

CALIBRATION AND OPTIMIZATION OF PRESSURIZED THERMAL SHOCK FOR BENCHMARKING DIRECT NUMERICAL SIMULATION

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ABSTRACT

Pressurized Thermal Shock (PTS) is considered as an important issue that challenges the integrity of the Reactor Pressure Vessel (RPV). PTS denotes the occurrence of a rapid cooling of the internal RPV surface under pressurized conditions. This overcooling may induce the criticality of an existing or postulated defect inside the vessel wall. The most severe PTS scenario concerns the Emergency Core Cooling (ECC) injection during a LOCA (Loss Of Coolant Accident). The injected cold ECC water mixes with the hot primary water present in the cold leg and the mixture flows towards the downcomer, where further mixing takes place, leading to large temperature gradients at the vessel surface. PTS is identified as one of the safety issues where CFD can bring real benefits complementary to the system codes' analyses. However, to gain the confidence in CFD codes' results, a comprehensive validation programme is necessary to demonstrate the capability of such codes to reliably predict PTS-related phenomena. In absence of detailed experimental data for the RPV cooling for CFD codes validation, DNS databases constitute a valid alternative for experiments.

The aim of the work is to assess the capability of the spectral element code NEK5000 to perform a high quality DNS of a PTS scenario. For this purpose, a single phase PTS scenario is considered, which is based on the ROCOM facility. The main idea is to design a numerical experiment, in the form of a DNS, which takes into account the jet impingement on the RPV wall, the resulting turbulent mixing in the downcomer and the evolution of the temperature distribution for both structures and fluid in an ECC scenario. However, such a DNS analysis represents a demanding application, including the simulation challenges of T-junction thermal mixing and conjugate heat transfer. The present work consists of two parts. In the first part, a calibration study has been performed in order to obtain a feasible and well representing PTS computational domain. This calibration analysis has been performed using RANS simulations and the computational domain has been optimized in terms of boundary conditions, properties and dimensions. In the second part, the DNS capabilities of NEK5000 have been tested for a well-known channel flow configuration. Different numerical parameters have been tested and their influence has been studied to obtain high quality turbulence statistics.

KEYWORDS

Pressurized Thermal Shock, DNS, NEK5000

1. INTRODUCTION

Pressurized Thermal Shock (PTS) consists of a rapid cooling of the Reactor Pressure Vessel (RPV) wall under pressurized conditions. The most severe PTS scenario is Emergency Core Cooling (ECC) injection into the cold leg during a Loss Of Coolant Accident (LOCA). The injected cold water mixes with hot water present in the cold leg, and flows towards the downcomer, causing further thermal mixing and, therefore, large temperature gradients. This sudden change in temperature may induce high stresses in the RPV wall, leading to propagation of flaws inside the vessel wall, especially in the embrittled region adjacent to the core. A proper knowledge of these loads is important for the RPV remnant lifetime assessment. For such purpose, thermal-hydraulic analysis has an important role in evaluating temperature distributions in downcomer, RPV, and nozzles. The existing thermal-hydraulic system codes, which are currently applied for Nuclear Reactor Safety (NRS) related issues, are based on simplified one-dimensional representations, and, therefore, cannot reliably predict the complex three-dimensional flows occurring during ECC injection. On the other hand, Computational Fluid Dynamics (CFD), particularly turbulence models, can be helpful in predicting these complex flow features. However, a proper validation of these available turbulence models against the reference databases needs to be done. The definition of a high quality reference database can be either an experiment or a high fidelity DNS.

The assessment of CFD for PTS has been the subject of many international research projects, and a number of test facilities are involved to produce reference experimental databases. For example, the Rossendorf Coolant Mixing Model (ROCOM) test facility [1] represents the primary circuit of a German KONVOI type reactor on a 1:5 linear scale. In this facility, the investigation of coolant mixing in the primary circuit of pressurized water reactors has been performed. Experimental data from such facility have been used for the assessment of CFD codes for PTS, e.g. [2]. However, due to the simplifications present in the facilities, experimental data are not always sufficient to capture all the involved phenomena. For example, acrylic glass is used for the vessel of the ROCOM facility, and, therefore, wall heat transfer data are not obtained from ROCOM experiments. Moreover, the spatial resolution in the measurements near the wall is not sufficient to catch velocity and temperature fluctuations. On the other hand, a high quality DNS database of a relatively simplified PTS case could be helpful for the scientific community in order to understand the complex turbulent flow and heat transfer phenomena. More in detail, such database could serve as a reference to validate the low order turbulence modelling approaches, such as Large Eddy Simulation (LES), Unsteady-Reynolds-averaged Navier-Stokes simulations (URANS) and Hybrid (LES/(U)RANS), which can be applied for realistic PTS scenarios. The aim of the present work is to generate a high quality reference DNS database in order to validate the low order turbulence modelling approaches for PTS configurations. These targeted DNS computations are planned to be performed by using the spectral element code NEK5000 [3]. Since performing such expensive DNS for an actual PTS configuration is not realistic, hence, a simplified configuration has to be designed.

The present paper consists of two parts. In the first part, the PTS numerical experiment has been designed and optimized to perform DNS. The design of such a computational domain is a delicate issue. On one hand, it has to reproduce a physically meaningful and challenging scenario. On the other hand, it has to be simple enough to fulfill the foreseen computational challenges of the DNS. Therefore, a wide range of RANS calculations have been performed to calibrate the domain in terms of boundary conditions, flow properties, and domain's sizes. All this calibration related work is given in Section 2. The second part deals with the assessment of NEK5000 in order to perform high quality DNS. For such investigation, a planar turbulent channel flow has been selected and is discussed in Section 3. This is followed by summary and conclusions.

2. PART I: CALIBRATION OF PTS DESIGN

The main objective of this research work is to calibrate a simplistic PTS design in order to perform a numerical experiment. This numerical experiment will serve as a reference CFD database to validate lower order turbulence modelling approaches. This section illustrates the selection of the computational domain and its respective calibration for the final DNS computations.

2.1. Domain configuration & Numerical method

The prime 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. This numerical experiment has been optimized in terms of fluid properties, boundary conditions, and sizes, in order to perform DNS computations with the spectral element code NEK5000 [3]. The computational domain consists of cold leg (Inlet 1), downcomer, vessel wall, and barrel wall, as shown in Figure 1. The original design is based on the ROCOM test facility, for details see [4]. However, in the present work, some simplifications have been introduced to facilitate the high fidelity DNS requirements. For example, instead of a real curved geometry of RPV, a simplistic planar configuration is considered. Moreover, the lower plenum is not considered. The targeted DNS is planned to be performed with constant flow properties. Therefore, in order to simulate a more realistic scenario in the downcomer, i.e. with buoyancy effects, an additional velocity inlet (Inlet 2) has been considered on the upper side of the downcomer. Inlet 1 and Inlet 2 are filled with relatively cold and hot water, respectively. Figure 1 displays the final design of the simplistic PTS domain along with the geometric parameters in Table I. These parameters are non-dimensionalized by the cold leg diameter, i.e. $L^*=L/D_p$ ($D_p = 0.15$ m, from ROCOM facility). A detailed description of these geometric parameters can be found in [4].

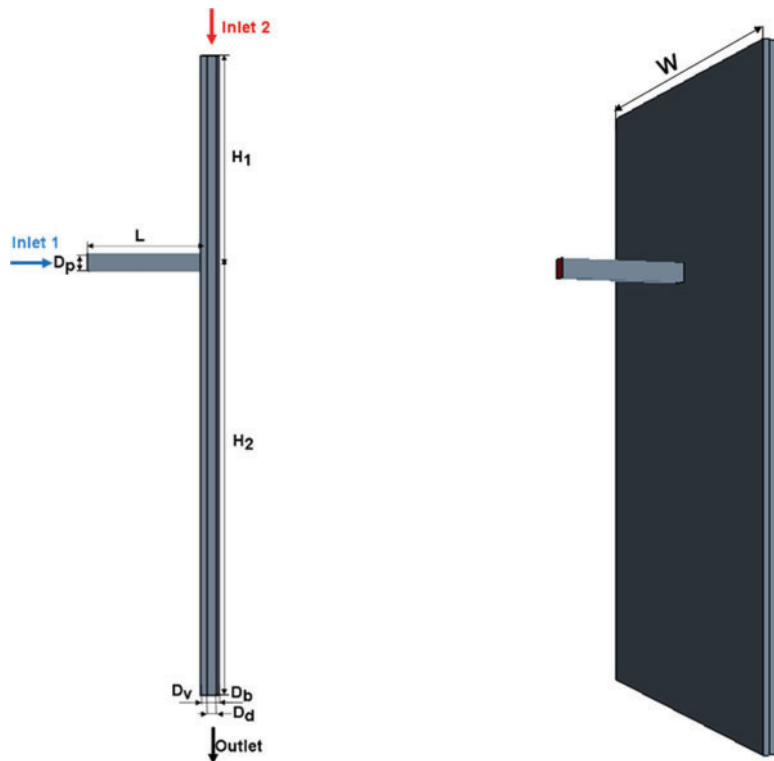


Figure 1. Front (left) and iso-metric (right) views of the final PTS design.

Table I. Initial and calibrated geometric dimensions of the numerical experiment.

(* = values non-dimensionalized by D_p , i.e. $L^*=L/D_p$)

Parameter	Initial value*	Final value*
D_p	1	1
L	~7	~7
H_1	~7	10
H_2	~23.3	~23.3
D_v	~0.33	~0.33
D_b	~0.16	~0.16
D_d	~0.48	~0.48
W	~14	20

2.1.1. CFD Code and Model

The calibration of the aforementioned PTS design is performed by a wide range of RANS simulations. These computations are carried by using the commercial CFD software STAR-CCM+ version 8.06 [5]. A non-linear cubic formulation of low-Reynolds $k-\epsilon$ is selected as a turbulence model. In addition, a second order upwind scheme is used for spatial discretization.

2.1.2. Mesh

The mesh used in all simulations presented in this calibration study consists of hexahedral trim cells along with structured prism layer in the near wall region to capture high flow gradients. The cross-sections of this mesh are shown in Figure 2. The value of average y^+ is kept less than 1 for the first cell. The resulting mesh consists of ~3.7 million cells.

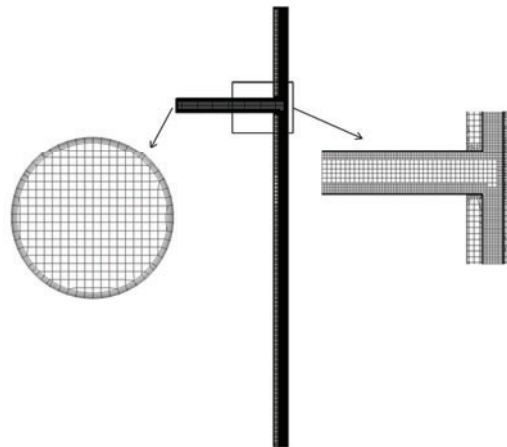


Figure 2. Front (left) and iso-metric (right) views of the final PTS design.

2.1.3. Fluid and solid properties

In this work, single-phase water is considered as working fluid. Whereas, 16MND5 steel is selected for the solid material. Constant properties are considered for both fluid and solid. The properties of the solid

material are selected at the average temperature of hot and cold fluids (i.e. 323 K) and are given in Table II. By considering water properties at the cold temperature of the fluid, i.e. 293 K, the corresponding Prandtl number (Pr) is ~ 7 . This means that the Batchelor scales are much smaller than the Kolmogorov scales. Consequently, the resultant DNS computation may be very expensive. Hence, the Prandtl number has been scaled down in terms of increasing the reference temperature (T_{ref}) for water properties. In total, four reference temperatures are considered, i.e. 293 K, 313 K, 323 K, and 353 K, and the corresponding Pr numbers are 7, 4.34, 2.99, and 2.23, respectively. Moreover, since the viscosity of water is strongly affected by the increase in temperature, the level of turbulence also increases. Hence, the resulting friction Reynolds number (calculated by using the Dean's correlation [$Re_{\tau} = 0.175(Re/2)^{(7/8)}$]) passes from 96 to 232 for $T = 293$ K to 353 K, respectively. The obtained results, not reported here due to the page limitation, have shown that despite small differences, the overall topology of the thermal field remains similar for the aforementioned four Pr cases. Therefore, the properties of water at 353 K have been selected to perform all the simulations presented in this work, and are given in Table II.

Table II. Properties of water and 16MND5 at 353 K and 323 K, respectively [6] [7].

T_{ref} [K]	ρ [kg/m ³]	c_p [J/kg-K]	μ (10 ⁻³) [Pa-s]	k [W/m-K]
<i>Water</i>				
353	971.79	4196.8	0.3544	0.67
<i>16MND5</i>				
323	7840	476.5	-	45.98

2.1.4. Boundary conditions

Adopting the mass flow rate of a ROCOM test case [8], a fully developed turbulent profile with a bulk velocity of $U_1 = 0.018$ m/s is applied at Inlet 1. The velocity at Inlet 2 is being calibrated as a percentage of Inlet 1 velocity, and is discussed in the following section. Temperature at Inlet 1 is relatively cold, i.e. 293 K, whereas a relatively hot temperature of 353 K is considered for Inlet 2. The standard no-slip boundary condition is applied at the fluid-side walls. An adiabatic boundary condition is imposed at the outer surfaces of the domain.

2.2. Calibration of boundary conditions, dimensions, and flow Reynolds number

This section presents the main part of the calibration work. The effects of the variation of each parameter on flow fields have been extensively investigated. However, because of the page limitation, only a brief overview is given here. A more detailed description can be found in [4]. As already mentioned, Inlet 2 has been created in order to force the downward cold jet downstream in the downcomer, reproducing buoyancy effects. For this inlet, four different velocities have been tested, as a percentage of Inlet 1 velocity, i.e. 0%, 5%, 10%, 15% of U_1 . A velocity of $U_2 = 10\% U_1$ is found to be a good compromise in terms of not increasing too much the level of turbulence in the upper part of the downcomer, and, therefore, the mesh requirement in that region for the targeted DNS computations. The resultant temperature and velocity fields at different cross-sections (i.e. fluid-vessel interface, fluid-vessel interface+0.007Dp, middle of downcomer, fluid-barrel interface, and symmetry plane), are shown in Figure 3. This configuration has been further optimized. Firstly, in order to minimize meshing difficulties in NEK5000, the geometry of the cold leg has been simplified, i.e. a square duct is considered. This square duct has same hydraulic diameter, bulk velocity, and, therefore, the Reynolds number as the circular pipe. Then, the height and the width of the domain have been increased in order to have complete development of the thermal field without increasing considerably the overall computational cost. These

final dimensions of the PTS design are given in Table I. Finally, the velocity of Inlet 1 has been scaled down to achieve, in the square duct, a friction Reynolds number equal to $Re_\tau = u_\tau D_p / 2\nu = 180$. Consequently, the velocity of Inlet 2 has been also reduced, remaining as 10% of the new scaled Inlet 1 velocity. The resultant temperature and velocity fields of the final domain are given in Figure 4. A comparison with Figure 3 highlights a more complex flow path in the downcomer, due to the square duct shaped cold leg.

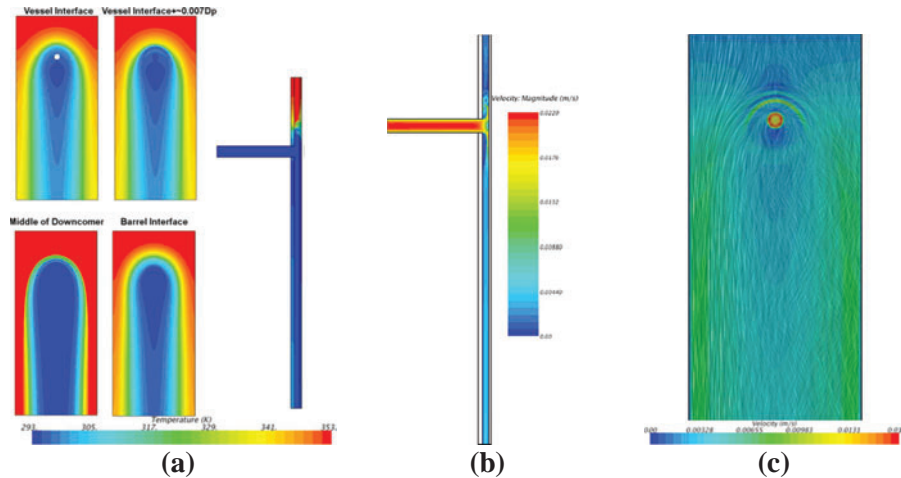


Figure 3. (a) Temperature distribution at different cross-sections (left) and at the symmetry plane (right) for the initial domain. (b) Velocity iso-contours at the symmetry plane for the initial domain. (c) Iso-contours of the integrated line convolution at the mid cross-section of the downcomer for the initial domain.

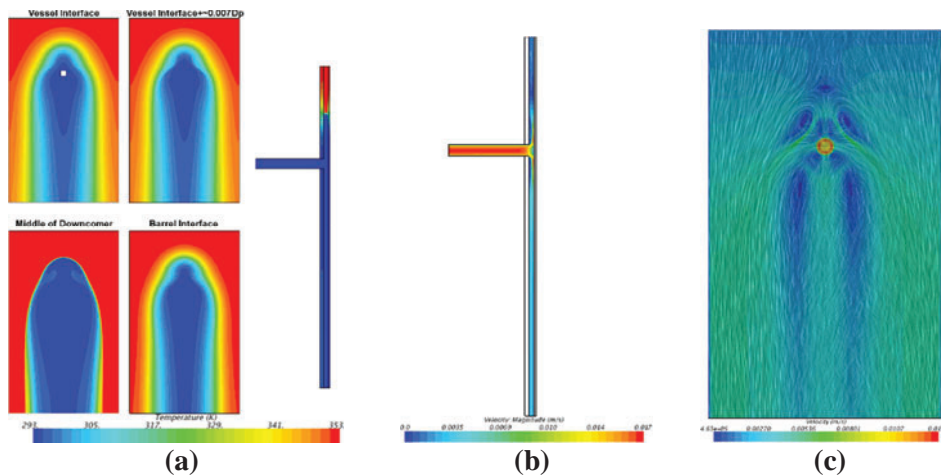


Figure 4. (a) Temperature distribution at different cross-sections (left) and at the symmetry plane (right) for the calibrated domain. (b) Velocity iso-contours at the symmetry plane for the calibrated domain. (c) Iso-contours of the integrated line convolution at the mid cross-section of the downcomer for the calibrated domain.

2.3. Preparation for the final DNS

2.3.1. Isothermal vs adiabatic boundary conditions

In the original PTS design, as shown in the previous section, adiabatic conditions have been applied at the outer surfaces. In this section, isothermal conditions at the outer surfaces in the interfaces-normal direction of vessel and barrel are investigated. Results are compared with the original adiabatic domain and are shown in Figure 5. It is clearly noticeable that temperature field is strongly affected by such boundary condition. Whereas, since constant properties are used, velocity field is not influenced by the thermal boundary condition applied and, therefore, it is not shown here.

In a PTS scenario, a high temperature gradient is present through the wall thickness after the transient initiation, and is decreasing during the course of time. Results show that both adiabatic and isothermal cases can be a representative scenario of different temporal stages of the PTS. The starting phase can be represented by isothermal conditions, because of the temperature gradient within the wall thickness. At a later stage, the phenomenon is more stationary and such temperature gradient diminishes. Adiabatic boundary conditions are more a correct representation of this latter phase.

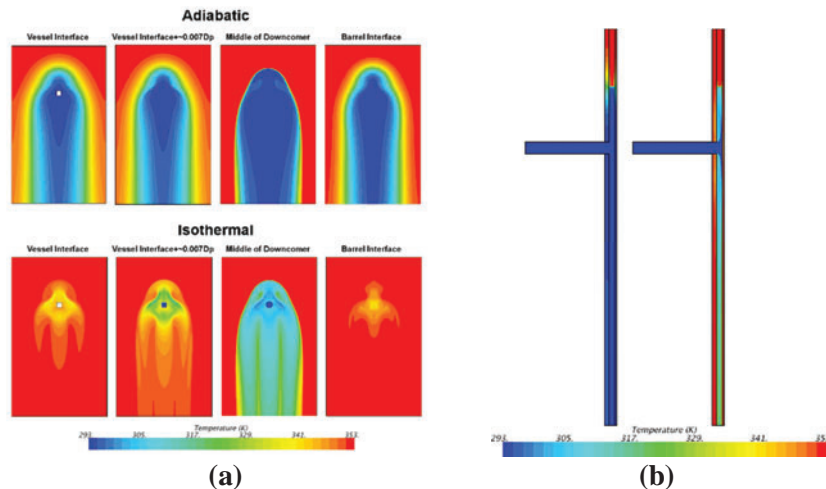


Figure 5. (a) Temperature distribution at four different cross-sections for adiabatic (top) and isothermal (bottom) boundary conditions. (b) Temperature distribution at the symmetry plane for adiabatic (left) and isothermal (right) boundary conditions.

2.3.2. Scaling of Prandtl number to 1

After a mesh sensitivity analysis, not shown here (for details see [4]), Kolmogorov and Batchelor length scales have been extrapolated from the obtained RANS solution. These scales have shown a very complex distribution throughout the domain, as fully described in [4]. From these scales, it has been possible to estimate the total number of grid points required for final DNS computations. The first estimation, based on a quasi-uniform distribution, gives a rough value of ~ 4 billion grid points. However, this mesh is highly resolved. Therefore, a smart meshing strategy, based on block structures, has been used and results in a final value of about 1.6 billion grid points (930 and 650 million grid points for fluid and solid, respectively). This total number of grid points is still challenging to perform DNS computations with the currently available computer power. Therefore, in order to make this computation feasible, the original thermal conductivity of water has been increased to scale down the Prandtl number of the fluid to 1. Although the velocity is not affected by this modification, however, the thermal field has shown small

differences, e.g. more cooling of the walls is present, see Figure 6. Nonetheless, the overall flow topology is remained well preserved. By reducing the Prandlt number to 1, a feasible mesh size has been reached. It consists of about 0.9 billion grid-points (550 million for fluid and 350 million for solid).

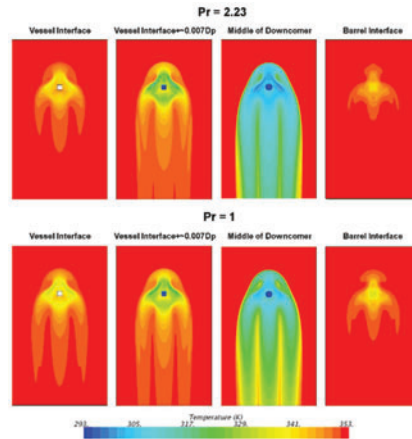


Figure 6. Temperature distribution at four different cross-sections for Pr = 2.23 (top) and Pr = 1 (bottom).

3. PART II: ASSESSMENT OF NEK5000 TO PERFORM DNS

As already mentioned, the objective of the present work is to generate a high fidelity DNS database for a simplistic PTS design, which will be used to validate the available turbulence models. To perform these DNS computations, a higher order spectral element code NEK5000 has been selected [3]. In this section, a preliminary assessment of this code has been carried out by performing high quality DNS for a well-known turbulent channel flow. Several statistical descriptors for the obtained turbulent quantities have been extensively analysed and compared with the available reference DNS databases.

3.1. NEK5000 Code

NEK5000 is an open source code, which adopts a Spectral Element Method (SEM), i.e the finite element method is coupled with a high-order weighted residual technique. In each element, velocity and pressure are expressed as Lagrange polynomials, computed on a N -th order Gauss-Lobatto-Legendre (GLL) points distribution [9]. Two different formulations for the spatial discretization of the Navier-Stokes equations are available in NEK5000. The P_N - P_N formulation is used in this work for two different cases, with a N -th polynomial order equal to 5 and 9, respectively. Moreover, the temporal discretization of the Navier-Stokes equations is based on a third order backward-difference formula, to evaluate velocity time derivatives, and on a third order extrapolation for explicit evaluation of the nonlinear and pressure boundary terms [3].

3.2. Turbulent Planar Channel case

The assessment of NEK5000 is performed for a planar turbulent channel flow case, with a friction Reynolds number of 180. This is an extensively investigated flow configuration w.r.t. the DNS computations. Therefore, a relative good number of DNS databases are available, and the selected ones

are reported in Table III [10, 11, 12, 13]. The geometry and coordinates system are displayed in Figure 7. The domain consists of two parallel walls, normal to the y direction and infinite in the x and z directions, bounding the fluid that is flowing in the x direction. In order to reproduce such an infinite domain, periodic boundary conditions are imposed for both the x and the z directions. The geometric parameters of the selected computational domain are as follows: $L_x=4\pi$; $L_y=2.0$, $L_z=4\pi/3$. Table III reports the main computational parameters of selected databases, also including the present work. All these databases were obtained for the same computational domain as the present work, with an exception of Hoyas and Jimenez's one, which was performed over a larger domain. Among all listed databases, it is noticeable that Vreman and Kuerten's data, henceforth called as V&K, were obtained on a very fine mesh with a relatively long averaging time. Hence, this database is expected to be the most accurate among all the listed cases and could be considered as a reference.

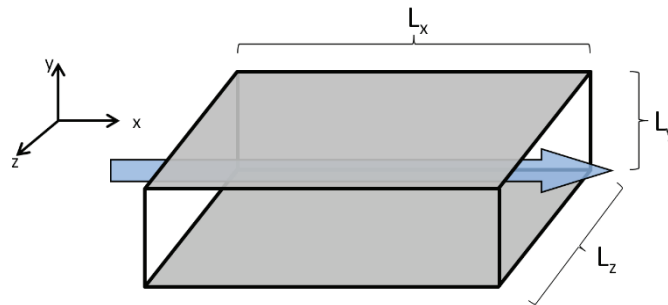


Figure 7. Planar Turbulent Channel Flow case's domain. Periodic Boundary Conditions are applied in the streamwise (x) and spanwise (z) directions.

3.3. Mesh and time step

NEK5000 implements a SEM, so that the final mesh grid is given by a combination of the finite elements mesh and the GLL points inside each element, the latter being dependent on the chosen polynomial order N . Two different values of N have been selected for this analysis, $N=5$ and $N=9$ respectively. It is worth mentioning that the first mesh point is located at a non-dimensional distance (y^+) from the wall less than 0.5. In both cases $N5$ and $N9$, it results in a total number of mesh points equal to $\sim 7.5 \div 8$ million. Mesh details are reported in Table III. A constant time step has been adopted in both the simulations in order to limit the CFL to 0.2. As previously described, a 3rd order temporal discretization has been adopted.

3.4. Results and Discussion

Turbulence appearing in the selected channel flow has been investigated through the statistical analysis of the velocity and pressure fields along with their respective fluctuations. In more detail, several moments of pressure and velocity have been elaborated, and the analysis of the Reynolds stresses and of the Turbulent Kinetic Energy (TKE) has been performed. Because of the page limitations, only the results for case $N9$ are presented. It is worthwhile to mention that these results are consistent with the case $N5$, of course with slight differences. Averaging is started only after the velocity field has reached the turbulent convergence. The averaging time is large enough in order to assure fully convergence of mean parameters. Its value is reported in Table III, compared against each database. In order to compare the results among different databases, all data have been non-dimensionalized via the friction velocity u_τ and the kinematic viscosity ν . Furthermore, because of domain's intrinsic periodic nature, variables are ensemble averaged on planes parallel to the two walls. As shown in Figure 8, all databases indicate a similar trend for the low order moments, i.e. the velocity magnitude and the r.m.s. of the velocity components. A very good agreement among all databases is noticeable.

Table III. DNS databases for the Planar Turbulent Channel Flow case. The first four databases are obtained adopting Spectral (SM) or Pseudo-Spectral (PSM) Methods. NEK5000 adopts a Spectral Elements Method (SEM). Mesh dimensions are non-dimensionalized by $L^+ = L \cdot u_\tau / \nu$. The averaging time is expressed in non-dimensional form, via $t^+ = t \cdot u_\tau^2 / \nu$.

	Method	Re_τ	Size [10^6 pts]	Δx^+	Δy^+	Δz^+	CFL	t^+
Moser et al. [10]	SM	178.1	2.1	17.7	0.05-4.4	5.9	-	-
Hoyas & Jimenez [11]	SM	186.3	-	13.7	0.1-6.1	6.9	-	11600
Tiselj & Cizelj [12]	PSM	180.7	2.1	17.7	0.05-4.4	5.9	<0.1	10800
Vreman & Kuerten [13]	SM	180.0	14.2	5.9	0.02-2.9	3.9	-	36000
NEK5000 - N5	SEM	179.4	7.5	9.0	0.36 - 4.5	4.5	<0.1	14400
NEK5000 - N9	SEM	179.8	7.9	9.8	0.34 - 3.6	4.2	<0.2	16100

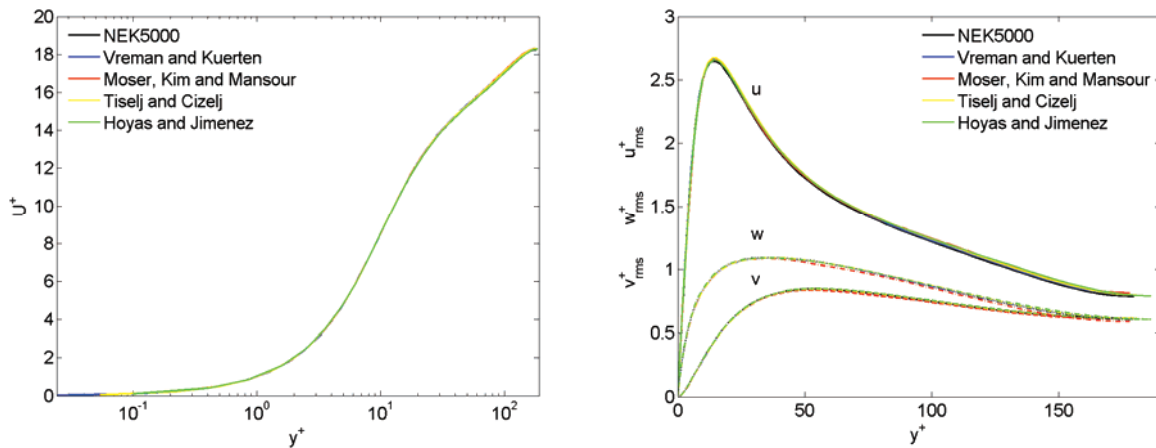


Figure 8. Normalized mean velocity U^+ and r.m.s. profiles for the three velocity components, u , v and w .

In order to better characterize the turbulent quantities, the analysis of the higher moments is needed. Figures 9-10 show a comparison of the skewness and kurtosis, defined as functions of the third and the fourth central moments, respectively. Such data are not available for Hoyas and Jimenez's database. It can be noticed that a general trend for all the three velocity components and the pressure is reproduced by the compared results. Moser, Kim and Mansour's database is the only one showing a slightly different general behaviour, mainly for the pressure term, for both skewness and kurtosis. Among the other databases, it is clearly noticeable that the results obtained via NEK5000 are in closer agreement with Vreman and Kuerten than with Tiselj and Cizelj.

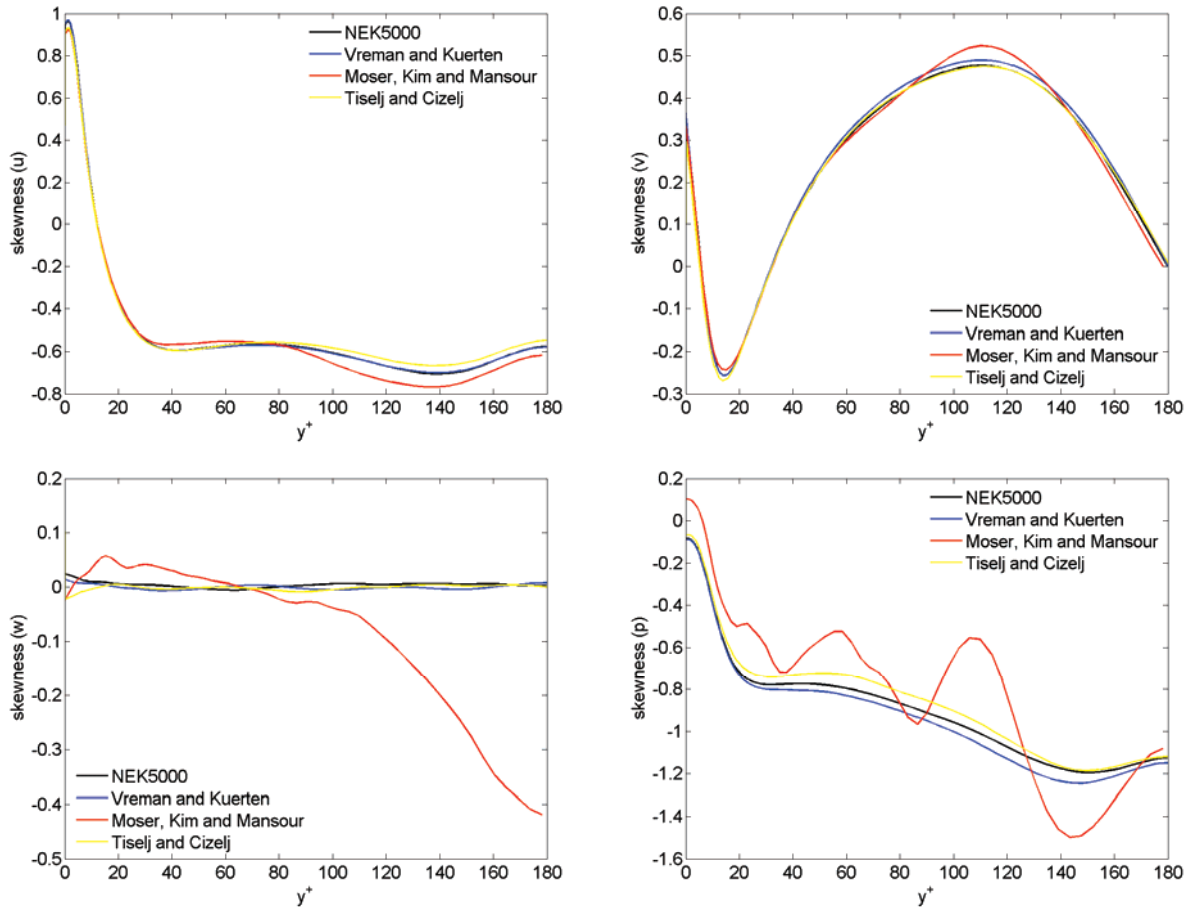


Figure 9. Skewness profiles for the three velocity components u , v and w , and the pressure p .

In addition, the balances of Turbulent Kinetic Energy (TKE) are also compared. Because of the periodicity and the regularity of the domain, it is expected that the global balance of TKE should be zero. Figure 11 depicts that the DNS of V&K shows the best results. Moreover, it is also noticeable that NEK5000 also produces good results and it is in good agreement with V&K. Whereas, all other databases show higher deviations from the expected values.

Although the TKE distribution has been extensively compared, however, due to page limitation, no additional figures are presented. The six notorious terms determining the global balance of TKE (Production, Dissipation, Molecular diffusion, Turbulent transport, Pressure strain and Pressure diffusion) have been investigated independently, considering the three velocity components both together and separately. The behavior highlighted for the global balance is reflected even for those single terms. Once again, the results suggest that NEK5000 is closer to V&K database than to the others.

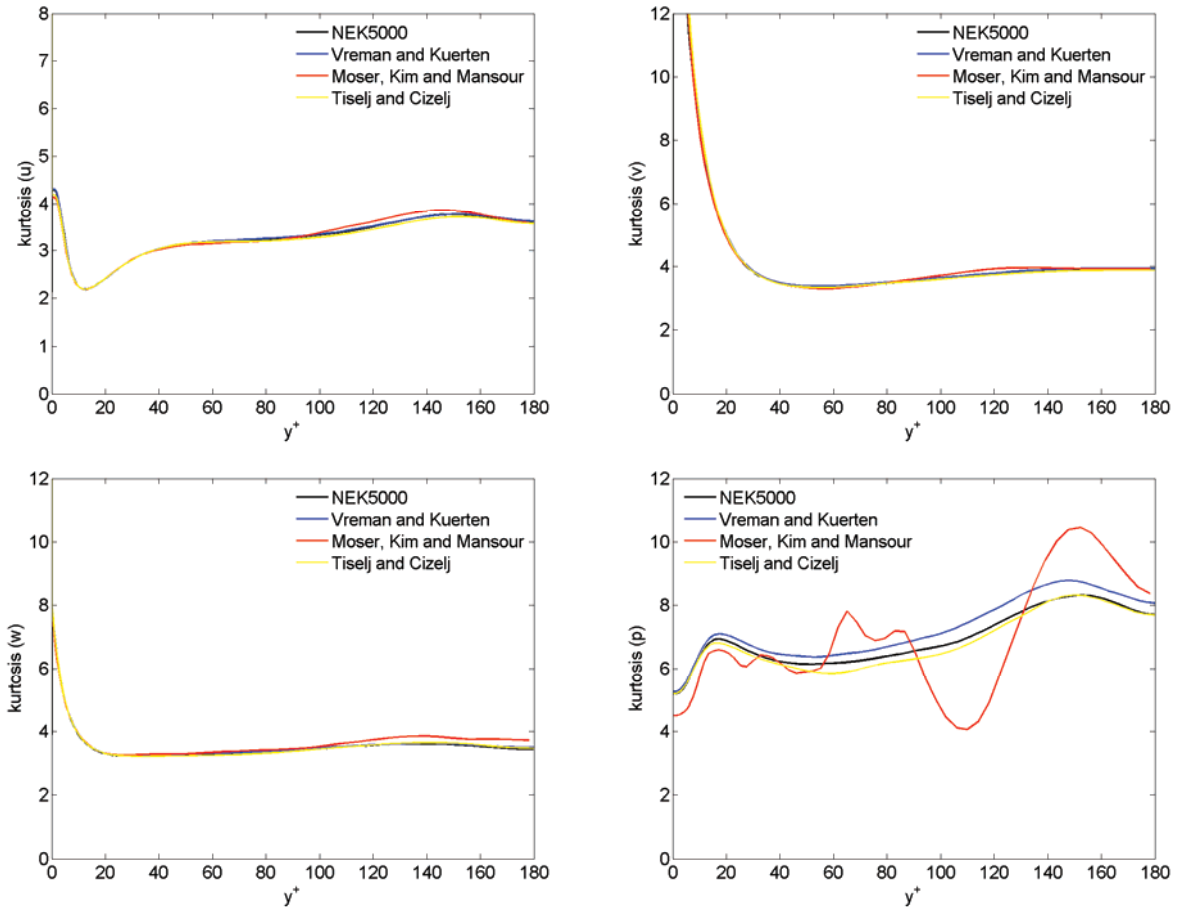


Figure 10. Kurtosis profiles for the three velocity components u , v and w , and the pressure p .

4. SUMMARY AND CONCLUSIONS

The present work aims to perform high quality DNS computations for a single-phase PTS. The targeted DNS are intended to serve as a reference database to validate lower order modelling approaches, such as Large Eddy Simulation (LES), (Unsteady) Reynolds-averaged Navier-Stokes (U)RANS, and Hybrid (LES/URANS) methods.

In the first part of the present paper, a single-phase PTS numerical experiment, initially based on the ROCOM test facility, was defined and optimized for the aimed DNS computations. For such purpose, a wide range of RANS calculations were performed to calibrate several aspects of the computational domain. Starting from the optimization of the cold leg design, the effect of all geometric parameters and their influence on the overall flow topology was studied. Secondly, the imposed boundary conditions were calibrated with particular attention to their effects on thermal field. Furthermore, both Reynolds and Prandtl numbers were scaled down to meet a feasible computational cost. As a result, a computational domain's configuration, that is a compromise between the reproduction of a physically meaningful and challenging PTS scenario and the fulfilment of the high fidelity DNS requirements, was obtained.

The second part of the present work involves the assessment of NEK5000 to perform DNS of a planar turbulent channel flow. The DNS computations are performed for the 5th and the 9th polynomial order. Among them, the latter one has shown superior quality. Moreover, the obtained results are extensively

compared with the available DNS databases. It is found out that NEK5000's results are in excellent agreement with the most recent database of Vreman and Kuerten.

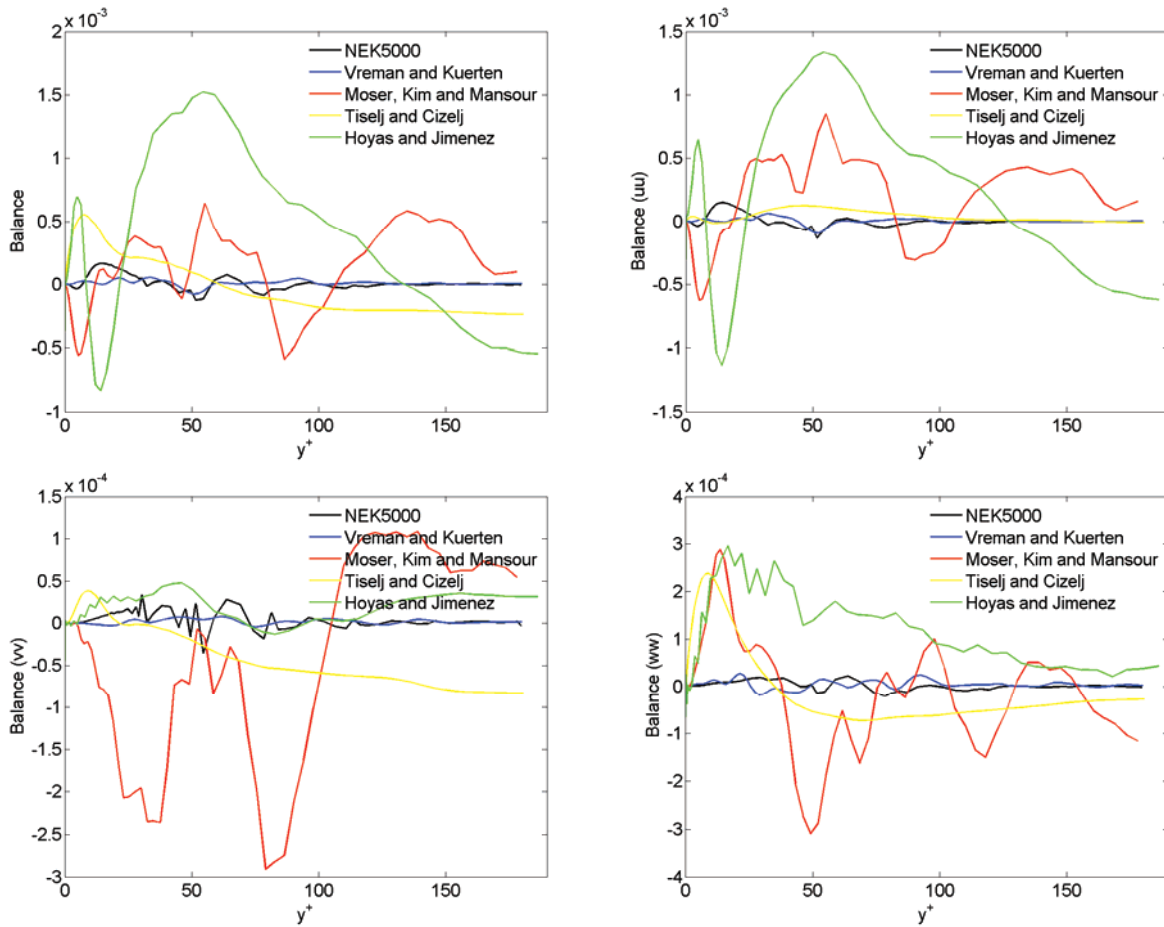


Figure 11. Turbulent Kinetic Energy global balance (upper-left corner) and balances for the single velocity components u, v and w.

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