<td>0.013</td>
</tr>
<tr>
<td>5a</td>
<td>120%$U_1$</td>
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<td>293 + 353</td>
<td>EBRSM</td>
<td>$H + 3D_h W + 6D_h$</td>
<td>3%</td>
<td>0.021</td>
</tr>
<tr>
<td>5b</td>
<td>150%$U_1$</td>
<td>0</td>
<td>293 + 353</td>
<td>EBRSM</td>
<td>$H + 3D_h W + 6D_h$</td>
<td>3%</td>
<td>0.024</td>
</tr>
<tr>
<td>5c</td>
<td>200%$U_1$</td>
<td>0</td>
<td>293 + 353</td>
<td>EBRSM</td>
<td>$H + 3D_h W + 6D_h$</td>
<td>3%</td>
<td>0.032</td>
</tr>
<tr>
<td>6</td>
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<td>0</td>
<td>303 + 343</td>
<td>EBRSM + Boussinesq</td>
<td>$H + 3D_h W + 6D_h$</td>
<td>2%</td>
<td>0.020</td>
</tr>
<tr>
<td>7</td>
<td>Fully turbulent</td>
<td>0</td>
<td>303 + 343</td>
<td>EBRSM + Boussinesq + Periodicity</td>
<td>$H + 3D_h W + 6D_h$</td>
<td>2%</td>
<td>0.020</td>
</tr>
</tbody>
</table>

Table 2: Work table

- $h$: distance between the leg nozzle and the outlet ($H_2$)
- $(\rho_1 - \rho_2)$: density difference between the cold water injected and the hot fluid present in the downcomer

**Numerical setup**

All the simulations presented in this paper are performed using the open source code Code_Saturne [14]. The URANS approach is used to design the numerical experiment of the selected PTS configuration. The Elliptic Blending Reynolds Stress Model (EBRSM) has been chosen as turbulent model [11]. In addition, a second order upwind scheme has been used for spatial discretization and a Pressure Implicit with Splitting of Operator (PISO) algorithm is adopted to solve the coupling between pressure and velocity field.

Computation are performed on a mesh of approximately 3.000.000 hexahedral elements for the fluid domain, while a mesh of around 900.000 tetrahedral elements is adopted on the solid walls.

**Calibration of the PTS**

In Tab.2 the complete list of parameter and their variations is reported for the whole calibration process.

**Velocity calibration**

The first parameter to be calibrated is the second inlet in the PTS configuration: this setup is mandatory in the case of constant density simulation, in fact the flow coming from the upper side of the downcomer is meant to push the cold water down the outlet, and the magnitude of the second inlet velocity has been calibrated in the previous
work of Shams et al., in particular it has been optimized at $U_2 = 10\% U_1$. On the other hand, when buoyancy effects are taken into account the cold fluid is expected to naturally flow down due to the gravity. For this reason, from the baseline configuration with $U_2 = 10\% U_1$, the value of the velocity at the downcomer has been reduced gradually: from $U_2 = 5\% U_1$ to a zero inlet velocity.

From the analysis of the results it is possible to notice that:

- For the whole set of simulations, in the square leg a temperature stratification is induced by the mixing of the cold water injected and the the hot fluid present in the domain

- Due to the presence of gravity and the different weight of the water, the cold fluid flows down even when the inlet velocity at the downcomer is zero

These are the reasons for which we decided to eliminate the second inlet from our configuration. The evolution of the temperature field in middle section of the downcomer along time is reported in Fig.2. Five samples of the temperature field are reported, along a real-time of around five minutes.

**Geometry calibration**

The behavior of the cold vein in the downcomer is heavily influenced by the bounding walls, the fluid falls down and starts oscillating, but after a while it attaches to the wall bounding the span-wise direction, and continues to imping this wall from there after, the heavy influence of the side walls is not acceptable, since these walls are not present in the actual configuration of the reactor. That is why the size of the domain must be calibrated, five cases have been studied:

- Base case: $H_2 = 3.5 \ m$, $W = 2 \ m$

- $H_2 = H_2 + 3D_h = 3.95 \ m$, $W = 2 \ m$
The results showed how a bigger domain helped the flow oscillating more freely, but the configuration with $H + 3D_h, W + 6D_h$ has been chosen to continue the calibration, since it is the compromise between a large domain and a reasonable number of elements of the computational grid for the future DNS. The evolution of the temperature field in the middle-downcomer is reported in Fig. 3.

**Buoyancy effects calibration**

In order to further mitigate the influence of the boundaries on the mixing and hence try to isolate the phenomenon occurring in the downcomer, buoyancy effects have been calibrated. Different strategies have been adopted in this calibration, in order to analyze the different influence of $U_1$ and $\frac{\rho_1 - \rho_2}{\rho_1}$ on the flow behavior, here are reported the cases that have been studied:

- $\Delta \rho = 2\%, Fr = 0.020$: the temperature difference between cold fluid injected and hot fluid in the downcomer is reduced, from $\Delta T = 60$ to $\Delta T = 40$, density and hence Froude number change accordingly
- $\Delta \rho = 4\%, Fr = 0.013$: larger temperature difference, $\Delta T = 90$
- $\Delta \rho = 3\%, Fr = 0.022$: same density difference of the base case but different magnitude of the inlet velocity, $u_{in} = 120% u_{in}$
- $\Delta \rho = 3\%, Fr = 0.024$: $u_{in} = 150% u_{in}$
- $\Delta \rho = 3\%, Fr = 0.032$: $u_{in} = 200% u_{in}$

The results showed how a bigger domain helped the flow oscillating more freely, but the configuration with $H + 3D_h, W + 6D_h$ has been chosen to continue the calibration, since it is the compromise between a large domain and a reasonable number of elements of the computational grid for the future DNS. The evolution of the temperature field in the middle-downcomer is reported in Fig. 3.

Figure 3: Temperature evolution in the middle-downcomer for expanded domain $H + 3D_h, W + 6D_h$
Figure 4: Temperature evolution in the middle-downcomer for case $\Delta \rho = 2\%, Fr = 0.020$

It has been found that for an higher $Fr$ the oscillations of the fluid vein are reduced, this is an interesting feature for the calculations, since the smaller the oscillations are the smaller the width of the domain is required, hence the influence of the boundaries is reduced; further more this feature is interesting from the point of view of the future DNS simulation, in fact if the area interested by the turbulence of the fluid vein is contained, the region that requires a finer mesh is smaller and hence the time expenditure for the simulation is also reduced. The first setup with $\Delta \rho = 2\%, Fr = 0.020$ (Fig.4) has been chosen to continue the calibration, because the Froude number is higher respect to the previous configuration, so as aforementioned this helps the flow stabilization, and also the smaller temperature difference is useful for the next calibration.

Final remark on the temperature gradient over the solid walls: in Fig.5 is reported the temperature evolution on the walls interfaces. It is interesting to notice the presence of temperatures gradients only on the shroud interface, that is because the flow after impinging the shroud wall it falls down, and it has not the time to adhere to the vessel wall and hence induce the gradients. This is a critical feature of the PTS event, that with actual laboratory experiments such as the ROCOM’s [6], it is impossible to replicate, giving to the future DNS simulation, and more generally to the CFD analysis an indisputably relevance in the study of such manners.

**Boussinesq approximation**

It was interesting to test a further simplification of the problem, applying the Boussinesq approximation: with this approach all the fluid properties inside the governing equations are constant, except for the density when multiplied by the gravity vector, in this case $\rho$ varies according to a linear law depending on temperature, reducing the nonlinearity of the problem:

$$\rho = \rho_0 - \rho_0 \beta \Delta T$$

where $\beta$ is the coefficient of thermal expansion. The approximation is extremely accurate for many industrial applications, and makes the mathematics and physics much simpler. The results presented in Fig.6 showed that the approximation maintains the feature in which this work is interested: the flow vein oscillates freely, but the area cov-
Periodic boundary conditions

The geometry simplification of the reactor pressure vessel imposed by the "cost" limitations of the future DNS is radical, in fact all the simulations reported in this work are performed on a planar domain, while an actual RPV has a cylindrical shape. Since a more complex geometrical configuration is not feasible, from the point of view of the DNS simulation, it is useful in this preliminary study to understand the influence, on the mixing occurring in the downcomer, of periodic boundary conditions (PBC) compared to the no-slip wall conditions. The PBCs configuration can be considered closer to the actual cylindrical geometry of the RPV, therefore in the last simulation periodic boundary conditions are applied on the walls enclosing the span-wise direction. In Fig.7 it is possible to notice how with the calibration process endured until this step, the oscillations of the fluid vein are contained, so that the flow passing through the periodic boundaries has small impact on the mixing occurring in the downcomer. This demonstrates how in this case the no-slip wall conditions do not differ too much from a more accurate configuration such as the one with periodic boundary conditions.

Figure 5: Temperature evolution at wall interfaces: (a) shroud, and (b) vessel
Figure 6: Temperature evolution in the middle-downcomer for case $\Delta \rho = 2\%, Fr = 0.020$, with Boussinesq approximation.

Figure 7: Temperature evolution in the middle-downcomer for case with periodic boundary conditions.
Turbulence length scales
The final step of this work is the estimation of the Kolmogorov and Batchelor turbulence length scales, this is fundamental to build up a proper meshing strategy for the future DNS. The knowledge of the tendency of such scales throughout the computational domain is necessary to identify the regions where the mixing phenomena require a very fine mesh and the regions where the cell size can be higher. In Fig. 8 the turbulence length scales have been extrapolated from the RANS solution, and it is possible to notice how a special attention is required in the region under the square leg nozzle, where the flow oscillations are concentrated. Based on such scales, a first estimation has been made, identifying the lowest values of Batchelor scales, considering a growth rate of 1.05 from the wall interfaces, a block structured meshing technique for the fluid domain and a conformal mesh for the walls discretization, the resulting mesh counts around 1.8 billion cells. This includes one billion grid points for the fluid region, and 800 million cells for the solid parts.

Conclusion
A large number of URANS calculations was carried out to design a reference single-phase buoyancy-driven PTS numerical experiment in order to perform an high quality DNS. This DNS is intended to serve as a reference database to validate the turbulent modeling approaches such as LES, Hybrid (LES/URANS) and URANS methods. The selection of the PTS design was based on the ROCOM facility. Due to numerical constrains, the design was further simplified for the target DNS study. Several aspects of this PTS design were calibrated and further optimized to achieve a realistic case for the final DNS computations. Starting from the optimization of the second inlet velocity, the effect of the geometric parameters and their respective influence on the over-all flow topology was studied. This eventually allowed to achieve an optimized final PTS configuration. Second, the influence of the buoyancy forces on the flow regime was investigated. Furthermore, the impact of periodic boundary conditions applied in the span wise direction was studied. Finally, the Kolmogorov and Batchelor length scales were extracted. These length scales have been proved quite instrumental in devising an optimized meshing strategy for the final DNS numerical experiment.
Summary

Along the lifetime of a Nuclear Power Plant (NPP), Pressurized Thermal Shock (PTS) is one of the most dangerous scenarios that can affect the Reactor Pressure Vessel (RPV) integrity. The term PTS encompasses all those events that involve the rapid cooling of the vessel internal wall, of which the most critical one is the Emergency Core Cooling (ECC) injection during a Loss Of Coolant Accident (LOCA). The injected cold water mixing with the hot working water produces thermal shocks at the solid wall of the vessel, that can put the solid walls under fatigue and can induce structural damages due to the presence of pre-existing material flaws.

The traditional one-dimensional models, fail to reliably predict the complex three-dimensional thermal mixing phenomena in the downcomer, that occurs during the ECC injection. Hence, Computational Fluid Dynamics (CFD) can bring real benefits in terms of more realistic and more predictive capabilities. However, an extensive validation programme is necessary, and in absence of experimental data, Direct Numerical Simulation (DNS) can serve as reference, because it is accurate enough to characterize completely all flow and heat transport phenomena involved. DNS, though, is also the most expensive approach, in terms of time, and usually it is not yet feasible to perform DNS for real life applications with the computational resources currently available. That is why the purpose of the project ongoing at the Nuclear Research and Consultancy Group (NRG) is to provide a DNS database, for a simplified PTS configuration. A preliminary study is essential in order to simplify the real configuration, in order to make the problem reasonably simple for a DNS approach but, at the same time, remaining as realistic as possible to reproduce all the main features of the configuration considered. So the aim of this work is to study the turbulent mixing in the down-comer and the evolution of temperature field in both fluid and solid regions, and through a series of Reynolds Average Navier Stokes (RANS) calculations, much more flexible and less time consuming than DNS, to optimize geometry, boundary conditions, and fluid properties in order to meet the future constraints, and to describe accurately the physical phenomenon.
**Sommario**

Lungo la vita utile di una centrale nucleare, il Pressurized Thermal Shock (PTS) è l’incidente più grave che può verificarsi all’interno del reattore nucleare. Sotto la definizione di PTS ricadono tutti quegli eventi che presentano un rapido raffreddamento delle pareti interne del reattore, tra tutti il più pericoloso è stato identificato nel Loss Of Coolant Accident (LOCA): quando il sistema di raffreddamento della centrale, per qualunque ragione, viene meno al suo scopo il sistema di Emergency Core Cooling (ECC) inietta acqua fredda sulle pareti del reattore. Il miscelamento della acqua fredda iniettata e il fluido di lavoro caldo, produce lo shock termico che può interagire con difetti pre-esistenti all’interno della parete e provocare una frattura attraverso la struttura.

Lo studio di questo tipo di incidente, storicamente, era affidato a modelli monodimensionali che però fallivano nel predire correttamente un fenomeno così complesso come quello del PTS. Oggi, si propone di affrontare questo tipo di problema con un approccio diverso: la Computational Fluid Dynamics (CFD), che può portare a soluzioni più realistiche grazie alle migliori capacità predittive sui fenomeni tridimensionali. Per far sì che l’analisi numerica possa essere considerata affidabile, però, è necessario un accurato programma di validazione, e in assenza di dati sperimentali le simulazioni del tipo Direct Numerical Simulation (DNS) potrebbero essere usate come riferimento. Le DNS oltre ad essere lo strumento CFD più accurato sono anche quello più "costoso" in termini di tempo ed hardware, per queste ragioni è necessario uno studio preliminare che semplifichi la reale configurazione del reattore ma che allo stesso tempo riesca a mantenere una rappresentazione accurata del PTS.

L’obiettivo di questa tesi è proprio quello di preparare le basi per una simulazione DNS di un evento PTS semplificato, infatti attraverso una serie di simulazioni Unsteady Reynolds Average Navier Stokes (URANS), molto più flessibili e meno costose di una DNS, andremo ad ottimizzare la geometria del dominio del nostro "esperimento", le condizioni al contorno, le proprietà del fluido in modo tale da rispettare i limiti materiali della futura DNS, e tenendo a mente che la simulazione dovrà essere il più possibile coerente col fenomeno fisico.
Nomenclature

CFD Computational Fluid Dynamics
DNS Direct Numerical Simulation
URANS Unsteady Reynolds Average Navier Stokes
LES Large Eddy Simulation
NRG Nuclear Research and Consultancy Group
PTS Pressurized Thermal Shock
NPP Nuclear Power Plants
NRS Nuclear Reactor Safety
ROCOM Rossendorf Coolant Mixing Model
ECORA Evaluation of Computational Fluid Dynamics Methods for Reactor Safety Analysis
RPV Reactor Pressure Vessel
ECC Emergency Core Cooling
LOCA Loss Of Coolant Accident
PSA Probabilistic Safety Assessment
T-H Thermal Hydraulic analysis
PFM Probabilistic Fracture Mechanics
ρ Density \( [kg/m^3] \)
µ Dynamic viscosity \( [Pa \cdot s] \)
ν Kinematic viscosity \( [m^2/s] \)
β Coefficient of thermal expansion \( [Pa^{-1}] \)
ηκ Kolmogorov scale \( [m] \)
λB Batchelor scale \( [m] \)
u x component of velocity \( [m/s] \)
v y component of velocity \( [m/s] \)
w z component of velocity \( [m/s] \)
P Pressure \( [Pa] \)
T Temperature \( [K] \)
k Thermal conductivity \( [W/m/K] \)
Fr Froude number
Cp Specific heat \( [J/kg/K] \)
Re Reynolds number
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Chapter 1

Introduction

The lifetime of a Nuclear Power Plant (NPP), from construction to complete decommission, may be between 80-100 years and the trend in the near future is to have an even longer operational time [18]. During service years, the operating equipments are subjected to a variety of chemical, mechanical and physical conditions that with time lead to a change in the properties of materials, that could affect the performance of the systems or, in the worst case scenario, could get to a totally loss of their design function. Hence, the ageing process is taken in serious consideration from the design up to the manufacturing stage.

The Reactor Pressure Vessel (RPV) is obviously the main actor in the lifetime estimation of a NPP, being the only barrier between the radioactive products and the ambient. The structural strength of the RPV walls decreases with time, this is especially true for the region adjacent to the core due to the continue neutron irradiation [19], and a possible abrupt change of the temperature at the wall caused by the instantaneous injection of cooler fluid can result in structural failures of the solid wall, induced by pre-existing material flaws. This kind of transient is called Pressurized Thermal Shock (PTS), and is characterized by a rapid cooling of the downcomer and internal RPV surface, usually these events concern cold-water injections, like during a Loss Of Coolant Accident (LOCA): if the coolant system somehow fails the heat generated by the fission may damage the structure, in this case the Emergency Core Cooling System (ECCS) will inject cold water to the reactor, the mixing of the hot working water and the cold emergency water generates temperatures gradients that can compromise the structural integrity of the solid walls [13].

Even though RPVs are designed to resist under several critical conditions, and all the components are manufactured according to the highest safety standards, still ageing management programs check continuously safety margins, through In-Service Inspect-
Figure 1.1: PTS evaluation process

Identify PTS initiating events

Evaluate PTS sequences

Sequence quantification

Selection of sequences

Thermal Hydraulic Analysis

Downcomer Mixing analysis

Probabilistic Fracture Mechanics

Total RPV Failure Probability

CHAPTER 1. INTRODUCTION

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tions (ISI), surveillance programs and dosimetry [5]. PTS evaluation (Fig. 1.1) is part of the ageing management programme of NPPs and is based on three analyses:

- **Probabilistic Safety Assessment** (PSA): based on the plant safety analysis report, a review of all possible transients is made and the more significant are selected.

- **Thermal Hydraulic analysis** (T-H): fluid temperature distribution in the RPV nozzles, and downcomer are evaluated, hence the corresponding heat transfer coefficient with the RPV inner surface is calculated.

- **Probabilistic Fracture Mechanics** (PFM): according to fabrication, examinations, and conventional measure the crack location, size and shape are defined.

Finally, with the analysis of the results a safety margin factor that indicates the failure probability of the reactor vessel is estimated.
The Thermal Hydraulic analysis plays an important role in the evaluation of PTS, since it investigates the overall response of the system to the transient, and determines, via the Downcomer Mixing Analysis, the complex three dimensional thermal mixing phenomena occurring in the downcomer. Numerical and/or experimental approaches can be adopted to perform the analysis of a PTS scenario. The experimental approach is usually limited by the possibility to completely reproduce the event in the laboratory and to the capability to actually measure data in the experimental set-up. One of the best known experimental set-up is the Rossendorf Coolant Mixing Model (ROCOM), that worked on a wide spectrum of coolant mixing scenarios, in this case they are working on a vessel model made of acrylic glass (Fig.1.2), which is a 1:5 scaled facility of a Konvoi PWR, so they have large database on the mixing distribution but they cannot provide wall heat transfer data [6].

The results of numerical tools, on the other hand, has not been completely trusted in the past and still nowadays its use in the nuclear industry is not as common as in other engineering applications. However, Computational Fluid Dynamics (CFD) has been making giant strides in the last decades and it is used with growing confidence also in critical operations such as those involved in the design and safety evaluation of components of a nuclear power plant [10].

For these reasons, thanks to their flexibility, capability in representing complex flows and with the advent of increasingly powerful computers, it is now more interesting to propose numerical tools to solve these kind of problems. However, a validation programme is necessary [3], in order to meet the standard of quality and trust requested by the regulation. Many international research project dealt with the assessment of CFD models for PTS scenarios, for instance within the EU project "Evaluation of Computational Fluid Dynamics Methods for Reactor Safety Analysis" (ECORA), a list of best practice guidelines was published for application of CFD for Nuclear Reactor Safety (NRS) [12].

Among the different approaches that falls under the word CFD, Direct Numerical Simulation (DNS) is the one that has the highest level of fidelity because it does not rely on any modeling approximation and it introduces virtually no numerical error. Furthermore, and more importantly, high quality DNS databases could serve as a ref-
ference to validate the available lower order turbulence modeling methods, such as Large Eddy Simulation (LES), Unsteady Reynolds Averaged Navier-Stokes simulations (URANS) and Hybrid (LES/URANS). In the past, the use of DNS was restricted because of the limited computational power. In particular, the application of DNS was limited to flows at low Reynolds numbers and in simplified geometries. But, unfortunately, DNS is still the most expensive approach, in terms of computational resources, and the simulation of a realistic PTS scenario is simply not feasible for today hardware capacity. That is why the purpose of the project ongoing at the Nuclear Research and Consultancy Group (NRG) is to provide a DNS database, for a simplified PTS configuration. This can be very helpful for scientific community: to understand the complex flow and heat transport in detail, but more importantly, this case could serve as database for the validation of any other numerical methods studying PTS. In order to get to this simpler setup, we need a preliminary study, NRG already worked on this kind of calibration [17], the PTS event was studied at constant density (accounting only for the forced convection). Through a series of Reynolds Average Navier Stokes Simulations (RANS), much less time consuming and more flexible then DNS, several aspects of the PTS design were calibrated and further optimized to achieve a realistic case for the final DNS computations. The effect of all the geometric parameters and their respective influence on the overall flow topology was studied, and the imposed boundary conditions were calibrated to correctly reproduce the flow regimes. Finally from the obtained RANS solution, Kolmogorov and Batchelor length scales were extracted, in order to optimize the DNS mesh.

The present work will start from this experience, but:

- instead of the commercial code Star CCM+, Code_Saturne an open-source software will be used, due to the high cost of a commercial code license it is interesting for a research center like NRG to investigate the capabilities of open-source softwares

- PTS involves the mixing of two fluids at different temperatures, this means different density, hence buoyancy forces will rise, therefore in order to get to a more realistic representation of the phenomenon, and a more accurate future database, calculations will account also for the buoyancy effect. The physics of the problem changes drastically, from forced convection the calculations will simulate natural convection

That is why it is necessary to perform an accurate validation process of Code_Saturne, to understand the possibilities and limitations of the new code, but it is also fundamental to rethink the calibration of the test case, due to the different physics of the
phenomenon introduced with the buoyancy effects. The aim is then to create a benchmark for DNS calculation, of a single-phase buoyancy-driven PTS event, keeping in mind that the experiment must be simple enough to meet the DNS time-limitations, but still physically meaningful in order to validate other codes.
Chapter 2

Governing equations

Computational Fluid Dynamics (CFD) is a branch of fluid mechanics that uses numerical analysis and algorithms to solve and analyze problems that involve fluid flows. Computers are used to perform the calculations required to simulate the interaction of liquids and gases with surfaces defined by boundary conditions. The fundamental basis of almost all CFD problems are the Navier–Stokes equations, they describe the motion of viscous fluids, from a macroscopic point of view, and they find wide application in the scientific and engineering world, because they describe the physics of a large spectrum of phenomena, like: flow in pipes or around a wing, ocean currents, blood flow etc... (Fig. 2.1). Navier–Stokes equations are composed by the following set of equations:

\[
\begin{align*}
\frac{\partial (\rho u)}{\partial t} + \text{div}(\rho u u) &= -\frac{\partial P}{\partial x} + \text{div}(\mu \text{grad} u) + f_x \\
\frac{\partial (\rho v)}{\partial t} + \text{div}(\rho v u) &= -\frac{\partial P}{\partial y} + \text{div}(\mu \text{grad} v) + f_y \\
\frac{\partial (\rho w)}{\partial t} + \text{div}(\rho w u) &= -\frac{\partial P}{\partial z} + \text{div}(\mu \text{grad} w) + f_z
\end{align*}
\]

(2.1)

the momentum equation, where \(\rho\) is the density, \(u, v, w\) are the three components of the velocity vector, \(P\) is the pressure, \(\mu\) is the dynamic viscosity and \(f_i\) is the sum of the body forces

\[
\frac{\partial \rho}{\partial t} + \text{div}(\rho u) = 0
\]

(2.2)
the continuity equation
\[
\frac{\partial (\rho i)}{\partial t} + \text{div } (\rho i \mathbf{u}) = -P \text{ div } \mathbf{u} + \text{div}(k \text{ grad } T) + \Phi + S_i
\] (2.3)

and the energy equation, where \( i = i(\rho, T) \) is the internal energy, \( T \) is the temperature, \( k \) is the thermal conductivity, \( \Phi \) is the friction power loss and \( S_i \) is the source term.

This set of equations: three time-dependent conservation of momentum equations (2.1), a time-dependent continuity equation for conservation of mass (2.2) and a time-dependent conservation of energy equation (2.3), represents the governing equations of a viscous, compressible flow with variable-properties. The aforementioned system is actually very complex, it counts: four independent variables, the \( x, y, z \) spatial coordinates of the domain, and the time \( t \); six dependent variables, the pressure \( P \), density \( \rho \), temperature \( T \) and three components of the velocity vector \( (u, v, w) \); and all the dependent variables are functions of all four independent variables. Due to this complexity the analytic solution still remain one of the main challenge of the modern mathematics, only for extremely simplified case is possible to get to a closed solution. Hence another strategy has been proposed: numerical analysis.

## 2.1 Natural convection modeling

Natural convection is a mechanism in which the fluid motion is not generated by any external source but only by density differences in the fluid occurring due to temperature gradients. The driving force for natural convection is buoyancy, a result of differences in fluid density.

The idea behind this study is to create a database for the validation of different numerical strategies, as aforementioned NRG already worked on a similar matter, investigating the PTS scenario accounting only for the forced convection, but mixing water at different temperatures, hence different density, means that buoyancy forces will rise and will affect both velocity and temperature field. That is why, in order to increase the quality of the future DNS database, it is necessary, in the present work, to analyze the effects of the natural convection on the PTS phenomenon. Density is the key of the physics, and a measure of its interference is necessary: the ROCOM test facility performed a series of experiments trying to replicate a buoyancy driven mixing, and due to the structural constraints of the facility, they studied the mixing of water and “sweet” water (water + glucose), and to track the flow they injected a sodium chloride solution [7]. Different mass flow rates (inlet velocity) and different density difference were investigated, and to determine the conditions at which the mixing was driven by
the momentum and when instead was influenced by the buoyancy forces, they chose
the Froude number:
\[ Fr = \frac{u_{in}}{\sqrt{gh \left( \frac{\rho_1 - \rho_2}{\rho_1} \right)}} \] (2.4)

The $Fr$ number is a dimensionless parameter that can be seen as the ratio between
inertia ($u_{in}$) and weight ($\frac{\rho_1 - \rho_2}{\rho_1} g$), and at the ROCOM test facility they discovered that for:

- $Fr < 0.85$: the mixing is buoyancy driven
- $Fr > 1.5$: the momentum is predominant
- $0.85 < Fr < 1.5$: transition region

The results show that the density difference shrinks the area covered by the ECC water
in spawn wise direction (respect to the constant density case), and then the cold water
falls down almost in straight line under the nozzle (Fig. 2.2).

Figure 2.2: Tracer distribution inside the vessel (left), Froude number isolines (right) at
ROCOM test facility

2.1.1 Boussinesq approximation

In the simulations of this study the buoyancy effects are considered, this means that
the only body force acting on the flow is the weight of the fluid itself, hence the Navier-
Stokes equations can be written as:

\[
\begin{align*}
\frac{\partial (\rho u)}{\partial t} + \text{div}(\rho u u) &= -\frac{\partial P}{\partial x} + \text{div}(\mu \text{grad } u) + \rho g_x, \\
\frac{\partial (\rho v)}{\partial t} + \text{div}(\rho v u) &= -\frac{\partial P}{\partial y} + \text{div}(\mu \text{grad } v) + \rho g_y, \\
\frac{\partial (\rho w)}{\partial t} + \text{div}(\rho w u) &= -\frac{\partial P}{\partial z} + \text{div}(\mu \text{grad } w) + \rho g_z, \\
\frac{\partial \rho}{\partial t} + \text{div}(\rho u) &= 0, \\
\frac{\partial (\rho C_p T)}{\partial t} + \text{div}(\rho C_p T u) &= \text{div}(k \text{grad } T).
\end{align*}
\]

where \(g_x, g_y, g_z\) are the components of the gravity vector. The Boussinesq approximation ignores density differences except where they appear in terms multiplied by \(g\), the basic idea is that the difference in inertia is negligible but gravity is sufficiently strong to make the specific weight appreciably different between the two fluids. If the incompressible assumption is acceptable the previous system 2.5 is modified as follows:

\[
\begin{align*}
\frac{\partial u}{\partial t} + \text{div}(u u) &= -\frac{1}{\rho} \frac{\partial P}{\partial x} + \nu \text{div}(\text{grad } u) + g_x \beta \Delta T, \\
\frac{\partial v}{\partial t} + \text{div}(v u) &= -\frac{1}{\rho} \frac{\partial P}{\partial y} + \nu \text{div}(\text{grad } v) + g_y \beta \Delta T, \\
\frac{\partial w}{\partial t} + \text{div}(w u) &= -\frac{1}{\rho} \frac{\partial P}{\partial z} + \nu \text{div}(\text{grad } w) + g_z \beta \Delta T, \\
\text{div}(u) &= 0, \\
\frac{\partial (\rho C_p T)}{\partial t} + \text{div}(\rho C_p T u) &= \frac{1}{\rho} \text{div}(k \text{grad } T).
\end{align*}
\]

In the aforementioned set of equations density variations are assumed to have a fixed part and another that has a linear dependence on temperature:

\[
\rho = \rho_0 - \beta \rho_0 \Delta T
\]

where \(\rho_0\) is the reference density and \(\beta\) is the coefficient of thermal expansion. The approximation is extremely accurate if the temperature difference \(\Delta T\) is contained, and makes the mathematics and physics simpler, in the following pages the Boussinesq approximation will be tested against the variable density approach.

### 2.2 Turbulence

Turbulence is a complex phenomenon that can be observed in our everyday life, the coffee stirred by a spoon, or the smoke of a cigarette. A turbulent flow is characterized by tridimensionality, unsteadiness, and more generally by chaotic movement, but inside this randomness we can recognize coherent spatial structures called *eddies*. We
can distinguish these arrangements for their seize and purpose: the large-scale turbulent motion extract energy from the mean flow, that through an energy cascade is transferred to the small-scale eddies (Kolmogorov’s scale), at this point the viscous effects is dominant and the kinetic energy is dissipated through heat (Fig. 2.3). Even though the random nature of the phenomenon, different non-dimensional parameters are used to predict similar patterns and describe turbulent flows:

- **Reynolds number**: defined as the ratio between inertia and viscous forces

  $$Re = \frac{\rho u L}{\mu}$$  \hspace{1cm} (2.8)

  - **Low Re**: flows with dominant viscous effect are called *laminar flows*, they show an ordered pattern, with streamlines parallel to the main axis of the flow
  
  - **High Re**: *turbulent flows* consist of chaotic vortices and eddies, where inertia forces are dominant

- **Prandtl number**: defined as the ratio between the momentum diffusivity and the thermal diffusivity

  $$Pr = \frac{c_p \mu}{k}$$  \hspace{1cm} (2.9)

to the Pr number is related the relative thickness of the momentum and thermal boundary layer near the wall. A low Pr number means that heat diffuses very
quickly compared to the velocity, hence the thermal boundary layer is thicker than the velocity boundary layer.

Now, assuming that the characteristic length of the domain studied is $L$, while the Kolmogorov’s scale is $\eta_K$, then:

$$\frac{L}{\eta_K} \approx Re^{3/4}$$  \hspace{1cm} (2.10)

the discretization of the domain leads to a number of cells of:

$$N \approx Re^{9/4}$$  \hspace{1cm} (2.11)

for each grid points we have to compute all the unknowns through the time and the computational efforts is proportional to $Re^3$.

### 2.3 Turbulence modeling

Turbulence modeling is a key issue in most CFD simulations, virtually all engineering applications are turbulent and hence it is fundamental to predict the effects of turbulence. In Fig.2.4 the principal approaches to the solution of the turbulence problem are reported:

- **DNS**: is a simulation in which the Navier-Stokes equations are numerically solved without any turbulence model, this means that the whole range of spatial and temporal scales of the turbulence are resolved.

- **LES**: the principal idea is to ignore the smallest length scales, which are the most computationally expensive to resolve, via low-pass filtering of the Navier–Stokes equations. This feature allows to explicitly solve for the large eddies in a calculation and implicitly account for the effects of the small scales and fluctuating parts using a model.

- **RANS**: give an approximate time-averaged solution to the Navier–Stokes equations, modeling the behavior of the Reynolds stresses.

#### 2.3.1 Direct Numerical Simulation

Direct Numerical Simulation (DNS) is the most complete approach available in CFD. Theoretically is also very simple, since it numerically solves the Navier-Stokes equations without any turbulence model, but this means to solve the fluid motion in the
whole range of spatial and temporal scales of the turbulence, from the smallest dissipative scales (Kolmogorov), up to the integral scale. This means that the domain must be discretized in space such that also the smallest spatial scales of the fluid flow are well resolved. A huge computational power is required to perform such simulation and that is why, even with the use of the most powerful computer available at the moment we are not able to solve realistic industrial problems, but only simplified scenarios, like flow in pipes or through diffusers etc...

2.3.2 Unsteady Reynolds Averaged Navier Stokes

The numerical approach does not seek the exact solution of the Navier-Stokes equations, instead it is concerned with obtaining approximate solutions while maintaining reasonable bounds on errors. The instantaneous description of the fluid motion, coming from the Navier-Stokes equations, has poor interest in industrial applications, since the quantities at a certain instant will never have the same value. Hence neglecting the instantly fluctuations, it is possible to introduce another system of equations derived from the NS, called: Unsteady Reynolds Average Navier Stokes (URANS). The idea is to represent every quantity involved in the fluid motion description, as the sum of a mean and a fluctuating component:

$$\phi(x, t) = \Phi + \phi'$$

(2.12)
the advantage is that when applying the time average the turbulent component disappears:

$$\bar{\phi} = \frac{1}{\Delta t} \int_0^{\Delta t} (\Phi + \phi') \, dt = \Phi$$  \hspace{1cm} (2.13)

Introducing this formulation in previous set of equations and applying the time average to all terms we get the URANS system:

$$\begin{align*}
\frac{\partial \rho}{\partial t} + \text{div}(\rho \mathbf{U}) &= 0 \\
\frac{\partial (\rho U)}{\partial t} + \text{div}(\rho U \mathbf{U}) &= -\frac{\partial P}{\partial x} + \text{div}(\mu \text{grad} \mathbf{U}) + (\rho u'v') - (\rho w') + F_x \\
\frac{\partial (\rho V)}{\partial t} + \text{div}(\rho V \mathbf{U}) &= -\frac{\partial P}{\partial y} + \text{div}(\mu \text{grad} \mathbf{V}) + (\rho u'v') - (\rho w') + F_y \\
\frac{\partial (\rho W)}{\partial t} + \text{div}(\rho W \mathbf{U}) &= -\frac{\partial P}{\partial z} + \text{div}(\mu \text{grad} \mathbf{W}) + (\rho u'w') - (\rho v') + F_z \\
\frac{\partial (\rho C_p T)}{\partial t} + \text{div}(\rho C_p T \mathbf{U}) &= \text{div}(k \text{grad} T)
\end{align*}$$  \hspace{1cm} (2.14)

With the averaging we neglect the instantaneous fluctuations of the velocity, but we have six more unknowns, the Reynolds stresses, that will take into account the influence of the turbulence on the flow:

$$\tau_{ij} = -\rho u'_i u'_j$$  \hspace{1cm} (2.15)

Both RANS and URANS approaches base their formulation on the Reynolds averaging [20] but in case of RANS simulations the term $\frac{\partial (\rho U)}{\partial t}$, the mean flow quantity variation along time, goes down to zero. URANS calculations are adopted in this work since the nature of buoyancy-driven flows is unsteady and a steady state solution is not achievable.
Chapter 3

Numerical setup

3.1 Code

All the simulations reported in this work were performed with Code_Saturne (CS), an open-source code developed by the Recherche et Développement (R&D) of Électricité de France (EDF). The software is designed to solve the Navier-Stokes equations in the cases of 2D, 2D axis-symmetric or 3D flows. Several turbulence models are available, from Reynolds-Averaged models to Large-Eddy Simulation models. In addition, a number of specific physical models are also available: gas, coal and heavy-fuel oil combustion, semi-transparent radiative transfer, particle-tracking with Lagrangian modeling, Joule effect, electrics arcs, weakly compressible flows, atmospheric flows, rotor/stator interaction for hydraulic machines. It relies on a finite volume discretization and allows the use of various mesh types: structured, block-structured, unstructured, hybrid etc.; with any elements: tetrahedral, hexahedral, etc.[14]. In order to solve the temperature field also inside the solid domain of the system, Code_Saturne is coupled with another software developed by EDF: Syrthes, that simulates conduction and radiation, only on tetrahedral meshes [16]. When coupled together it is possible to solve the conjugate heat transfer between the fluid and solid domain, Code_Saturne solves the interaction, while Syrthes sees the change at the boundary conditions and solves the conduction equation accordingly.

For a research center such like NRG it is interesting to investigate the possibilities of an open-source code, due too the high cost of other commercial softwares, but Code_Saturne is never been used by NRG before, hence a validation process is necessary [A].
3.2 EBRSM

During the validation process all turbulence models available in Code_Saturne have been tested, and from this study, due to the outstanding performance, the Elliptic Blending Reynolds Stress Model ($R_{ij}$-EBRSM) has been chosen to perform this study. The Reynolds Stress Models are elaborate turbulence models in which the eddy viscosity isotropicity has been discarded and the Reynolds stresses are directly computed. The effects of solid walls on turbulent flows is still a challenge for the scientific society. Different strategies have been adopted to model this problem:

- **Wall functions**: widely used in the industry, because of the confirmed results on simple cases, and the drastic reduction of grid points needed. But this technique is deficient in non-equilibrium flows, such as separated streams, natural convection, three-dimensional flows, etc.

- **Damping functions**: allow the integration of equations up to the wall, less popular among the industry because of the very refined mesh requirement

- **Elliptic relaxation method**: formulated by Durbin, enables the integration down to the wall, with acceptable grid density. But introduces some instability due to the elliptic equations introduced

The EBRSM, proposed by Manceau and Hanjalic in 2002 and here implemented [11], preserves the main feature of Durbin’s Reynolds stress model, but instead of six elliptic equations, it involves only one scalar equation. The purpose is to eliminate the numerical stiffness induced by the boundary conditions of the additional elliptic equations, and meet the industrial needs for a simple and robust model while still satisfying the main theoretical constraints.

Hereby the formulation of the turbulence model implemented in this work is reported:

$$\frac{Du'_i u'_j}{Dt} = P_{ij} + D_{ij}^V + D_{ij}^T + \Phi_{ij}^* - \varepsilon_{ij}$$  \hspace{1cm} (3.1)

transport equation for the Reynolds-stress tensor $u'_i u'_j$ where $P_{ij}$ is the production term, $D_{ij}^V$ the viscous diffusion term, $D_{ij}^T$ the turbulent diffusion term, $\Phi_{ij}$ the pressure-strain redistribution term and $\varepsilon_{ij}$ is the dissipation term.

$$\frac{D\varepsilon}{Dt} = \frac{C_{e_1}p - C_{e_2}c}{T} + \frac{\partial}{\partial x_i} \left( \frac{C_{\mu}}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_m} \right) + v \frac{\partial^2 \varepsilon}{\partial x_k \partial x_k} + C_{e_3} \frac{k}{\varepsilon} \frac{\partial^2 U_i}{\partial x_i \partial x_m} \left( \frac{\partial^2 U_j}{\partial x_j \partial x_m} \right)$$  \hspace{1cm} (3.2)
The model equations for the Reynolds-stress are then closed with the low-Re-number version of the transport equation for the turbulence dissipation rate $\varepsilon$.

$$\alpha - L^2 \nabla^2 \alpha = \frac{1}{\varepsilon T}$$

(3.3)

The ellipticity of the model is preserved by solving an elliptic differential equation for $\alpha$. The blending function $\alpha$ is introduced in the pressure-velocity gradient correlation term:

$$\Phi_{ij}^* = (1 - k\alpha) \Phi_{ij}^w + k\alpha \Phi_{ij}^h$$

(3.4)

and in the model of the dissipation:

$$\varepsilon_{ij} = (1 - A\alpha) \frac{u_i u_j}{k} \varepsilon + A\alpha \frac{2}{3} \varepsilon \delta_{ij}$$

(3.5)

Where the budgets introduced are:

$$T = \max \left( \frac{k}{\varepsilon}, C_T \left( \frac{v}{\varepsilon} \right)^{1/2} \right)$$

$$L = C_L \max \left( \frac{k^{3/2}}{\varepsilon}, C_{\eta} \frac{v^{3/4}}{\varepsilon^{1/4}} \right)$$

$$C_{\varepsilon_1} = 1.4$$

$$C_{\varepsilon_2} = 1.85$$

$$C_{\varepsilon_3} = 0.55$$

$$C_{\eta} = 80.0$$

$$C_T = 6.0$$

(3.6)

The budget $\Phi_{ij}^* - \varepsilon_{ij}$ reproduces the constraints (no-slip boundary condition and fluid incompressibility) in the near-wall region, limiting the Reynolds stresses. This setting avoids writing the six elliptic relaxation equations, and provide a smooth transition between the near-wall form of the Reynolds stresses and the one far from the wall, thanks to the blending formulas for $\Phi_{ij}^*$ and $\varepsilon_{ij}$.

### 3.3 Spatial discretization of the fluid equation

The following step, after the Reynolds averaging of the Navier-Stokes equations, is the spatial discretization. The Finite Volume Method (FVM) is a method for representing and evaluating partial differential equations, such as Navier-Stokes, in the form of algebraic equations. "Finite volume" refers to the small volume surrounding each node point on a mesh. In the finite volume method, volume integrals in a partial differential equation that contain a divergence term are converted to surface integrals, using the divergence theorem. These terms are then evaluated as fluxes at the surfaces of each
finite volume. Different strategies for the convective terms of the Navier-Stokes are
available, for the simulations here reported the Second Order Linear Upwind (SOLU)
has been chosen:

\[ C_{ij}(\dot{m}_{ij}, Y) = (Y_{fi} - Y_i) \dot{m}_{ij} \]  

(3.7)

with

\[ Y_{fi} = \begin{cases} 
Y_i + \nabla_i Y \cdot I F & \text{if } \dot{m}_{ij} \geq 0 \\
Y_j + \nabla_j Y \cdot J F & \text{if } \dot{m}_{ij} < 0 
\end{cases} \]  

(3.8)

In the incompressible Navier-Stokes equations the transport for pressure does not ap-
pear, but the pressure gradient is present in every equation, so either the pressure field
is known and the velocity field is solved consequently or it is necessary to introduce a
strategy to manage the pressure-velocity coupling.

The Pressure Implicit with Splitting of Operator (PISO) algorithm is one of the possibili-
ties that can solve the coupling between pressure and velocity. It is an iterative process
that involves one predictor step and two corrector steps and can be summarized as
follows:

1. Set the boundary conditions
2. Solve the discretized momentum equation to compute an intermediate velocity
   field \((u^*)\)
3. Compute the mass fluxes at the cells faces \((\dot{m}^*)\)
4. Solve the pressure equation \((p')\)
5. Correct the mass fluxes at the cell faces \((\dot{m}^{**})\)
6. Correct the velocities on the basis of the new pressure field \((u^{**} = u^* + u')\)
7. Update the boundary conditions
8. Repeat from step 3 for the prescribed number of times
9. Increase the time-step and repeat from step 1

The PISO algorithm is highly recommended for transient calculations, and allows to
implement a large time-step. This feature is very interesting for our study, since can
balance the sensitivity of the EBRSM turbulence model to the time-step magnitude
and therefore decrease the computational cost.
3.4 Temporal discretization of the fluid equation

The time scheme is a $\theta$-scheme. At first, the physical properties of the flow are computed (density, viscosity, specific heat etc...). For the Reynolds stress model, the variables (turbulent stresses and dissipation) are solved sequentially, without coupling. Next, the equations for the scalars (enthalpy, temperature, tracers, concentrations, mass fractions...) are solved. Finally, all the variables are updated and another time step may start.

3.5 Conduction

When different parts of a solid body have different temperatures, the heat spreads from the hot regions to the cold ones. If the heat is transferred within the material itself, we have conduction.

\[ \rho C_p \frac{\partial T}{\partial t} = -\nabla \cdot q + \Phi \]  

(3.9)

Where $\rho$ is the density, $C_p$ is the specific heat and $T$ is the unknown. The right side of the equation characterizes the way the heat propagates, $q$ represents the heat flux, $\Phi$ is the source term.

Different models can be adopted for the heat flux, depending on the kind of material we want to simulate $q$ can be either a scalar or a matrix:

- **Isotropic**: solids diffuse heat isotropically in space, isothermal contours are concentric spheres, so we can assume that the flux and the temperature are co-linear

\[ q = -k \nabla T \]  

(3.10)

- **Anisotropic**: when different conductive behaviors of a material cannot be aligned to the reference axes, the conductivity matrix is no more diagonal and can be adapted to any circumstances

In this work the solid parts are treated as isotropic materials, and as aforementioned Syrthes will solve the solid domains.

3.6 Conjugate heat transfer

In the following simulations it is crucial to understand and represent the thermal interaction between the flow field and the walls enclosing it. For many simulations of real
world engineering applications, the predictions of heat transfer properties are as im-
portant as the actual flow field, and when the combination of heat transfer in solids and
heat transfer in fluids must be studied, the Conjugate Heat Transfer (CHT) model can
describe the conduction, often dominating the solid domain, and the convection in-
side fluids. As already mentioned Code_Saturne cannot solve the conjugate heat trans-
fer between the injecting cold fluid and the hot walls, but EDF offers another software,
Syrthes [16], which has been developed to simulate specifically thermal problems, and
it can be used alone if users are interested only in conduction/radiation problems or
coupled with fluid mechanics codes, such as Code_Saturne, to simulate thermal phe-
nomena couple fluid and solid. Once the two codes are coupled the physical processes
and solutions of the governing equations are considered separately for each domain:
Code_Saturne will solve the flow field and the conjugate heat transfer, providing the
distributions of temperature and heat flux along the body/flow interface, eliminating
the need for a heat transfer coefficient, Syrthes starting form the interface will solve the
conduction inside the walls.
Chapter 4

Calibration of the PTS experiment

In this chapter, the numerical simulations for a single-phase buoyancy-driven simplified PTS scenario will be performed. Through a series of RANS calculations: boundary conditions, fluid properties and computational domain will be calibrated and optimized in order to perform the DNS computation in a future work. As aforementioned, the correct design of such experiment is crucial since the setup must be simple enough to isolate the event and fulfill the "cost" limitations of the DNS, but still physically meaningful in order to include all the main features of this problem.

4.1 Baseline configuration

The main idea of the present work is to design a numerical experiment to simulate the thermal mixing in the downcomer and the evolution of temperature distribution for both fluid and structures in an ECC injection event. During such a scenario, the injected cold ECC water mixes with hot water present in the cold leg and the mixture flows downward in the downcomer in the form of density driven cold plumes. Previous studies focused on the mixing process in the injecting leg [9], therefore this work will deal with the mixing process occurring in the downcomer, in particular the influence of the buoyancy effect and the evolution of temperature distribution in the fluid and solid regions. NRG already worked on a similar matter, a calibration was performed on the same phenomenon but at constant density [17], the optimized set-up: domain size, boundary conditions and fluid properties, represents the baseline configuration of this work.

The computational domain, reported in Fig.4.1, consists of:

- **Square leg**: where the relatively cold fluid is injected (Inlet 1), and it is characterized by the hydraulic diameter $D_h$
• **Downcomer**: where the mixing takes place. In the upper-side the hot fluid is injected (*Inlet 2*), at the bottom the outlet is present.

• **Shroud** and **Vessel**: bounding walls enclosing the fluid.

The initial domain configuration is based on the ROCOM test facility, however, some simplifications have been introduced to facilitate the high quality DNS requirements. For example, instead of a real curved geometry for a vessel, a planar configuration is considered. Moreover, the lower plenum and the internal vessel cladding are not considered. In the following table (Tab.4.1) the dimensions and initial setup of the PTS experiment are reported.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>( U_1 = 0.018 , m/s )</th>
<th>( T = 293 , K )</th>
<th>( \rho = 997.16 , kg/m^3 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet 1</td>
<td>Inlet with relatively cold water. Initially a constant velocity profile is applied.</td>
<td>( U_2 = 0.0018 , m/s )</td>
<td>( T = 353 , K )</td>
<td>( \rho = 970.19 , kg/m^3 )</td>
</tr>
<tr>
<td>Inlet 2</td>
<td>Inlet with relatively hot water. Fictitious inlet to push down the cold fluid.</td>
<td>( D_h = 0.15 , m )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( D_h )</td>
<td>Diameter of the cold leg, taken from the ROCOM facility.</td>
<td>( H_1 = 1 , m )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( L )</td>
<td>Cold leg length.</td>
<td>( W = 2 , m )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( H_2 )</td>
<td>Downcomer height. It is intended to be calibrated in order to mitigate the influence of the outlet</td>
<td>( H_2 = 3.5 , m )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( W )</td>
<td>Width of the downcomer. It is intended to be calibrated in order to mitigate the influence of the bounding walls</td>
<td>( D_v = 0.05 , m )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( D_v )</td>
<td>Thickness of the vessel, a 1:5 scale of a real reactor vessel design.</td>
<td>( D_s = 0.025 , m )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( D_s )</td>
<td>Thickness of the shroud, a 1:5 scale of a real reactor vessel design.</td>
<td>( D_d = 0.075 , m )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( D_d )</td>
<td>Thickness of the downcomer, taken from the ROCOM facility.</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 4.1: Initial setup of the PTS experiment
CHAPTER 4. CALIBRATION OF THE PTS EXPERIMENT

We must underline, once again, that this configuration is just the starting point of this work and it comes from a different calibration that had completely different assumptions, for these reasons the domain will be optimized further on in this paper.

4.2 Boundary conditions

The mass flow rate imposed in the square leg is the same used in a ROCOM test case [8], the fluid is entering the domain at a bulk velocity of $U_1 = 0.018 \text{m/s}$ and a relatively cold temperature of 293 K. At the Inlet2 the flow is injected at 353 K and the velocity has been calibrated during the previous experience at NRG, this is a fictitious inlet since it is not present in the real configuration of the RPV, but it is needed in the numerical simulation to push down the outlet the cold fluid entering the domain. At the outlet a gauge pressure equal to 0 is imposed. No-slip boundary conditions are imposed on all the walls bounding the fluid domain, while adiabatic conditions are applied at external boundaries of the solid.

The initial boundary conditions, as aforementioned, come from the previous work at NRG, due to the basic difference between this work and the one at constant density, the calibration of the boundary conditions will be the first issue to be investigated. In particular the presence of two inlets seems redundant if we introduce the buoyancy effect inside the simulation.

4.3 Fluid and solid properties

The working fluid is water, whose properties are considered to depend only on the temperature and here, in particular, are approximated with the following quadratic functions:

- Density: $\rho = 777.214 + 1.7469T - 0.0034T^2 \text{[kg/m}^3\text{]}$
- Dynamic viscosity: $\mu = 0.019 - 1.06 \cdot 10^{-4}T + 1.48 \cdot 10^{-7}T^2 \text{[Pa} \cdot \text{s]}$
- Thermal conductivity: $k = -0.788 + 0.008T - 1.361 \cdot 10^{-5}T^2 \text{[W/m} \cdot \text{K]}$
- Specific heat: $C_p = 5186.439 - 6.443T + 0.011T^2 \text{[J/kg} \cdot \text{K]}$

The not constant water properties is the key difference from the previous work on the PTS, in the following pages we will show how this feature affects the mixing in the downcomer, and how the calibration will work around the buoyancy effect in order to
Figure 4.1: Numerical domain of the PTS experiment
isolate the event, to observe the DNS constraints and still produce a physically meaningful experiments. Moreover a simplification for the modeling of water behavior will be investigated.

The solid parts are made of 16MND5 steel, with constant properties at 323 K:

- Density: $7840 \text{ kg/m}^3$
- Thermal Conductivity: $45.98 \text{ W/m/K}$
- Specific heat: $476.50 \text{ J/kg/K}$

4.4 Mesh

As previously mentioned, the initial geometry and fluid mesh are the same used in the previous calibration work of Shams et al. [17], in particular:

- the mesh consists of approximately 3.000.000 hexahedral elements
- the spatial resolution in the wall normal direction is such that the distance of the cell center from the wall in terms of friction units is $y^+ << 1$, this assures that the velocity profile near the wall is well resolved

Since the solver Syrthes can handle only meshes with tetrahedral elements, a new mesh for the solid domain has been generated. It consists of approximately 200.000 elements for the shroud and 700.000 elements for the vessel (see Fig.4.2 center and right).

Figure 4.2: Fluid and solid meshes
4.5 Work structure

The calibration reported in this work is structured as follows:

- The starting point is the same configuration used in the previous at NRG in which the fluid density was assumed to be constant, but here buoyancy effects are also taken into account.

- In the first step, due to the not constant properties of the working fluid, the inlet velocity in the upper side of the downcomer will be calibrated.

- In the second step, using the value of the inlet velocity chosen in the previous step, the geometrical dimensions of the downcomer will be calibrated.

- Finally, the buoyancy effects on the selected configuration are studied.

In Tab. 4.2 the complete list of parameter and their variations is reported for the whole calibration process.

<table>
<thead>
<tr>
<th>Case</th>
<th>$U_1 [m/s]$</th>
<th>$U_2 [m/s]$</th>
<th>$\Delta T [K]$</th>
<th>Model</th>
<th>Domain</th>
<th>$\Delta \rho$</th>
<th>Fr</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.018</td>
<td>10$% U_1$</td>
<td>293 $\pm$ 353</td>
<td>EBRSM</td>
<td></td>
<td>3%</td>
<td>0.018</td>
</tr>
<tr>
<td>1a</td>
<td>0.018</td>
<td>10$% U_1$</td>
<td>293 $\pm$ 353</td>
<td>EBRSM</td>
<td></td>
<td>3%</td>
<td>0.018</td>
</tr>
<tr>
<td>1b</td>
<td>0.018</td>
<td>5$% U_1$</td>
<td>293 $\pm$ 353</td>
<td>EBRSM</td>
<td></td>
<td>3%</td>
<td>0.018</td>
</tr>
<tr>
<td>2a</td>
<td>0.018</td>
<td>0</td>
<td>293 $\pm$ 353</td>
<td>EBRSM</td>
<td>$H + 6D_h$</td>
<td>3%</td>
<td>0.016</td>
</tr>
<tr>
<td>2b</td>
<td>0.018</td>
<td>0</td>
<td>293 $\pm$ 353</td>
<td>EBRSM</td>
<td>$H + 6D_h W + 6D_h$</td>
<td>3%</td>
<td>0.016</td>
</tr>
<tr>
<td>2c</td>
<td>0.018</td>
<td>0</td>
<td>293 $\pm$ 353</td>
<td>EBRSM</td>
<td>$H + 6D_h W + 12D_h$</td>
<td>3%</td>
<td>0.016</td>
</tr>
<tr>
<td>3a</td>
<td>0.018</td>
<td>0</td>
<td>293 $\pm$ 353</td>
<td>EBRSM</td>
<td>$H + 3D_h$</td>
<td>3%</td>
<td>0.017</td>
</tr>
<tr>
<td>3b</td>
<td>0.018</td>
<td>0</td>
<td>293 $\pm$ 353</td>
<td>EBRSM</td>
<td>$H + 3D_h W + 6D_h$</td>
<td>3%</td>
<td>0.017</td>
</tr>
<tr>
<td>4a</td>
<td>0.018</td>
<td>0</td>
<td>303 $\pm$ 343</td>
<td>EBRSM</td>
<td>$H + 3D_h W + 6D_h$</td>
<td>2%</td>
<td>0.020</td>
</tr>
<tr>
<td>4b</td>
<td>0.018</td>
<td>0</td>
<td>278 $\pm$ 368</td>
<td>EBRSM</td>
<td>$H + 3D_h W + 6D_h$</td>
<td>4%</td>
<td>0.013</td>
</tr>
<tr>
<td>5a</td>
<td>120$% U_1$</td>
<td>0</td>
<td>293 $\pm$ 353</td>
<td>EBRSM</td>
<td>$H + 3D_h W + 6D_h$</td>
<td>3%</td>
<td>0.021</td>
</tr>
<tr>
<td>5b</td>
<td>150$% U_1$</td>
<td>0</td>
<td>293 $\pm$ 353</td>
<td>EBRSM</td>
<td>$H + 3D_h W + 6D_h$</td>
<td>3%</td>
<td>0.024</td>
</tr>
<tr>
<td>5c</td>
<td>200$% U_1$</td>
<td>0</td>
<td>293 $\pm$ 353</td>
<td>EBRSM</td>
<td>$H + 3D_h W + 6D_h$</td>
<td>3%</td>
<td>0.032</td>
</tr>
<tr>
<td>6</td>
<td>Fully turbulent</td>
<td>0</td>
<td>303 $\pm$ 343</td>
<td>EBRSM + Boussinesq</td>
<td>$H + 3D_h W + 6D_h$</td>
<td>2%</td>
<td>0.020</td>
</tr>
<tr>
<td>7</td>
<td>Fully turbulent</td>
<td>0</td>
<td>303 $\pm$ 343</td>
<td>EBRSM + Boussinesq + Periodicity</td>
<td>$H + 3D_h W + 6D_h$</td>
<td>2%</td>
<td>0.020</td>
</tr>
</tbody>
</table>

Table 4.2: Work table
4.6 Constant density

Before starting with the actual calibration, since the antecedent work was performed with the commercial code Star CCM+ [2] while the present simulations will be performed on Code_Saturne, it is interesting to compare the results obtained with the two codes on a preliminary simulation of the optimized PTS test case at constant density. We must recall that the two simulations were performed on the same domain and with same boundary conditions but different turbulence models: low Reynolds cubic $k – \epsilon$ for Star CCM+ while the EBRSM for Code_Saturne.

In Fig.4.3 the velocity field in the perpendicular section to the downcomer and the velocity profile along the middle-line of the downcomer are reported, and it is possible to see how the major features of the flow field are similar. In Fig.4.4 the temperature evolution in the middle section of the downcomer is reported, we can notice how the overall shape of the temperature field is the same.

In the end nevertheless the differences between the configurations this simulation confirmed the robustness of code and turbulence model.

![Figure 4.3: Velocity field in perpendicular section to the downcomer (left), and velocity profile along the middle-line of the downcomer (right)](image)

4.7 Velocity calibration

After the preliminary simulation at constant density the actual calibration can start, this means that all the calculations that are about to be mentioned will take into ac-
The first issue addressed is the presence of the second inlet: the boundary conditions of the following simulation are the same applied in the previous PTS calibration process without buoyancy effect, this mean that cold fluid is injected in the square leg while an hot flow is imposed at the upper side of the downcomer. This configuration is mandatory in the case of constant density simulation, in fact the second inlet is meant to push the cold water down the outlet, and the magnitude of the second inlet velocity has been calibrated in the previous work of Shams et al. [17], in particular it has been optimized at $U_2 = 10\% U_1$. On the other hand, when buoyancy effects are taken into account the cold fluid is expected to naturally flow down due to the gravity. For this reason, in the calibration of the inlet velocity at the downcomer, a zero inlet velocity is also considered.

In the following pages, for the analysis of the results, we will concentrate especially on the investigation of the temperature field inside the downcomer, because we find it more explicative of what is happening in the domain, since it is the temperature and hence the density that is driving the mixing.

Therefore the instantaneous temperature fields for three different values for the second inlet velocity are reported in Fig.4.5. From the baseline configuration with $U_2 = 10\% U_1$, coming from the previous experience at NRG, the value of the velocity at the downcomer has been reduced gradually: from $U_2 = 5\% U_1$ to a zero inlet velocity. From the analysis of the results it is possible to notice that:

- For the whole set of simulations, in the square leg a temperature stratification is induced by the mixing of the cold water injected and the the hot fluid present in
CHAPTER 4. CALIBRATION OF THE PTS EXPERIMENT

Figure 4.5: Temperature field in the perpendicular section to the downcomer (left), and in the middle of the downcomer (right) for three different values of the inlet velocity at the downcomer

- Due to the presence of gravity and the different weight of the water, the cold fluid flows down even when the inlet velocity at the downcomer is zero.

These are the reasons for which we decided to eliminate the second inlet from our configuration: because the code is dealing well with buoyancy driven flows, how has been shown also in the validation process (Appendix A), and finally now, with the buoyancy forces introduced, the second inlet is no more needed to push down the flow. However, due to the unsteadiness of the phenomenon, only a snapshot of the temperature field is not enough to understand what is happening in the downcomer, so also the evolution of the temperature field along time is reported in Fig. 4.6. Five samples of the temperature field are reported, along a real-time of around five minutes. From this set of images, it possible to understand that:

- As aforementioned, the cold water falls down the cold leg nozzle without the presence of a second inlet at the top of the downcomer.

- The behavior of the cold vein in the downcomer is heavily influenced by the bounding walls, the fluid falls down and starts oscillating, but after a while it attaches to the wall bounding the span-wise direction, and continues to imping this wall from there after.

The way the mixing is occurring in the downcomer is not acceptable, since the bounding walls are not present in the real configuration of the RPV, so they cannot
affect the flow behavior so heavily, for this reason the size of the domain will be calibrated in the following chapter.

A final remark must be done on the value of the Froude number, in order to continue the simulations. As said before, in order to simulate a buoyancy driven mix $Fr$ must be less than 0.85. In this case has been calculated as $Fr = 0.018$, we are well under the buoyant limitations, hence we shall continue our calibration with the zero velocity configuration.

### 4.8 Domain calibration

With the previous calibration of the second inlet velocity we have insured that natural convection is represented correctly in the simulations, but the heavy influence of the side walls on the flow behavior is not acceptable, since these walls are not present in the actual configuration of the reactor. That is why the size of the domain must be calibrated, five cases are here reported (Fig.4.7):

- **Base case**: $H_2 = 3.5 \text{ m}, \ W = 2 \text{ m}$
- $H_2 = H_2 + 3D_h = 3.95 \text{ m}, \ W = 2 \text{ m}$
- $H_2 = H_2 + 3D_h = 3.95 \text{ m}, \ W = W + 6D_h = 2.9 \text{ m}$
- $H_h = H_2 + 6D_h = 4.4 \text{ m}, \ W = W + 6D_h = 2.9 \text{ m}$
- $H_2 = H_2 + 3D_h = 4.4 \text{ m}, \ W = W + 6D_h = 3.8 \text{ m}$
where $H_2$ is the distance between the cold leg nozzle and the outlet, $W$ is the width of the downcomer and $D_h$ is the hydraulic diameter of the cold leg. The dimensions chosen for the calibration are: $H_2$ because of the outlet, that influences the mixing in the downcomer, and $W$ since, as we have seen previously, the cold vein can adhere to the walls enclosing the span-wise direction. The upper size of the downcomer $H_1$ has not been calibrated because, as mentioned before, the goal of the calibration is to isolate the event happening in the downcomer and a shorter section would affect the mixing, while a longer section would be too expensive to simulate in the future DNS.

The results show how a bigger domain helps the flow oscillating more freely, but it is important to keep in mind that the final configuration will be eventually used to perform a DNS simulation. For this reason, the optimal configuration must be a compromise between a large domain and a reasonable number of elements of the computational grid. That is why the second option ($H + 3D_h, W + 6D_h$) has been chosen to continue the calibration. From the initial three million cells, the computational domain now counts around four million cells. This setup allows the flow to oscillate without impinging the boundary walls, and in the mean time reduces the domain as geometrical dimensions such that a DNS simulation can be solved on a computational grid with a reasonable number of elements. It is important to check once again the value of the Froude number, and this time it is equal to $Fr = 0.016$, slightly less than the previous case, because of the higher jump between the square leg nozzle and outlet.

Also this time, to understand what is happening in the domain, the evolution of the temperature field in the middle-downcomer is reported in Fig.4.8, and from this observation it is possible to notice that even though the flow vein does not reach the boundaries, still the oscillations are too big, and the fluid could attach again to the walls. Therefore, we must find another way to reduce the amplitude of these oscillations, in the next chapter, the influence of the buoyancy forces on the cold vein will be studied, in particular the magnitude of the Froude number has been investigated in order to further reduce the influence of the walls bounding the span-wise direction.

### 4.9 Calibration of buoyancy effects

Having fixed the size of the domain, in order to further mitigate the influence of the boundaries on the mixing and hence try to isolate the phenomenon occurring in the downcomer, it is necessary to calibrate the buoyancy effects. In order to have an idea of the impact of the buoyancy forces on the mixing, based on the ROCOM’s experience
we chose the Froude number \((Fr)\) as measure of the buoyancy effect:

\[
Fr = \frac{u_{in} \rho_1}{\sqrt{g \cdot h \cdot \rho_1 - \rho_2}}
\]  

\(4.1\)

it is possible to look at the Froude number as the ratio between inertia and weight, hence it is the right parameter to determine if the mixing is driven by the buoyancy forces or it is inertia dominated. In our formulation the Froude number depends on:

- \(u_{in}\): inlet velocity \((U_1)\)
- \(h\): distance between the leg nozzle and the outlet \((H_2)\)
• \((\rho_1 - \rho_2)\): density difference between the cold water injected and the hot fluid present in the downcomer

Since we already fixed the domain size \((H_2)\), the parameters that can be tune are the inlet velocity \((U_1)\) and density difference \((\frac{\rho_1 - \rho_2}{\rho_1})\). Different strategies have been adopted in this calibration, in order to analyze the different influence of the two budgets on the flow behavior, here are reported the cases that have been studied:

1. \(\Delta\rho = 3\%, Fr = 0.016\): previous case
2. \(\Delta\rho = 2\%, Fr = 0.020\): the temperature difference between cold fluid injected and hot fluid in the downcomer is reduced, from \(\Delta T = 60\) to \(\Delta T = 40\), density and hence Froude number change accordingly
3. \(\Delta\rho = 4\%, Fr = 0.013\): larger temperature difference, \(\Delta T = 90\)
4. \(\Delta\rho = 3\%, Fr = 0.022\): same density difference of the base case but different magnitude of the inlet velocity, \(u_{in} = 120\%u_{in}\)
5. \(\Delta\rho = 3\%, Fr = 0.024\): \(u_{in} = 150\%u_{in}\)
6. \(\Delta\rho = 3\%, Fr = 0.032\): \(u_{in} = 200\%u_{in}\)

In Fig.4.9 the results for different density ratio \((\frac{\rho_1 - \rho_2}{\rho_1})\) are compared against the previous case, in Fig.4.10 the comparison is done at increasing inlet velocity \((U_1)\). For both calibrations it has been found that for an higher \(Fr\) the oscillations of the fluid vein are reduced, this is easily explained by the Froude number formulation, since an higher \(Fr\) means less dependence on the buoyancy forces and more on the inertia, this stabilize the oscillations in the downcomer.

This is an interesting feature for the calculations, since the smaller the oscillations are the smaller the width of the domain is required, hence the influence of the boundaries is reduced; further more this feature is interesting from the point of view of the future DNS simulation, in fact if the area interested by the turbulence of the fluid vein is contained, the region that requires a finer mesh is smaller and hence the time expenditure for the simulation is also reduced.

The first setup with \(\Delta\rho = 2\%, Fr = 0.020\) (Fig.4.11) has been chosen to continue the calibration, because the Froude number is higher respect to the previous configuration, so as aforementioned this helps the flow stabilization, and also the smaller temperature difference is useful for the following step.

Final remark on the temperature gradient over the solid walls: in Fig.4.12 is reported
the temperature evolution on the walls interfaces. It is interesting to notice the presence of temperatures gradients only on the shroud interface, that is because the flow after impinging the shroud wall it falls down, and it has not the time to adhere to the vessel wall and hence induce the gradients. This is a critical feature of the PTS event, that with actual laboratory experiments such as the ROCOM’s, it is impossible to replicate, giving to the future DNS simulation, and more generally to the CFD analysis an indisputably relevance in the study of such manners.

4.10 Fully turbulent profile

All the simulations performed at this point had a constant velocity profile at the inlet of the cold leg, instead for the following calibrations a fully turbulent profile will be set at the inlet of the squared leg. The reason of this choice is that we want to ensure a tur-
CHAPTER 4. CALIBRATION OF THE PTS EXPERIMENT

Figure 4.11: Temperature evolution in the middle-downcomer for case $\Delta \rho = 2\%$, $Fr = 0.020$

Figure 4.12: Temperature evolution at wall interfaces: (a) shroud, and (b) vessel
bulent mixing in the downcomer, so that it will be possible to calculate the turbulent length scales and hence evaluate the size of the mesh for the DNS simulation. In order to generate a fully turbulent profile with a bulk velocity of 0.018 m/s a separate RANS simulation of a pipe with the same hydraulic diameter of the cold leg is performed, applying periodic boundary conditions at the inlet and outlet sections. The results for the velocity of such simulation are reported in Fig. 4.13, this profile together with the profiles of the turbulent quantities (Reynolds stress tensor and turbulent dissipation rate) will be applied at the inlet section of the cold leg.

![Velocity profiles along the squared tube](image)

Figure 4.13: Velocity profiles along the squared tube

### 4.11 Boussinesq approximation

Now that the boundary conditions are set and the domain is fixed, we want to test a further simplification of the problem, applying the Boussinesq approximation: with this approach all the fluid properties inside the governing equations are constant, except for the density when multiplied by the gravity vector \( \mathbf{g} \), in this case \( \rho \) varies according to a linear law depending on temperature, reducing the nonlinearity of the problem:

\[
\rho = \rho_0 - \rho_0 \beta \Delta T
\]  
(4.2)
where $\beta$ is the coefficient of thermal expansion. The approximation is extremely accurate for many industrial applications, and makes the mathematics and physics much simpler.

The water properties are now set at the temperature of $T = 303K$ as follow:

- Density: $\rho = \rho_0 = 995.71 \text{ kg/m}^3$ or $\rho = \rho_0 - \rho_0\beta\Delta T$
- Dynamic viscosity: $\mu = 7.98 \times 10^{-4} \text{ Pa} \cdot \text{s}$
- Thermal conductivity: $k = 0.62 \text{ W/m/K}$
- Specific heat: $C_p = 4.18 \text{ kJ/kg/K}$

From the formulation of the density it is possible to understand that the configuration coming from the last calibration: $\Delta\rho = 2\%$, $Fr = 0.020$, with smaller density difference, hence temperature difference, reduces the error admitted in the density prediction, (0.5% in our case). The results presented in Fig.4.14 showed that the approximation maintains the feature in which this work is interested: the flow vein oscillates freely, but the area covered by the swirls is contained.

Obviously this configuration, as well as all the previous URANS simulations, will have to be validate by the future DNS in order to be relevant.

![Temperature evolution in the middle-downcomer for case $\Delta\rho = 2\%$, $Fr = 0.020$, with Boussinesq approximation](image)

Figure 4.14: Temperature evolution in the middle-downcomer for case $\Delta\rho = 2\%$, $Fr = 0.020$, with Boussinesq approximation

### 4.12 Periodic boundary conditions

The geometry simplification of the reactor pressure vessel imposed by the "cost" limitations of the future DNS is radical, in fact all the simulations reported in this work are
performed on a planar domain, while an actual RPV has a cylindrical shape (Fig. 4.15). Since a more complex geometrical configuration is not feasible, from the point of view of the DNS simulation, it is useful in this preliminary study to understand the influence, on the mixing occurring in the downcomer, of periodic boundary conditions (PBC) compared to the no-slip wall conditions. In topological terms, the space made by two-dimensional PBCs can be thought of as being mapped onto a torus meaning that when an object passes through one side, it re-appears on the opposite side with the same velocity. This configuration can be considered much closer to the actual cylindrical geometry of the RPV, therefore in the last simulation periodic boundary conditions are applied on the walls enclosing the span-wise direction.

In Fig. 4.16 the results with and without periodicity are compared along the time evolution. It is possible to notice how with the calibration process endured until this step, the oscillations of the fluid vein are contained, so that the flow passing through the periodic boundaries has small impact on the mixing occurring in the downcomer. This demonstrates how in this case the no-slip wall conditions do not differ too much from a more accurate configuration such as the one with periodic boundary conditions.

Figure 4.15: Numerical domain adopted in the simulations with periodic boundary conditions underlined (left), actual Reactor Pressure Vessel (right)
Figure 4.16: Temperature evolution in the middle-downcomer for: (a) periodic boundary conditions, and (b) no-slip wall conditions
4.13 Estimation of turbulent length scales

The estimation of the turbulence length scales is fundamental to build up a proper meshing strategy for the future DNS. The knowledge of the tendency of such scales throughout the computational domain is necessary to identify the regions where the mixing phenomena require a very fine mesh and the regions where the cell size can be higher.

The formulation of the Kolmogorov and Batchelor length scales are reported hereby:

\[
\eta_K = \left( \frac{\nu^3}{\varepsilon} \right)^{1/4} \\
\lambda_B = \left( \frac{\nu \left( \frac{k}{\rho C_p} \right)^2}{\varepsilon} \right)^{1/4}
\]

where \( \nu \) is the kinematic viscosity of the fluid, \( \varepsilon \) is the average rate of dissipation of turbulence kinetic energy, \( k \) is the thermal conductivity, \( \rho \) is the density and \( C_p \) is the specific heat capacity at constant pressure.

In Fig. 4.17 the turbulence length scales have been extrapolated from the URANS solution, and we can notice how a special attention is required in the region under the square leg nozzle, where the flow oscillations are concentrated. Results show that this phenomenon exhibits a very complex distribution of these length scales and, hence, a smart meshing technique would be extremely useful to reduce the overall mesh size.

Based on such scales, a first estimation has been made, identifying the lowest values of Batchelor scales, considering a growth rate of 1.05 from the wall interfaces, a block structured meshing technique for the fluid domain and a conformal mesh for the walls discretization, the resulting mesh counts around 1.8 billion cells. This includes one billion grid points for the fluid region, and 800 million cells for the solid parts.
Figure 4.17: Turbulent length scales in different section of the downcomer: (a) Kolmogorov length scale, and (b) Batchelor length scale
Chapter 5

Conclusion

In the present work a PTS scenario is investigated thought the use of numerical simulations. The main objective was to investigate the effect of different geometrical and fluid-dynamic parameters on the system by the means of URANS simulations. This step is necessary in order to design a future DNS simulation of this test case. These DNS computations will serve as a reference database to validate low order turbulence modeling approaches that will be applied for the analysis of PTS scenarios.

However, since DNS computations for a real PTS event are not feasible with the currently available computation power, a comprehensive work consisting of an extensive range of Reynolds-Averaged Navier Stokes simulations was performed in order to determine a simplified configuration for PTS that is physically meaningful and, at the same time, meets a feasible computational demand. In particular, starting from a configuration based on a previous experience at NRG that studied the PTS event at constant density, several aspects of the experiment were optimized, such as flow properties, boundary conditions, and domain size. In particular, the effects of the density variation on the temperature field was fully investigated. Furthermore, the smallest scales of turbulence, i.e. Kolmogorov and Batchelor scales, were extrapolated from the obtained solution in order to build up a mesh for the DNS.

The spectral element solver NEK5000 [4] has been selected to perform the targeted DNS calculations. A total number of 1.8 billion grid points was calculated. The CFD team of NRG is now involved in optimizing and generating this mesh and setting up the calibrated domain in NEK5000. The DNS computations will require a huge computational time, i.e. of the order of months.
Appendix A

Validation process

A.1 Introduction

The purpose of this work is to validate the results of the calibration of the Pressurized Thermal Shock, obtained with Code_Saturne. In order to do so, we choose to test two cases that have well established results, and that are significant to our project:

- Heated Channel Flow (HCF)
- Differentially Heated Cavity (DHC)

The following simulations, tested the general capabilities of the turbulence models (HCF case), and the behavior, of the two best performing models, on a buoyancy driven flow (DHC case).
A.2 Turbulence models

Two families of turbulence models are available in Code_Saturne:

- Eddy Viscosity Models (EVM), based on the Boussinesq hypothesis

\[ R_{ij} = \frac{2}{3}k\delta_{ij} - 2\nu_t \left( \frac{U_j}{x_j} + \frac{\partial U_j}{\partial x_i} \right) \]  

(A.1)

they account the Reynolds stresses as parallel to the mean strain rate

- Reynolds Stress Models (RSM), the code solves six equations for the Reynolds stresses transport

\[
\begin{align*}
\frac{\partial \rho u'_i u'_j}{\partial t} + \frac{\partial \rho \bar{u'_i} \bar{u'_j}}{\partial x_k} &= - \frac{\partial \rho u'_i u'_k u'_j}{\partial x_k} + \frac{\partial \rho u'_j u'_k u'_i}{\partial x_k} + \frac{\partial \mu \delta_{ij}}{\partial x_k} + \\
&- \rho \left( \bar{u'_i} \bar{u'_k} \frac{\partial \bar{u'_j}}{\partial x_k} + \bar{u'_j} \bar{u'_k} \frac{\partial \bar{u'_i}}{\partial x_k} \right) - \rho \beta \left( \bar{g}_i u'_j T' + \bar{g}_j u'_i T' \right) + p' \left( \frac{\partial \bar{u'_i}}{\partial x_j} + \frac{\partial \bar{u'_j}}{\partial x_i} \right) + \\
&- 2\mu \frac{\partial \bar{u'_i}}{\partial x_k} \frac{\partial \bar{u'_j}}{\partial x_k} - 2\rho u'_i u'_k \Omega_{k j} + u'_j u'_k \Omega_{i k} \\
\end{align*}
\]

A.2

and the transport of the turbulent dissipation rate

\[ \rho \frac{\partial \epsilon}{\partial t} + \text{div} \left( \rho U\epsilon - \mu \text{grad} \epsilon \right) = d_\epsilon + C_{\epsilon 1} \frac{\epsilon}{k} P - \rho C_{\epsilon 2} \frac{\epsilon^2}{k} \]  

(A.3)

The turbulence models available can also be accounted as:

- Low Reynolds (LR): models able to solve the flow quantities until the solid wall, but to do so they necessitate a mesh well refined next to the wall to catch all the rapid variations

\[ \nu^2 - f \]

\[ Bl - \frac{\nu^2}{k} \]

\[ R_{ij} - \epsilon \text{ EBRSM} \]
• High Reynolds (HR): these models are not valid in the neighborhood of the wall

  Standard $k - \epsilon$
  $k - \epsilon$ Linear Production
  $R_{ij} - \epsilon$ SSG
  $R_{ij} - \epsilon$ LRR

• In between: they are supposed to be adapted to all mesh size

  $k - \omega$ SST
  Splalart-Allmaras

A.2.1 Wall functions

In the immediate vicinity of a bounding surface, we can distinguish a particular area where: the viscous forces are comparable to the inertia of the fluid, and the velocity of the stream is reduced by 99% with respect to the free-stream velocity. This region is called boundary layer and can be divided in:

• Sub-layer: viscous effects predominates inertia forces

• Log-law layer: the two effects are equivalent

• Outer-layer: inertia dominated region

Because of their inability to solve correctly the flow region near the boundaries, High Reynolds models are coupled with wall functions. The idea is to replicate the effect of the wall on the fluid, through empirical laws. With these laws it is possible to express the mean velocity parallel to the wall and turbulence quantities outside the viscous sub-layer in terms of the distance to the wall. Hence, the wall functions can be used to provide near-wall boundary conditions for the momentum and turbulence transport equations, rather than conditions at the wall itself, so that the viscous sub-layer does not have to be resolved and the need for a very fine mesh is circumvented.

\[
\begin{cases}
  u^+ = y^+ , & y^+ \leq y^+_{lim} \\
  u^+ = \frac{1}{k} \ln (y^+) + 5.2 , & y^+ > y^+_{lim}
\end{cases}
\]  

(A.4)

In Code_Saturne three different wall functions are available:
APPENDIX A. VALIDATION PROCESS

Figure A.1: Dimensionless velocity profile

- 2-scale: based on two ways to evaluate the friction velocity

\[ u_k = C_{\mu}^{1/4} k^{1/2} \]

\[ u_\tau = \sqrt{\frac{\tau_w}{\rho}} \quad u^+ = \frac{u}{u_\tau} \quad y^+ = \frac{u_k y}{v} \tag{A.5} \]

- 1-scale: classic wall function

\[ u_\tau = \sqrt{\frac{\tau_w}{\rho}} \quad u^+ = \frac{u}{u_\tau} \quad y^+ = \frac{u_\tau y}{v} \tag{A.6} \]

- Scalable: allows to virtually "shift" the wall when necessary in order to be always in a logarithmic layer

A.3 Heated Channel Flow (HCF)

The Heated Channel Flow (HCF) case consists in studying a turbulent fluid flow between two infinite heated parallel plates. The meshes adopted for these simulations are reported in Fig. ??, they consists of one cell in the direction of the flow, and instead multiple cells in the direction of the boundary layer growth. It is possible to notice the large difference in number of cells between the two meshes, in particular how the low-Reynolds mesh is much more refined near the wall.
APPENDIX A. VALIDATION PROCESS

A.3.1 HCF results

The results, here listed, are compared to the DNS analysis of Kawamura [1], for $Re_\tau = 640$, where $Re_\tau$ is the friction Reynolds number, formulated as:

$$Re_\tau = \frac{u_\tau \delta}{\nu}$$

(A.7)

where $u_\tau = \sqrt{\frac{\tau_w}{\rho}}$ and $\tau_w$ is the statistically averaged wall shear stress, $\rho$ is the density, $\delta$ is the channel half width and $\nu$ is the kinematic viscosity.

About the EBRSM model also the Reynolds Stresses are pictured, since is the only Low Reynolds RSM model and so is the only turbulence model that can predict the near wall anisotropy of the Reynolds stresses.
APPENDIX A. VALIDATION PROCESS

Figure A.4: $u^+$ profile for EVM

Figure A.5: $u^+$ profile for RSM
APPENDIX A. VALIDATION PROCESS

Figure A.6: $T^+$ profile EVM

Figure A.7: $T^+$ profile RSM
APPENDIX A. VALIDATION PROCESS

Figure A.8: $k$ profile EVM

Figure A.9: $k$ profile RSM
APPENDIX A. VALIDATION PROCESS

Figure A.10: $\epsilon$ profile EVM

Figure A.11: $\epsilon$ profile RSM
Figure A.12: $u'u'$ profile EBRSM

Figure A.13: $v'v'$ profile EBRSM
Figure A.14: $w' w'$ profile EBRSM

Figure A.15: $T' \nu'$ profile EBRSM
APPENDIX A. VALIDATION PROCESS

A.4 Differentially Heated Cavity (DHC)

The Differentially Heated Cavity (DHC) case concerns a square cavity, filled with air, with two walls kept at different temperature and two adiabatic walls. 

![Figure A.16: Square cavity mesh](image)

A.4.1 DHC results

The results compare the different behavior of the two best models: $Bl - v^2/k$ for the EVM and EBRSM for the RSM. The work of Le Quéré for $Ra = 10^8$ and $Pr = 0.71$ is the benchmark used for the check.

<table>
<thead>
<tr>
<th></th>
<th>Le Quéré</th>
<th>$Bl - v^2/k$</th>
<th>EBRSM</th>
</tr>
</thead>
<tbody>
<tr>
<td>$v_{max}^+$</td>
<td>2222.39</td>
<td>2112.02</td>
<td>2111.74</td>
</tr>
<tr>
<td>$x_p^*$</td>
<td>0.012</td>
<td>0.010</td>
<td>0.010</td>
</tr>
<tr>
<td>$u_{max}^+$</td>
<td>321.88</td>
<td>315.72</td>
<td>315.63</td>
</tr>
<tr>
<td>$y_{u^+}$</td>
<td>0.928</td>
<td>0.930</td>
<td>0.930</td>
</tr>
<tr>
<td>$Nu_{1/2}$</td>
<td>30.22</td>
<td>30.01</td>
<td>30.02</td>
</tr>
</tbody>
</table>

Table A.1: Quantitative results
Figure A.17: $u^+$ profile at cavity mid-plane

Figure A.18: $v^+$ profile at cavity mid-plane

Figure A.19: $T^+$ profile at cavity mid-plane
A.5 Conclusion

Since the purpose of this thesis is to provide a database for DNS calculation, high Reynolds models are discarded. Between the low Reynolds models: $Bl - \frac{v^2}{k}$ and $R_{ij}$-EBRSM reach more accurate results. The two models are very similar in terms of formulation they both are based on Durbin’s elliptic parameter $\alpha$, in terms of performance:

- in the HCF case the dimensionless quantity profiles are coherent to the DNS and the difference between the models is almost null. Only exception is the turbulent kinetic energy and dissipation rate, for which EBRSM shows a better agreement to the Kawamura experiment

- about the DHC case the two models predict correctly magnitude and location of the peaks for the dimensionless velocity, and the behavior of the two models in vertical and horizontal middle planes is practically identical

The $R_{ij}$-EBRSM has been chosen to perform the current thesis: for the outstanding performance on the two classic cases, and because it is the only model that predicts correctly the near-wall anisotropy. Plus it is interesting for NRG to test Code_Saturne at the best of its capability.
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