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Requirements of LES in Modelling Natural Circulation Loops: Preliminary Study in a Pipe Geometry

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ABSTRACT

At Politecnico di Milano, the experimental facility DYNASTY has been built to study natural circulation of fluids with internal heat generation, and the reliability of passive safety strategies in the Generation IV molten salt reactor. In a preliminary step prior to the simulation of the entire facility with computational fluid dynamics and large-eddy simulation, in this work LES is applied to pipes with flow conditions similar to those found in DYNASTY. The rather low Reynolds number, typical of the laminar to turbulent transition region, and the focus of most of the available literature on channel flows, explain the need for further understanding of LES requirements and predictive capabilities in such conditions. An incompressible adiabatic flow at Re = 5300 is predicted in a cyclic pipe section with numerical solution meshes of increasing quality and refinement, and using the WALE sub-grid scale model. Comparison with direct numerical simulation results demonstrates good accuracy in predicting the turbulent flow field, and frictional pressure drops, essential for the stability features of natural circulation loops, are also successfully determined. As expected, accuracy of the results depends strongly on the grid refinement. More importantly, refinement levels appropriate to achieving a desired accuracy, but maintaining the model's computational tractability on the large spatial scales and long temporal transients of natural circulation loop studies, are identified.

1 INTRODUCTION

Natural circulation loops (NCLs) are experimental facilities aimed at increasing the knowledge on the dynamic behaviour of buoyancy-driven single phase fluid systems [1]. DYNASTY is a natural circulation loop based at Politecnico di Milano, which includes the possibility of heating the working fluid in a uniform and distributed manner, emulating the conditions occurring in the molten salt nuclear reactor. This Generation IV reactor design relies on the internal heat generation to achieve natural circulation of the liquid fuel in accident conditions and therefore enhance the safety of the system [2]. Due to the complex nature of the buoyancy-driven physics behind natural circulation, achieving good understanding and a predictive capability of the phenomena involved is imperative for the engineering design. Computational fluid dynamics (CFD) allows a detailed representation of thermal-hydraulic systems such as NCLs [2]. In recent years, high-resolution models of turbulent flows such as large eddy simulation (LES) have been progressively developed and employed for their potentially greater capabilities and reliability in predicting flow dynamic features with respect to RANS models [3]. In this work, LES is tested on a simple and easy to reproduce scenario that is, however, expected to be representative of the flow regimes encountered in the DYNASTY facility in order to be able to understand LES requirements for modelling such systems and efficiently simulating unstable transients in the full-scale facility. The work is focused on a $Re = 5300$ flow inside a circular pipe of diameter equal to $D = 0.038\mathrm{m}$. In available CFD research, much more importance has been given to the testing of LES capabilities in reproducing channel flows [4, 5, 6]. In contrast, much less effort has been dedicated to the analysis of of cylindrical geometries such as pipe flows, mainly because of the knowledge that the numerical mesh requirements for LES predictions in such systems could be derived from channel flow results [7, 8]. The objective of this work is to obtain the computational grid requirements and meshing criteria for the low-Reynolds number flow that will be employed in the study of natural circulation loops such as DYNASTY. Other than the scarcity of literature on the subject, this effort is motivated by the necessity to optimize the accuracy and computational requirements, and gain some confidence on the expected performance of the model, given the large spatial scales and long temporal transients usually characterizing natural circulation loop studies. The WALE sub-grid scale model [9] is employed, which has been shown in recent years to have good adaptability in situations it has been applied to, especially in comparison to the standard Smagorinsky model [10]. The work is composed of 16 simulations carried out on increasingly refined meshes, grouped by their tangential and longitudinal refinement and with constant radial refinement, imposed by the requirement to properly resolve the wall region. For each of the two directions, 4 refinement levels have been adopted, with a linear increase in the number of subdivisions for the selected dimension (i.e. 100, 200, 300, 400 streamwise steps). The bulk velocity of the flow is kept constant for each of the selected setups in order to maintain a fully developed turbulent flow, while the increasing refinement level allows the resolution of a greater number of turbulence scales, hence improving the prediction capabilities of the simulation and at the same time reducing the amount of the sub-grid scale contribution required by the WALE model.

2 COMPUTATIONAL FLUID DYNAMIC MODEL

In this work, an adiabatic flow is simulated and incompressible filtered continuity and momentum equations are solved with the $pimpleFoam$ solver of the open-source OpenFOAM CFD code. Similarly to $pisoFoam$, this type of solver is based on the Pressure Implicit Splitting of Operators (PISO) algorithm [11], which solves the incompressible time-dependent formulation of the Navier-Stokes equation with a predictor-corrector approach applied at each time-step. In $pimpleFoam$, the PISO algorithm is further iterated, allowing for larger time steps and/or a correct resolution of the advection non-linearity inside the time-step. Differently from a direct numerical simulation, in LES only the large scale turbulent motions are resolved by the filtered Navier-Stokes equations, while the effect of the smallest scale fluctuations on the resolved flow is modelled with the addition of a sub-grid scale (SGS) model.

2.1 Sub-grid scale model

In this work, the SGS eddy-viscosity Wall Adapting Linear Eddy-viscosity (WALE) model [9] is employed. Although relatively simple and with low computational requirements (the closure equations are algebraic and use data from the resolved flow), this model has shown promising results for several applications [12, 13]. Similarly to the more famous Smagorinsky model [14], it calculates a sub-grid scale turbulent kinematic viscosity, which is added to the molecular kinematic viscosity, from the filter width Δ (dependent on the volume of the computational cells in this work), the resolved strain rate tensor $\hat{S}_{ij}$ and its deviatoric part $\hat{S}^d_{ij}$:

$$\nu_t = (C_w\Delta)^2 \frac{(S^d_{ij}S^d_{ij})^{1.5}}{(\tilde{S}_{ij}\tilde{S}_{ij})^{2.5} + (S^d_{ij}S^d_{ij})^{1.25}} \tag{1}$$

The WALE model has been found to have improved capabilities in representing the alternating turbulent and laminar regimes typical of natural circulation flows, with the contribution given by the SGS model when the flow is laminar correctly dampened to zero, differently from the standard Smagorinsky model, which has instead been found to over-dampen the turbulent oscillations [15].

2.2 Computational grid

The geometry and mesh have been built using the CAD software Gmsh [16], which allows great control of geometry and mesh parameters, and a good user interface to visualize the work in progress. The pipe discretisation is based on a hybrid block-structured and unstructured mesh, with a central octagonal prism split into 4 hexahedrons, enclosed by 8 hybrid circular sections that contain the most refined part of the mesh near the wall. The mesh is built from a 2D cross-sectional surface that is extruded and discretised with a constant longitudinal step. Radial refinement is obtained by applying a 0.85 geometric progression in the radial dimension of the cell, i.e., moving from the pipe centre to the wall, such that each element length is equal to 0.85 of the length of the preceding element. This approach allows good control of the wall refinement, creating a very fine grid where it is needed close to the wall boundary and optimizing the resources needed for the simulations. In this analysis, the radial refinement in the outer layer has been kept constant, to obtain the required refinement of the boundary and a wall distance $(1 - r/R)^+$ in the first cell near the wall lower than 1. This is a common requirement for wall-resolved LES, and due to the abundance of literature confirming the validity of such an approach [17, 18], the sensitivity analysis conducted in this work will only focus on the refinement in the remaining 2 directions (θ, z). In any case, in the internal region, the radial discretisation is controlled and changes following the tangential refinement (See Fig 1). In a pipe, the tangential refinement depends also on the radial coordinate. This means that, with a constant number of elements in the angular direction, shorter arcs are created in the centre of the grid and longer ones closer to the wall, even though their angular distance is the same. To avoid this and change the tangential refinement along the radius, at the expense of a decrease in the speed of the simulation [19], a layer of prismatic elements has been included between the internal and external hexahedral regions, obtaining the hybrid mesh shown in Figure 1. The calculation meshes used for this work are shown in Table 1, where the first numerical values identify the streamwise refinement and the second the tangential value.

Table 1: Number of cells for each combination of streamwise and tangential refinement.

	Δz			
$R \cdot \Delta\theta$	**M1-x**	**M2-x**	**M3-x**	**M4-x**
Mx-1	$1.55 \cdot 10^5$	$3.1 \cdot 10^5$	$4.64 \cdot 10^5$	$6.19 \cdot 10^5$
Mx-2	$2.27 \cdot 10^5$	$4.54 \cdot 10^5$	$6.82 \cdot 10^5$	$9.09 \cdot 10^5$
Mx-3	$3.2 \cdot 10^5$	$6.39 \cdot 10^5$	$9.59 \cdot 10^5$	$1.278 \cdot 10^6$
Mx-4	$4.21 \cdot 10^5$	$8.42 \cdot 10^5$	$1.262 \cdot 10^6$	$1.683 \cdot 10^6$

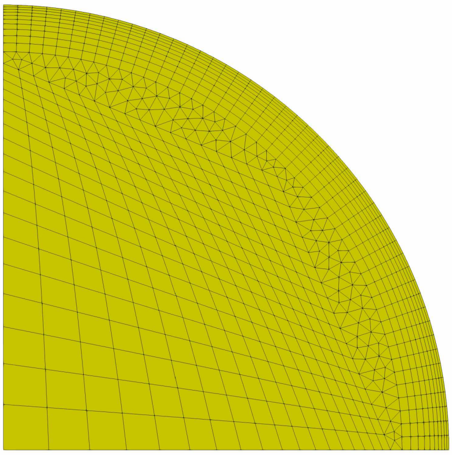

Figure 1: Cross-sectional view of the finest calculation mesh (M4-4 from Table 1).

2.3 Initial and boundary conditions

A 0.5 m long section of the pipe is simulated, with cyclic conditions applied on the inlet and outlet sections. To sustain the flow, a positive pressure gradient is applied by the code, adjusting the mass flow-rate in order to overcome the friction losses and maintain the $Re = 5300$ flow. At the wall a $no - slip$ $(u_r = u_\theta = u_z = 0)$ condition is imposed for the velocity field, and zero gradient conditions $\frac{\partial p}{\partial r} = \frac{\partial \nu_t}{\partial r} = 0$ are used for the pressure and the turbulent viscosity ν_t. To obtain turbulent conditions at the beginning of the simulation, sinusoidal perturbations are introduced in the initial velocity field that with time develop into a fully turbulent flow. [20].

3 RESULTS

Geometric parameters, refinement values and flow quantities are made non-dimensional, in order for them to be general and independent of the specific case studied. The normalisation parameters are the kinematic viscosity $\nu = 2.94837 \cdot 10^{-6} \mathrm{m}^2\mathrm{s}^{-1}$, in this case taken as the reference value for water-propylene glycol mixtures that will be used in DYNASTY to reproduce the behaviour of molten salts, and the friction (or shear) velocity, defined as $u_\tau = \sqrt{\nu \left(\frac{\partial u}{\partial n}\right)_{wall}}$. A preliminary value for this quantity is obtained from DNS data at the same bulk Reynolds number of 5300 [21], for which a friction Reynolds number $Re_\tau = \frac{u_\tau \cdot D}{\nu}$ of 181.0541 was obtained. Therefore, the value of the friction velocity is $u_\tau = 0.028095 \mathrm{~m\,s^{-1}}$.

To obtain consistent values between the different meshes, these values are always used as the velocity scale for the normalisation of the mesh refinement. The flow parameters, instead, to be compared against DNS data are normalised using the friction velocity derived from the resolved flow. The normalised quantities are defined as $a^+ = a \cdot \frac{u_\tau}{\nu}$. Using these normalisation criteria, the streamwise and tangential refinement reported in Table 2 is obtained. It is important to note

Table 2: Refinement in the streamwise and tangential directions for each mesh.

Δz^+			
M1-x	M2-x	M3-x	M4-x
47.65	23.82	15.88	11.91
$(R \cdot \Delta\theta)^+$			
Mx-1	Mx-2	Mx-3	Mx-4
3.77	2.83	2.26	1.89

that while the streamwise refinement is constant, the tangential value is provided at the external wall, where the tangential spacing is a maximum for the same angular distance.

3.1 Qualitative analysis of the flow regimes

A first comparison between the coarsest and the finest meshes is shown in Figure 2. The increase in resolution allows for the simulation of increasingly small turbulent eddies, the contribution of which is instead accounted for by the SGS model for mesh M1-1, where the velocity field is still turbulent but with only a limited number of very large eddies present in the flow. On a related note, previous simulations with a standard Smagorinsky SGS model [14] showed an excessive energy dissipation for very coarse meshes [15]. This effect usually resulted in the dampening of the turbulent structures with the instantaneous velocity field eventually converging to laminar. This is not the case for the WALE SGS model, even at the lowest level of resolution adopted in this work (mesh M1-1). Therefore, the LES methodology coupled to the WALE SGS model seems to be able to sustain and allow the development of low-Reynolds number turbulent flows even on reasonably coarse meshes.

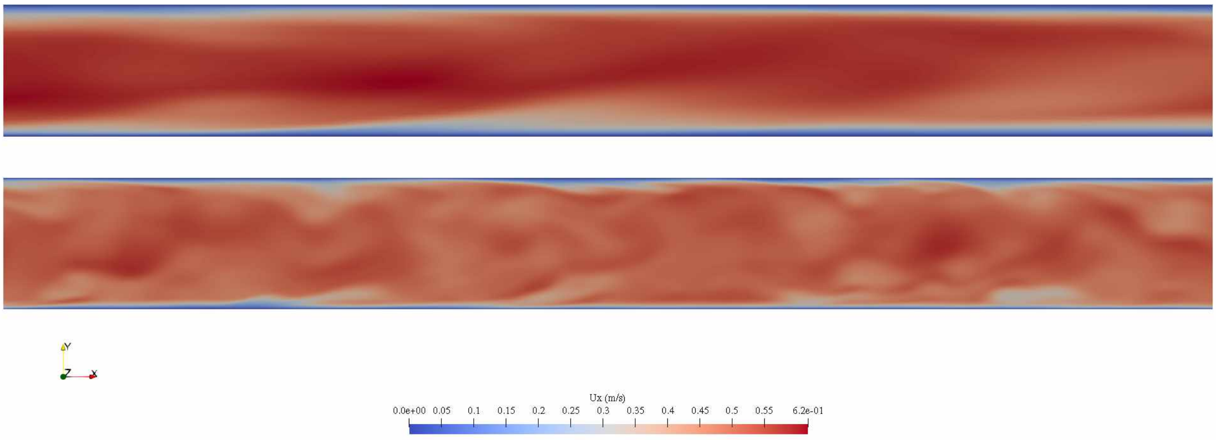

Figure 2: Longitudinal view of the instantaneous velocity distribution for meshes M1-1 (Upper picture) and M4-4 (Lower picture).

3.2 Pressure drop analysis

Especially for the simulation of natural circulation loops, one of the most important parameters a CFD simulation should be able to predict are the pressure losses occurring inside the computational domain, since they are one of the main drivers of the fluid motion [22]. The pressure losses are calculated from the friction shear stress at the wall:

$$\frac{\Delta p}{\rho} = \Delta\tilde{p} = 2 \cdot u_\tau^2 \cdot \frac{L}{\frac{1}{2}D} \tag{2}$$

The sensitivity analysis on the pressure losses demonstrated a peculiar behaviour, with the increase in accuracy with respect to DNS mostly related to an increase of refinement in the longitudinal direction, as shown in Table 3.

As per the numbers presented, it is clear that the tangential refinements used in this work do not significantly modify the accuracy of the simulations, with an increase in performance relegated to about 2%–3% with respect to the predicted pressure losses. In view of this, the first mesh seems already relatively well resolved in the tangential direction. On the other hand, the longitudinal refinement employed in the the M1-x and M2-x meshes leads to large errors, whereas accuracy greatly improves for the finer meshes, when the non-dimensional refinement falls below $\Delta z^+ <\approx 20$–15. This observation underlines the importance that must be given to all the 3 directions of motion when dealing with LES, and this is linked to the necessity of resolving 3-dimensional turbulent structures. From this quantitative analysis it becomes apparent that LES is able to predict the pressure losses occurring in low-Reynolds number scenarios with an acceptable degree of accuracy ($e_{\%} \approx 10$–15%) for values of the non-dimensional tangential refinement below $(r \cdot \Delta\theta)^+ <\approx 3$ and longitudinal (or streamwise) below $\Delta z^+ <\approx 20$–15. This criterion must always be coupled to the well-established requirement that the normalised radial step in the first cell of the boundary layer is less than 1 ($\Delta r^+_{wall} < 1$).

Table 3: Prediction errors of pressure losses with respect to DNS data [21].

	Δz^+			
$(R \cdot \Delta\theta)^+$	**M1-x**	**M2-x**	**M3-x**	**M4-x**
Mx-1	-37.95%	-21.84%	-15.39%	-11.92%
Mx-2	-36.19%	-20.08%	-13.63%	-10.16%
Mx-3	-35.25%	-19.13%	-12.68%	-9.22%
Mx-4	-34.68%	-18.57%	-12.12%	-8.65%

3.3 Average flow quantities

Figure 3 shows a comparison of the 16 simulations grouped by the longitudinal refinement adopted and the flow quantity of interest. It is clear that an increase in refinement in either direction moves the results of LES closer to the real (DNS) behaviour of the fluid flow. The trends in the mean streamwise velocity (first row), the turbulence-related component of the shear stress (second row) and the velocity turbulent fluctuations in the 3 directions (summed up to the turbulent kinetic energy - third row) all show a similar behaviour, with the biggest improvement in the predictions obtained via streamwise refinement (different for each column of Figure 3). An increase in tangential refinement, instead, leads only to a small increase in accuracy. This behaviour confirms previous observations from the pressure losses, and at the same time confirms that a certain convergence of the results, and the resolution of a sufficient amount of turbulence structures, is reached for the most refined meshes, where a portion significantly higher than 90% of the total turbulence energy is resolved. This can be noted in the similarity of the curves for the M3-x ($\Delta z^+ = 15.88$) and M4-x ($\Delta z^+ = 11.91$) meshes, which, although different, present only a small improvement when the streamwise refinement is increased. As a consequence, it can be assumed that a further increase in resolution ($\Delta z^+ < 10, (r \cdot \Delta\theta)^+ < 3$),

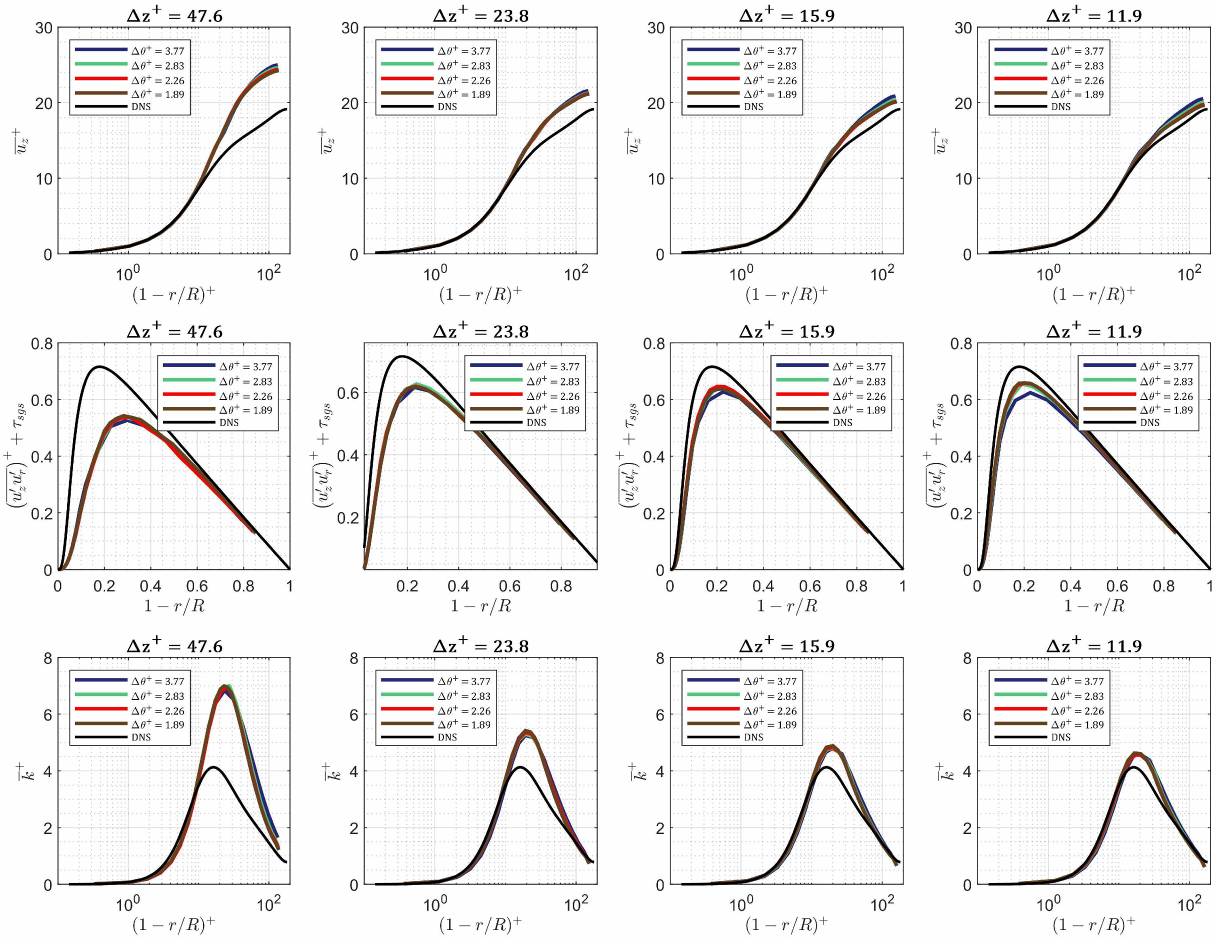

Figure 3: Results comparison for the mean streamwise velocity, the turbulent shear stresses and the turbulence kinetic energy.

in the context of the simulation of natural circulation loops, would increase the computational burden of the simulations up to a level not justifiable by the improved accuracy of the results.

4 CONCLUSIONS

LES has been successfully adopted to flow on a simple pipe geometry representing the typical flow conditions present in a natural circulation loop built at Politecnico di Milano. The study focused on incompressible adiabatic flow conditions, and showed the reliability of the methodology without excessive damping of the buoyancy-driven turbulence structures and a satisfactory accuracy when a sufficient refinement of the computational grid was employed. Most importantly for the application to natural circulation loops, refinement criteria for the numerical mesh have been obtained for the pipe geometry, whilst most of other literature works are based on channel geometries. These criteria are based on a-priori evaluation of the expected errors in the prediction of the flow field and the pressure losses, the latter of fundamental importance for the correct representation of natural circulation loops. More specifically, the analysis showed the importance of refinement in all the 3 directions of motion, and judging from the reported results, in order to achieve a certain a-priori confidence in the pressure loss estimates ($e_{\%} \approx 10$–15%) and the predicted turbulent flow parameters, it is advisable to keep the streamwise non-dimensional refinement below $\Delta z^+ <\approx 20$–15 and the tangential step below $(r \cdot \Delta\theta)^+ <\approx 3$. Further increases in resolution in either direction only slightly improve the accuracy of the simulation (with respect to the predictions of DNS), while significantly increasing the computational cost of the simulations. This aspect is of major importance for natural circulation loops, which are usually characterized by large spatial scales and long temporal transients ($t \approx 10^2$–10^4), often requiring an optimum between accuracy and computational load to maintain the simulation with CFD LES methods manageable.

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