HIGH-FIDELITY NUMERICAL SIMULATION OF THE FLOW THROUGH AN INFINITE WIRE-WRAPPED FUEL ASSEMBLY

A. Shams, F. Roelofs and E.M.J. Komen
Nuclear Research and Consultancy Group (NRG)
Petten, The Netherlands
shams@nrg.eu

ABSTRACT

The present study is an attempt towards generating a high fidelity reference database for a wire-wrapped fuel assembly of a liquid metal fast reactor (LMFR). This database will be open to the scientific community and will serve to validate RANS based turbulence modelling approaches. In the present paper, the calibration of an infinite wire wrapped fuel assembly is performed for such high fidelity numerical reference simulations. The selection of the fuel assembly has been made on the present MYRRHA design. A wide range of RANS calculations are performed to calibrate the computational domain, boundary conditions, meshing parameters, and the turbulence quantities. This paper also reports the meshing strategy that has been adopted for the reference high fidelity calculations along with some preliminary results obtained from the on-going quasi Direct Numerical Simulation (q-DNS).

KEYWORDS
LMFR, wire-wrapped fuel assembly, MYRRHA, q-DNS, RANS

1. INTRODUCTION

Nuclear power plays an important role in power generation and produces about 11% of the total electricity worldwide. The rapidly growing energy demand suggests an important role for nuclear power in the future energy supply, as for example denoted in the projections of the World Energy Outlook 2014 [1]. They consider that nuclear fission will play a large role towards a low-carbon energy mix. The IAEA [2] attributes a large role to the deployment of fast reactors in a sustainable nuclear energy mix. For an elaborated overview of the status of fast reactor development the reader is referred to a technical report made by the IAEA [3]. Most of the described fast reactors employ a liquid metal as coolant showing the importance of liquid metal coolants.

The nuclear chain reaction, which is the source of nuclear fission energy production, takes place in the core of a nuclear reactor. Within this core, heat is produced in nuclear fuel and transported to the coolant. Typically, a nuclear core consists of a few hundred fuel assemblies which in turn consist of a large number of fuel rods. Most fast reactor designs, employ wire wraps as spacer design (see e.g. [3]). For the design and safety analysis of such reactors, the heat transport in the fuel assemblies of the core is very important. The main challenges related to fuel assembly thermal hydraulics are the occurrence of hot spots, the thermo-mechanical loads, effects of partial blockage and deformation, and the different flow regimes and their transition e.g. when the reactor switches from forced cooling to other types of cooling in decay heat removal situations. For the design and safety analyses of nuclear reactors, simulations of the heat transport within the core are essential. However, the specific, mostly empirical, correlations for heat transport often contain large uncertainties for liquid metal coolants as e.g. clearly demonstrated by [4]. Therefore, experiments and detailed Computational Fluid Dynamics (CFD) simulations play an important role. As experimental data for liquid metals is often hard to obtain and very costly, nuclear reactor designers rely more and more on simulation techniques like CFD. However, CFD approaches first need to be validated against experimental data or very fine computational data. In order to simulate the heat transport in the core of a liquid metal fast reactor, a correct description of the flow behavior in fuel assemblies employing wire wraps is essential. In the past few decades, many experiments were performed world-wide to characterize the flow in such fuel assemblies. An elaborate overview of these studies is provided in [5] . However, most of these data aimed at obtaining global information on the heat transport. These experiments do not provide sufficiently detailed information required for the validation of CFD approaches. More recently, some attempts have been recorded to derive sufficiently detailed experimental data. A summary of these works obtained from [6]. In order to obtain such detailed experimental data required for validation of CFD approaches, all reported studies employ transparent simulant fluids replacing the liquid metal. Such experiments are restricted to the hydraulic behavior and do not encompass the heat transport.

In order to overcome this issue of not having reference data for flow and heat transport simultaneously, high fidelity numerical simulations can be performed. Such analyses are reported by [6]. They compare their high fidelity numerical reference data, again only for flow hydraulics, with more pragmatic Reynolds Averaged Navier Stokes (RANS) simulations which enable fuel assembly simulations for industrial purposes. They conclude that application of advanced RANS turbulence models does not show much added value compared to standard RANS models for wire wrapped rod bundles. More recently, [7] used the 7-pin data from a large eddy simulation dataset to benchmark pragmatic RANS simulations. These data are restricted to a 7-pin bundle including housing. Obviously, the presence of the housing has a large effect on the flow behavior and has to be taken into account. However, there is still clearly a need of more high fidelity numerical reference data. Firstly, in order to exclude the effect of the housing from the comparison. Secondly, to create reference data for different rod configurations (the existing dataset is related to sodium reactor designs, whereas the configuration of lead reactor designs typically allows for larger spaces between the individual rods). And finally, to include the heat transport in the comparison.

Therefore, the objective of the current work is to calibrate an infinite wire wrapped fuel assembly in order to perform high fidelity numerical reference simulations. Such simulations require calibration of the computational domain, boundary conditions, mesh parameters, and turbulence quantities. Principally, this paper is divided into two parts. The selection of the flow configuration along with the calibration of the boundary conditions are reported in Part-I: section 2. Whereas, in Part-II: section 3, the meshing strategy to perform high fidelity simulations is documented. This part also reports some preliminary results of on-going q-DNS computations. This is followed by the summary.

2. PART I: SELECTION AND CALIBRATION OF FLOW CONFIGURATION

The main objective of this research work is to perform high fidelity CFD calculations, which will serve as a reference database to validate lower order turbulence modelling approaches. Performing such high fidelity simulations is extremely expensive. Hence, the selection of a geometric configuration and its respective calibration is extremely important in terms of reducing the overall computational cost. This section illustrates the selection of the computational domain and its respective calibration.

2.1. Computational domain

The selection of a computational domain is performed using the dimensions of the MYRRHA design as presented by [8]. A MYRRHA fuel assembly consists of 127 wire wrapped fuel pins, and the related geometric dimensions are given in Table I.

Table I. Dimensions of MYRRHA design wire wrapped rod bundle.

Parameters	Values	Units
Diameter of rod	6.55	mm
Diameter of wire	1.75	mm
Wire (wrapping) pitch	262	mm
Gap (between wire and rod)	0.1	mm
Pitch to diameter ratio (P/D)	1.279	-

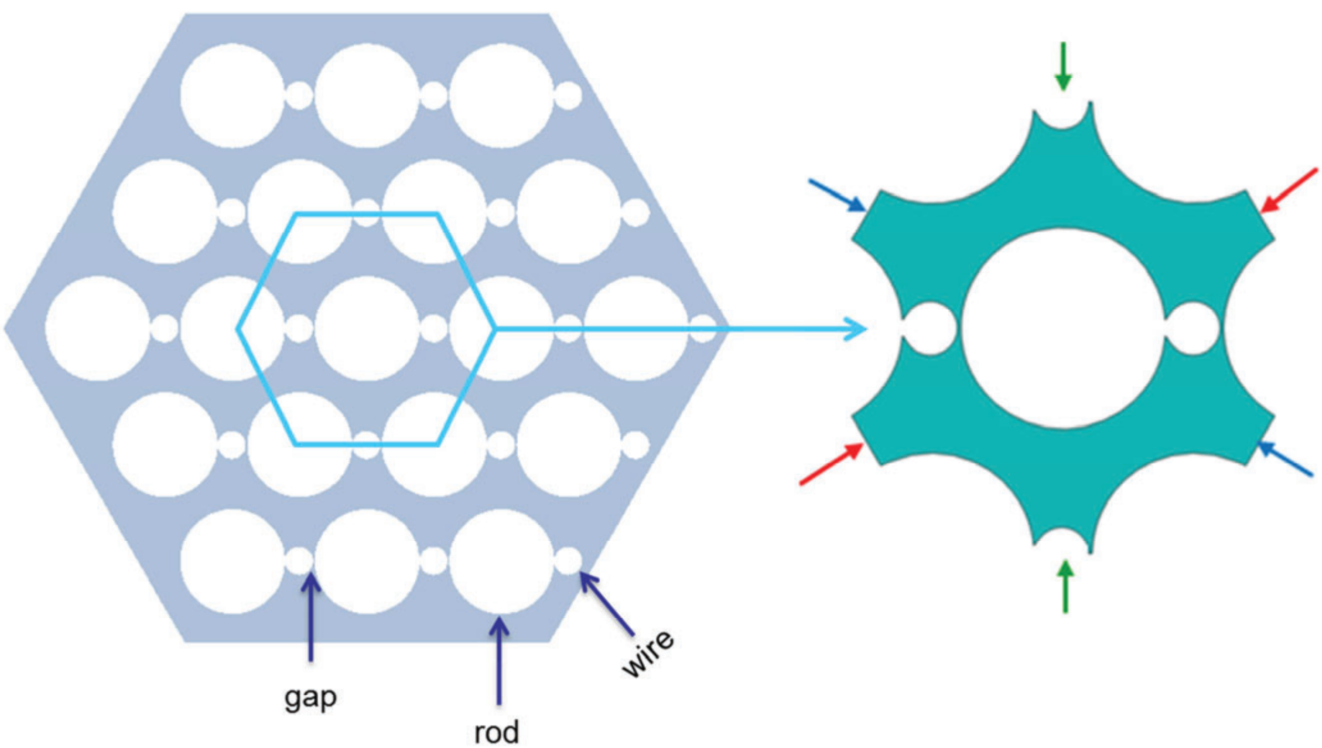

Figure 1. (Left) A 19 pin wire wrapped rod bundle and (Right) the selected single pin wire wrap domain: green, red and blue arrows indicate respective preiodic sides.

The selection of a computational domain is performed such that it can represent an infinite wire wrapped fuel assembly by keeping the realistic MYRRHA design parameters. To understand this selection, a 19-pin rod bundle is shown in Figure 1.

To create an infinite wire wrapped fuel assembly, a hexagonal section is selected, as shown in Figure 1. This hexagonal section consists of 1/3rd of six rods clustered around a full-centralized rod in a systematic arrangement. This hexagonal section is explicitly shown in Figure 1 (right) and represents a geometrically symmetric configuration. Thus, allowing to numerically impose periodic boundary conditions to their respective opposite side, see Figure 1 (right). Furthermore, the length of the computational domain is kept to one wire wrap pitch. This also allows to impose periodic boundary conditions, for the mass flow rate, in the principle flow direction, see Figure 2. Hence, the resulting wire wrapped domain represents an infinite wire wrapped rod bundle configuration.

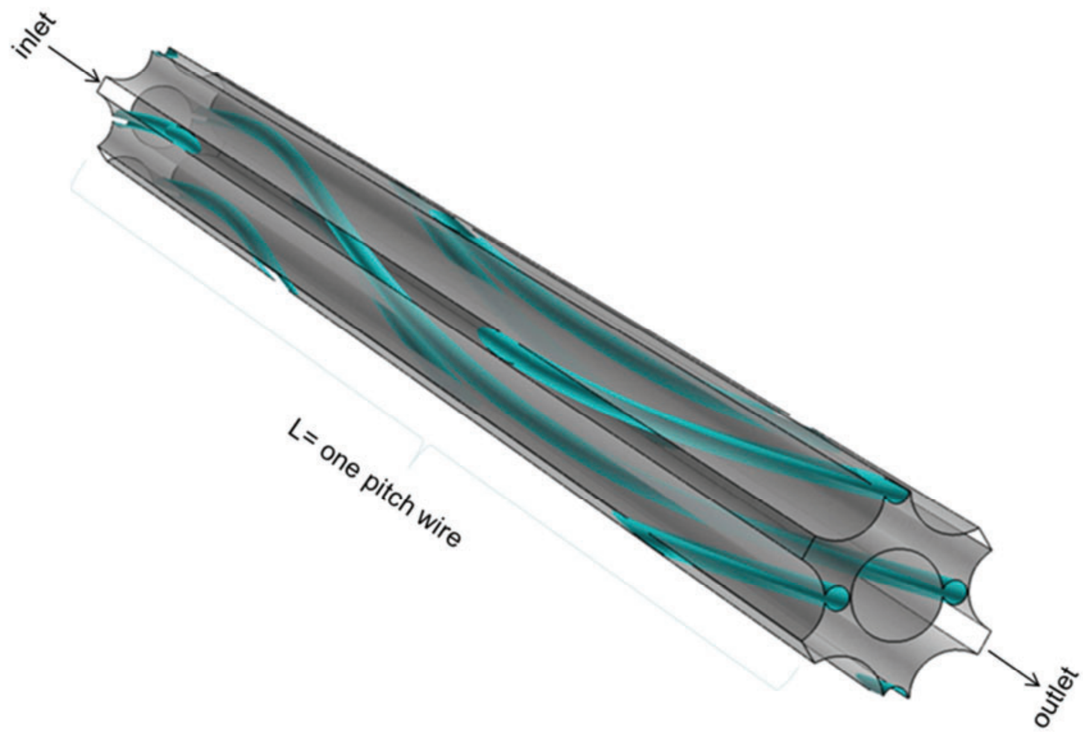

Figure 2. Selected computational domain with the boundary conditions [9].

2.1. Flow parameters

Following the MYRHHA design, lead bismuth is considered as a working fluid with an average inlet temperature and velocity of 340 °C and 2 m/s, respectively. The properties of lead bismuth corresponding to the inlet temperature conditions are given in Table II. The computed bulk Reynolds number (based on the hydraulic diameter) for the selected computational domain is Re = 46137. The resulting mesh estimation (based on a preliminary RANS calculation) for a DNS computation for this Reynolds number gives a total of ~ 200 million grid points. Hence, it would result in a very expensive simulation. Therefore, a wide range of RANS calculations are performed to scale down the Reynolds number. These are discussed in Section 2.4.

Table II. Properties of lead bismuth at T=340 ^{o}C.

Property	Value	Units
Density	10284.63	Kg/m^3
Dynamic viscosity	1.69×10^{-3}	Kg/m.s
Thermal conductivity	12.25	W/m.K
Specific heat	145.0	J/kg.K

2.2. Numerical Methods and Turbulence Modelling

All numerical simulations presented in this paper are performed by using the commercially available STAR-CCM+ code [10]. The scaling of Reynolds number requires a wide range of RANS calculations. Hence, a linear k-ω SST model has been selected. Moreover, a second order upwind scheme is used for space discretization. The present discretization is performed by using collocated and a Rhie-and-Chow type pressure-velocity coupling combined with a SIMPLE-type algorithm.

Mesh generation for such a complex geometric configuration is not an easy task. Thanks to the versatile meshing technique provided in [10], it was possible to generate a trimmed hexahedral mesh consisting of ~6 million grid points with relatively low efforts. A cross-section at the mid of the computational domain is extracted to display the generated trim mesh, see Figure 3. It is worth mentioning that the size of the first cell close to the wall is fine enough to ensure y^+ values < 1.

2.3. Scaling of Reynolds number

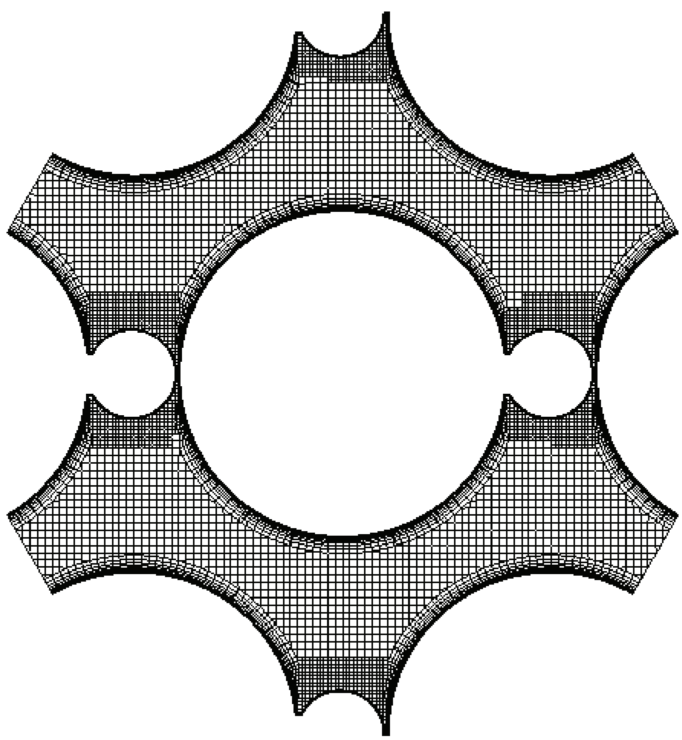

Figure 3. Trim mesh over a cross-section.

Performing a high fidelity simulation of an infinite wire wrapped rod bundle at Re = 46137 is challenging in terms of computational resources. Hence, following the work of [11], the Reynolds number is scaled in order to reach a feasible computational workload. This scaling is performed in such a way that the overall flow remains in the turbulent regime. Hence, RANS computations for seven different Reynolds numbers, given in Table III, have been performed.

Table III. List of the Reynolds numbers for calibration study.

Case	Reynolds number
1	43167
2	19582
3	14687
4	9791
5	7000
6	5000
7	3571

Before comparing the results obtained corresponding to these seven Reynolds numbers, it is worthwhile to understand the flow physics exhibited by this complex flow configuration. The iso-contours of the velocity magnitude for Re = 46137 are shown in Figure 4. It gives an indication of the extensive range of velocity scales appearing throughout the computational domain. Low velocity regions appear in the small gap between the wire and the central rod. These low velocity regions develop into turbulent flow along the wire in the principle flow direction.

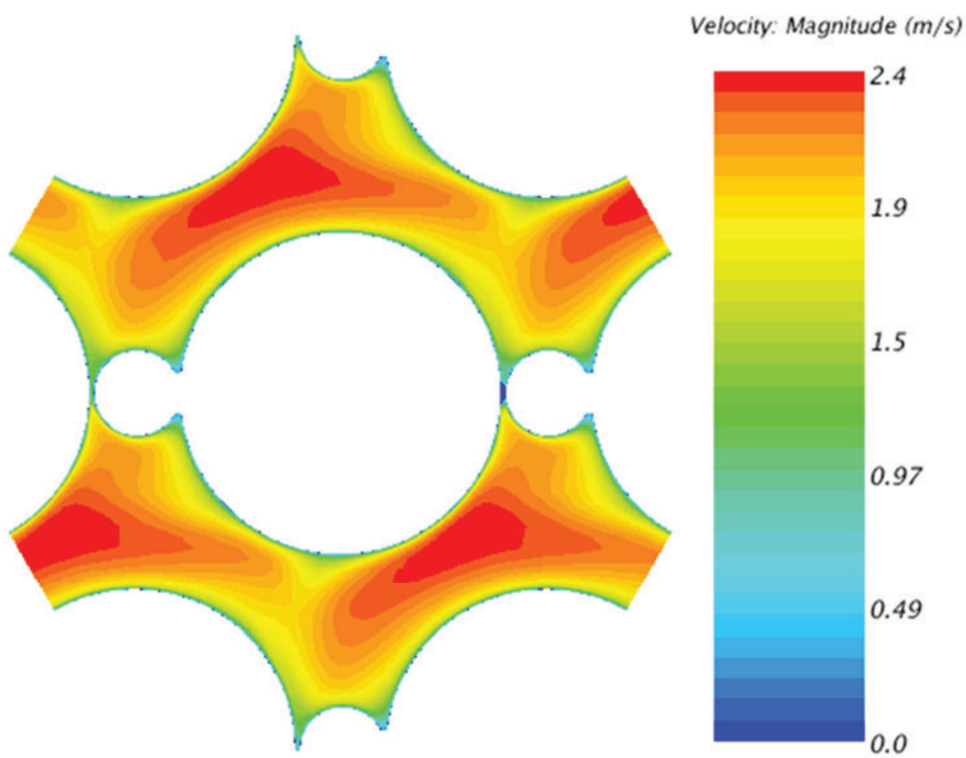

Figure 4. Iso-contours of velocity magnitude at Re = 46137.

The obtained results corresponding to the seven Reynolds are presented in a perspective of a 7-pin fuel assembly, see Figure 5. This highlights the connectivity of scaled Reynolds number with the original one. It is noticeable that with decreasing Reynolds numbers the low velocity region (indicated by a blue color) increases. Hence, a decrease in the flow gradient appears in the near wall region. Nonetheless, all the Reynolds numbers qualitatively reproduce a similar flow topology. Interestingly, the low velocity regions are more prominent for low Reynolds numbers, i.e. Re = 7000, 5000 and 3571, which could result in flow re-laminarization.

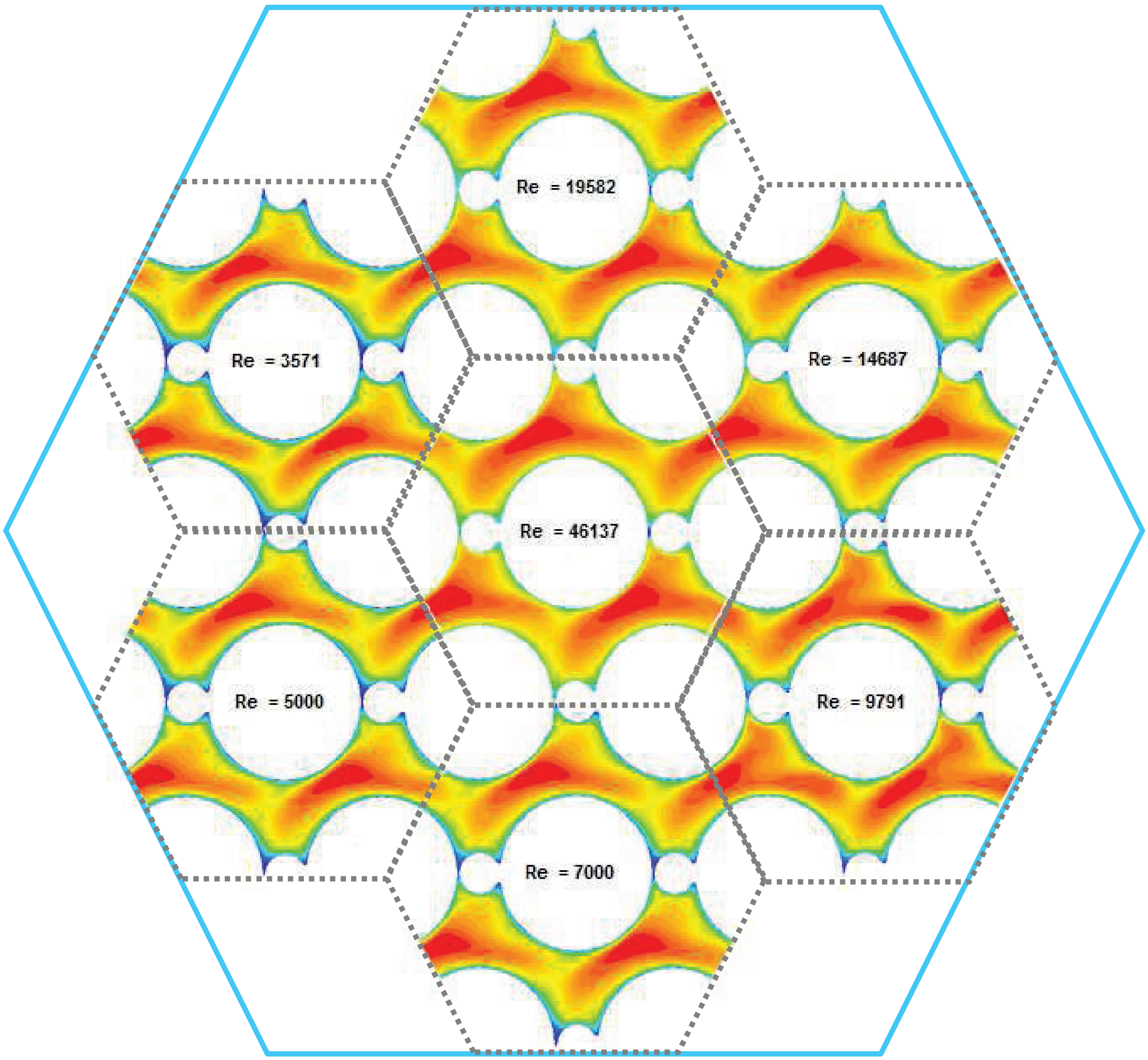

Figure 5. Scaling analyses in a fuel assembly perspective: iso-contours of velocity field.

In addition to these qualitative results, an extensive comparison of quantitative results is also performed. These results are not shown here. Nevertheless, it can be mentioned that the quantitative results suggest that except Re = 5000 and 3571, all the Reynolds numbers are able to reproduce a similar and turbulent flow regime. These low Reynolds numbers both seem too close to the transitional flow regime. Hence, to be on the safe side, Re = 7000 is selected to perform the target high fidelity simulations, which is a feasible choice corresponding to the available computational resources.

3. PART II: HIGH FIDELITY SIMULATIONS OF AN INFINITE WIRE WRAP

This section focuses on the meshing strategy to perform the aforementioned high fidelity reference simulations. In addition, some preliminary results of the on-going high fidelity computation are reported and discussed here.

3.1. Meshing strategy for high fidelity simulations

3.1.1. Mesh sensitivity of RANS calculations

The extensive calibration study in the previous section has shown that a scaled Reynolds number of Re = 7000 successfully reproduces the overall flow topology and is selected to perform the high fidelity numerical simulation. However, the feasibility of this selected Reynolds number in terms of mesh requirement is yet to be evaluated. Therefore, an estimation of Taylor (length) and Kolmogorov (length and time) scales needs to be made based on a RANS solution. To obtain a proper prediction of these scales, the RANS solution should be grid independent. Therefore, a mesh sensitivity study of the selected infinite wire wrap case at Re=7000 is performed. Three different meshes are used for this mesh study and are given in Table IV.

Table IV. List of the Reynolds numbers for calibration study.

Mesh	Points (millions)
M1	6
M2	8
M3	16

It is worth mentioning that all the previously mentioned simulations in section 2 are performed on mesh M1, which was accordingly modified for different Reynolds numbers. In addition to M1, two more meshes are tested. The comparison of the results (not shown in this paper, for details see [9]) suggests that the Mesh M1 is good enough to reproduce the overall flow topology. However, with a slight mesh refinement, such as for mesh M2, the obtained results get better. Moreover, no further changes in the results is observed for M3. This concludes that the selected flow configuration can be considered as grid independent for mesh M2. Therefore, the estimation of the turbulent length and times scales is performed on mesh M2.

3.1.2. Calculation of turbulence length and time scales

Two important turbulent length scales, i.e. Taylor and Kolmogorov, are computed to find out the mesh requirements for high fidelity CFD calculations. The Taylor micro-scale (TMS) is a good indicator for LES mesh dimensions and is given as $\lambda = (10\ k\ \upsilon / \varepsilon)^{1/2}$. The obtained results have shown that, for a well-resolved LES, the non-dimensionalized cell size in the bulk is found to be in the range of $\Delta^+ = 15\text{-}60$: $\Delta^+ = \Delta^* U_\tau / \upsilon$, where U_τ is the friction velocity. Whereas, the small length scales are only present in the near wall region. Moreover, the Kolmogorov length scales (KLS) are also computed, which are the best representative to obtain a resolved DNS mesh. The obtained KLS ($\eta = (\upsilon^3/\varepsilon)^{1/4}$) in the bulk give non-dimensionalized cell sizes (Δ^+) of 3-33. It is clearly noticeable that the KLS represent much finer scales than the TMS and hence would lead to a well-resolved DNS mesh. In addition, the Kolmogorov time scales ($\tau = (\upsilon/\varepsilon)^{1/2}$) are computed and are found to be in the range of $5.2\times10^{-5} - 1.34\times10^{-3}$ as non-dimensionalized time scale ($\tau^+ = \tau^* U_\tau / L$, where L is the length of the domain). This range of time steps is significantly larger than what was computed for Re = 46137. Hence, such time steps will allow for a sufficiently long integration time given the available computational power.

3.1.3. Mesh generation of DNS study

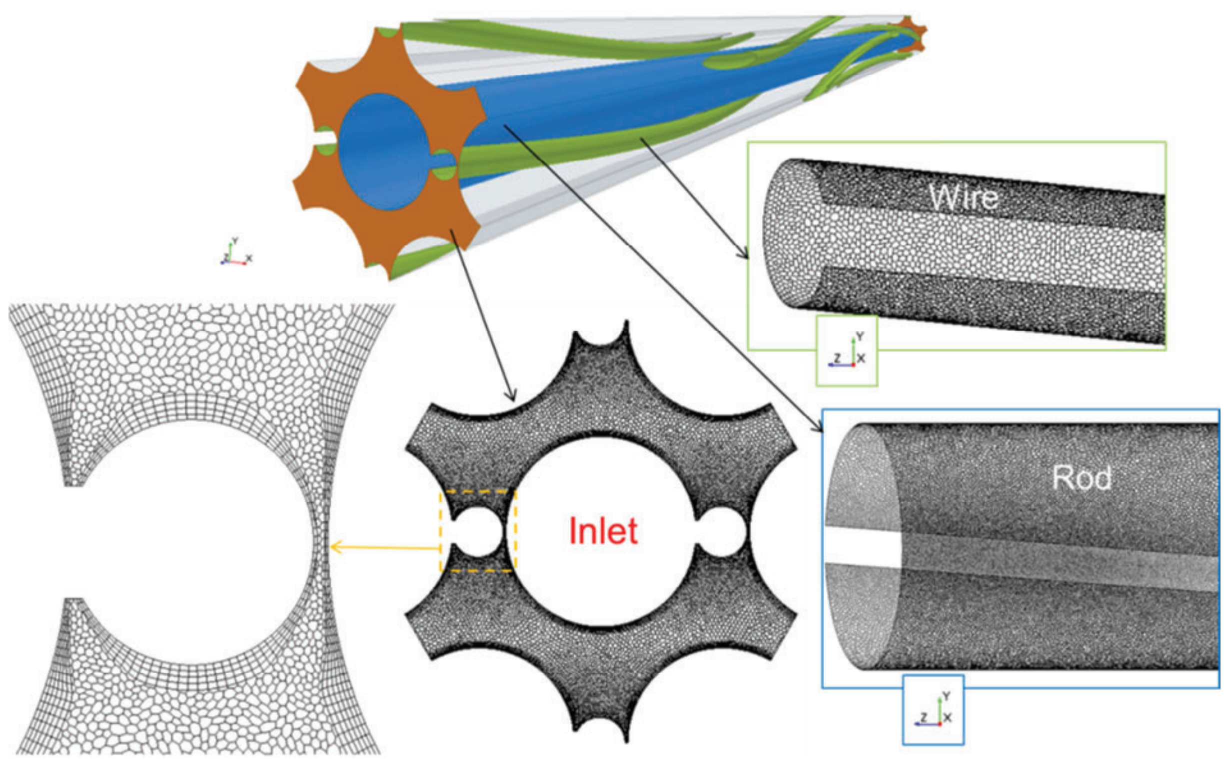

Figure 6. Q-DNS quality polyhedral mesh for a single pin wire wrapped fuel assembly [9].

Generating a high quality mesh for reference simulations, be it DNS or well resolved LES, traditionally requires a hexahedral type meshing to keep the numerical dissipation to the minimal. However, to generate a hexahedral mesh of DNS quality for a complex flow configuration like the one under consideration poses severe restrictions. Hence, a polyhedral meshing technique is chosen to generate the final mesh. Such meshing has been extensively tested by [12] and [13] for a wide range of channel, pipe and pebble bed flow configurations. The results have shown that simulations with such unstructured polyhedral meshes are found to be in good agreement with the available high quality DNS database employing typically structured hexahedral meshes. Hence, a similar strategy is applied and again thanks to the versatile meshing techniques available in STAR-CCM+, the mesh which is shown in Figures 6 & 7 could be generated. In the near wall region a structured prism layer mesh is generated to correctly capture the high flow gradient. Special care has been taken to generate a smooth transition from the prism layer (in the near wall region) to the bulk region. The work of [11] has shown that a sudden jump in the transition region would significantly affect the numerical solution. Figures 6 & 7, display different views of the generated mesh, which contains a total of ~25 million cells. The non-dimensionalized cell sizes of this generated mesh are ($\Delta x^+_{max} = 7$, $\Delta y^+ = 0.5$-7, $\Delta z^+_{max} = 9$). These cell sizes are much finer than the estimated KLS from the RANS solution and also the latest DNS meshing guidelines [14]. Thus, the obtained mesh is much finer than current DNS guidelines. However, when such a mesh is used in STAR-CCM+ to perform a 'DNS', it should be called a q-DNS merely because of the reason that at maximum second order schemes will be used to perform the simulations. These numerical schemes were also used and tested in the study of [12] and [13], where the authors have shown that the results of such a q-DNS are in excellent agreement with the existing high quality DNS databases.

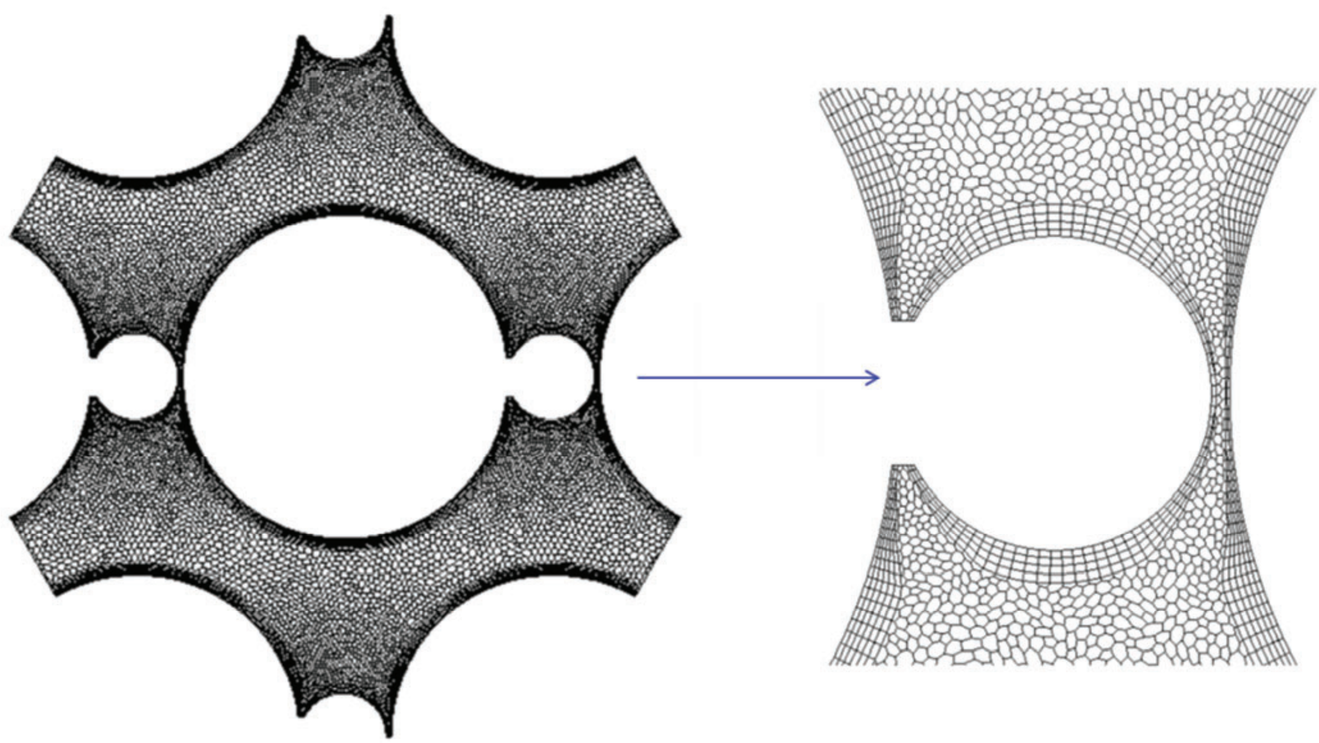

Figure 7. A zoom of polyhedral mesh at (Left) cross-section and (Right) near wire [9].

3.1.4. Preliminary Results and Discussion

The mentioned q-DNS computations are being performed by using the commercially available code STAR-CCM+. Following the work of [12] a second order central scheme with 5% boundedness (of second order upwind scheme) has been used for spatial discretization. The boundedness is introduced only when the local Normalized-Variable Diagram (NVD) value is outside the range [0,1], which means in the cells where central differencing (CD) would anyhow introduce an error. This means that in the fine grid of the DNS calculations, the boundedness introduced is in all effects negligible, as it is only rarely introduced in very few cells, i.e. less than 1%. In addition a second order implicit scheme is used for temporal discretization. The discretization is performed by using a collocated and a Rhie-and-Chow type pressure-velocity coupling combined with a SIMPLE-type algorithm. The synthetic eddy method (SEM) [15], available in STAR-CCM+, has been used to generate the initial turbulence in the computational domain. It is worth mentioning that the on-going q-DNS computations are performed for both flow and temperature fields. Therefore, a scaled heat flux of 0.15 MW/m^2 is imposed on the rod walls.

Iso-contours of instantaneous velocity and temperature fields are given in Figure 8. As expected, it is clearly noticeable that for this liquid metal flow, the thermal boundary layer is thicker than momentum boundary layer. This is evident, as the corresponding Pr numer for lead bismith is equal to 0.02. To identify the complex turbulent flow field, appearing in this flow configuration, the line integral convolution (LIC) are extracted and shown in Figure 9. The obtained solution exhibits a complex flow dominated by vortical structures, indicating a highly turbulent flow regime. Moreover, it highlights the appearance of small-scale structures throughout the computational domain. Hence, the q-criterion of the flow structures is extracted for the whole computational domain and is illustrated in Figure 10. It is evident that the flow regime exhibits an extremely complex flow, with highly three-dimensional flow structures. Nevertheless, the principle direction of the flow is dictated by the wire, which is wrapped around the main fuel rod. The small structures also highlight the fact that the generated mesh is fine enough to resolve all the Kolmogorov scales present throughout the selected computational domain.

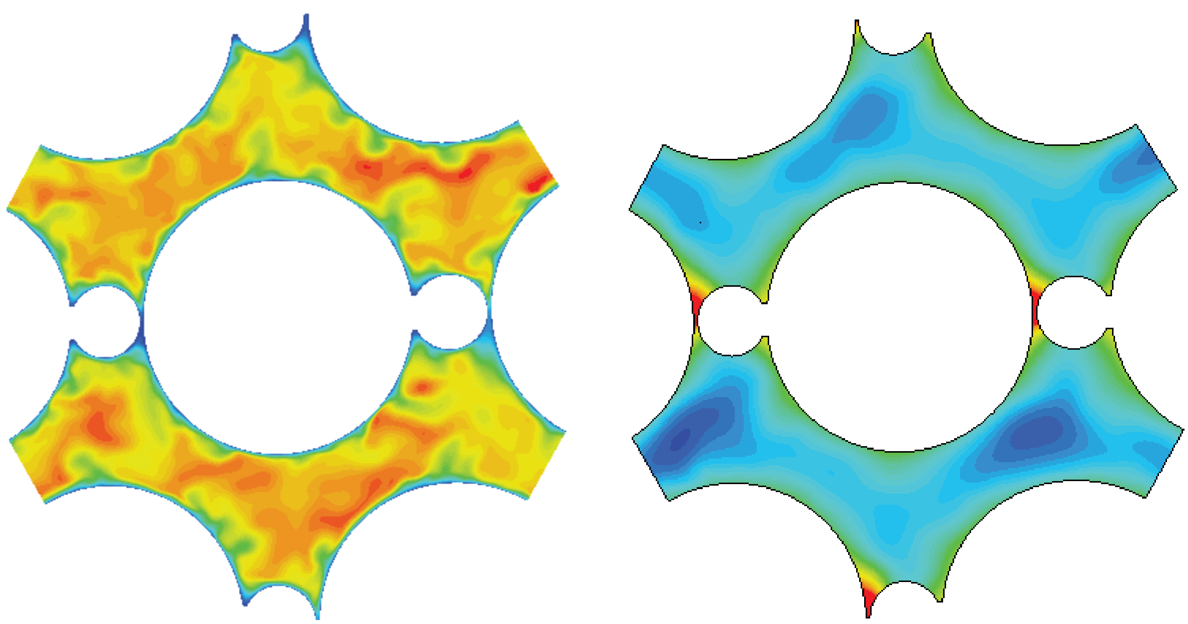

Figure 8. Iso-contours of instantaneous (Left) velocity and (Right) temperature field.

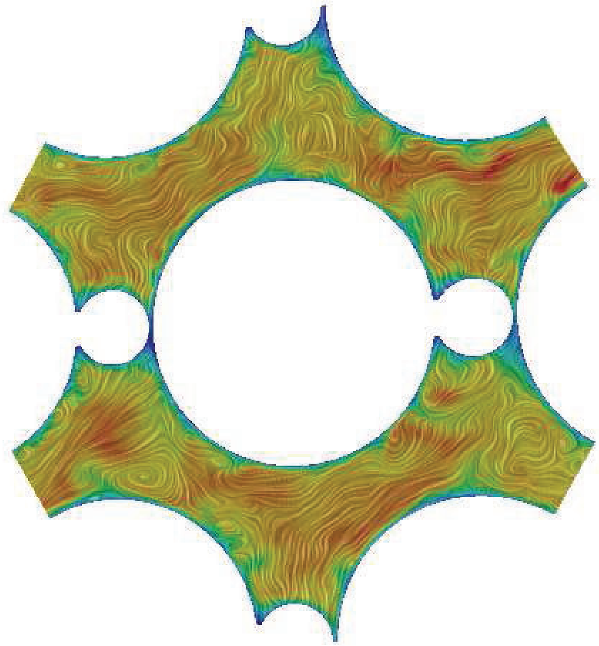

Figure 9. Iso-contours of line integral convolution.

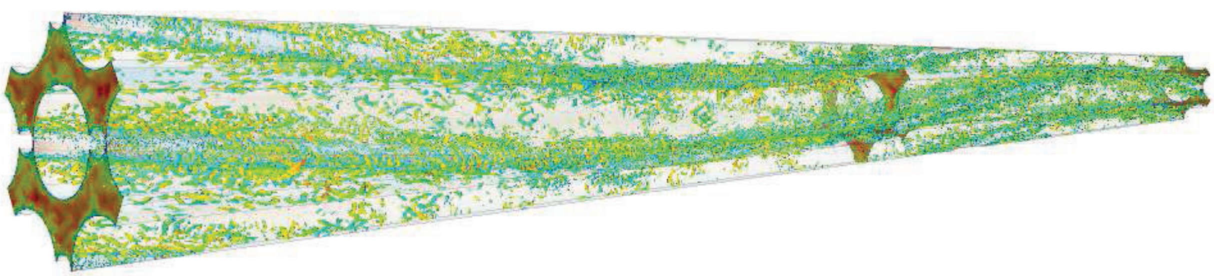

Figure 10. Iso-surface of Q-criterion coloured with velocity magnitude.

4. SUMMARY

A wide range of RANS calculations are performed to calibrate an infinite wire wrapped fuel assembly in order to perform high fidelity CFD calculations. The selection of the computational domain is performed on the present MYRRHA design and results in an infinite wire-wrapped fuel assembly. This selected computational domain is further calibrated to optimize the flow parameters and the respective boundary conditions. Special care has been taken to optimize this flow configuration in order to achieve a feasible computational challenge to perform the high fidelity simulations. Hence, scaling of the Reynolds number is carried out by ensuring that the overall flow topology remains in the turbulent flow regime. Results obtained from this RANS calibration are used to generate a meshing strategy for the final high fidelity CFD reference calculations. The generated mesh is found to be fine enough to meet the q-DNS quality. The simulations are currently running at NRG's cluster and preliminary results shown in this paper promises the awaited good quality reference q-DNS database.

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