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CALIBRATION OF A PEBBLE BED CONFIGURATION FOR DIRECT NUMERICAL SIMULATION

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Abstract

The appearance of hot spots in the pebble bed cores of High Temperature Reactors (HTR) may affect the integrity of the pebbles. A good prediction of the flow and heat transport in such a pebble bed core is a challenge for available turbulence models. Such models need to be validated in order to gain trust in the simulation of these types of flow configurations. Direct Numerical Simulation (DNS) can serve as a reference for validation, however, it poses restrictions in terms of flow parameters and numerical tools corresponding to the available computational resources. In the present study, a wide range of numerical simulations has been performed in order to calibrate a pebble bed configuration for DNS which may serve as reference for validation.

1. Introduction

High Temperature Reactors (HTR) are considered all over the world. An HTR uses helium gas as a coolant, and the moderator function is taken by carbon in the form of graphite. The fuel is embedded in the graphite moderator. This brings unequalled safety features of HTRs, basically preventing the fuel from melting. An important feature associated with the HTRs, is the high coolant temperature that can be achieved and therefore high electric efficiency. This also brings a high suitability for coupling the heat source to an industrial process requiring heat.

The core can be designed using a graphite pebble bed. Some experimental reactors have been operated over the world using this design [1]. They showed safe and efficient operation, however questions were raised about the occurrence of possible local hot spots in the pebble bed possibly affecting the pebble integrity [2]. Heat transfer around a curved surface varies noticeably for both laminar and turbulent flow regimes and the obvious appearance of the curved flow. The flow passages through the gaps between the pebbles could have concave and convex configuration and the manifestation of centrifugal forces comes into play in the form of suppression or stimulation of turbulence level [3]. In addition, pressure gradients strongly affect the boundary layers. Transition from laminar to turbulent, wake, flow separation and its respective reattachment make this flow configuration very complex. Hence a detailed evaluation of the pebble bed flow physics needs to be done.

On the experimental side, such phenomena can hardly be studied. In the recent past, few attempts have been made but quite a small amount of information is available [4]-[6]. Whereas on the CFD side, this has also become a big challenge for available turbulence models, which is of great importance in the accurate prediction of flow details [3], [7]-[17]. A number of attempts have already been made for flow around curved surfaces and pebble bed geometries by using Reynolds Averaged Navier Stokes (RANS) CFD approaches which have not been successful. This is not surprising because of the limitations imposed by the closure of these models, as explained well in [17], [18]. To gain trust in the numerical models and simulations, their validation is always an important step and needs to be done. A Large Eddy Simulation (LES) modeling approach has been reported recently for a pebble bed geometry but can't serve as a reference for validation purpose as it also includes modeling issues [3]. As a result, direct numerical simulation (DNS) which is considered as an advanced and accurate simulation technique may serve as an alternative that can be used to validate the turbulence models. However, DNS poses severe restrictions in terms of flow parameters, grid requirements and the computational domain for these types of flow configurations.

In the present study, the flow geometry (pebble stacking), boundary conditions, and mesh generation of a defined pebble bed geometry are analyzed with the help of a RANS modeling approach in to order to obtain an optimized and well defined computational domain to perform a DNS which can serve as reference. Details of flow configuration and the numerical tools which are used to perform the simulations are given in Section 2. A detailed discussion regarding calibration of the computational domain and boundary conditions are reported in Section 3 and 4, respectively. In section 5, the meshing strategy of the benchmark DNS of a pebble bed is documented along with the supporting pipe flow DNS. In the end, a short summary of these results and discussion is given.

2. Flow Configuration and Numerical Strategies

2.1 Flow Configuration

The flow configuration is a defined arrangement of spherical type pebbles. Following the specification of the PBMR-250MWth design, the diameter of a pebble is kept 6cm [5], [6]. Mimicking the real pebble bed configuration, which is random in a wide range of the reactor core, does not seem to be possible because of the limitations provided by the current experimental and numerical facilities. On the other hand, defined cubic crystal arrangements appear in the literature likewise, simple cubic, face cubic centered, body cubic centered etc [10]. In the present study, we have selected a Face Cubic Centered (FCC) configuration, as shown in Figure 1.

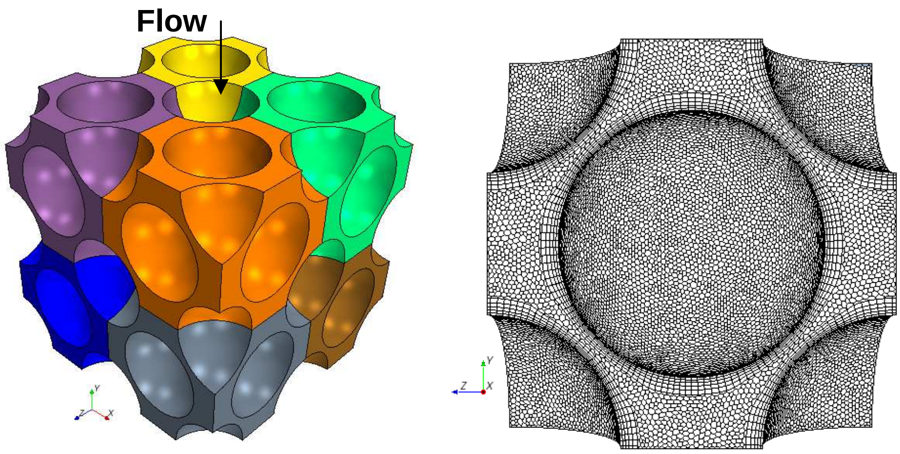

Figure 1: (Left) Isometric view of eight cubic FCC configuration (Right) Front view of single cubic FCC domain with mesh (~0.3 M, polyhedral mesh with an off-set layer).

It is important to recall here that the prime idea of this work is to perform a Direct Numerical Simulation of an arranged pebble bed geometry. In this regard, two different types of computational domains are studied here, single and eight cubic FCC configurations (see Figure 1), by performing RANS calculations in order to obtain an optimized pebble bed computational domain for a DNS study.

More explicitly, one can see from Figure 1 (left) that this eight cubic domain is composed of eight single cubic domains, shown by different colours. A single cubic domain is composed of four complete spherical pebbles in total, i.e. six half pebbles covering each face of the computational domain and eight quarter pebbles, see Figure 1 (right). In reality, there appears a point and/or area contact between the pebbles. However, this contact pebble strategy is not possible for DNS, due to the meshing issues. On the other hand, a gap between the pebbles could be possible by keeping an average porosity level close to the reality and/or experiments. Hence, a constant gap of 5mm is kept between the pebbles in order to get the porosity level near to the various experiments performed worldwide [1], [2],[4]. It is worthwhile to mention that the effects of the treatment of the contact and the gap between the adjacent pebbles have been numerically investigated by Lee et al. [12]. Their study has shown a significant difference in the flow topology for a contact and inter-pebble gap configurations.

2.2 Mesh Generation for RANS Study

Mesh generation for such a complex geometry is not an easy task and thanks to the versatile meshing technique provided in Star-CCM+ [19], it was possible to generate a full polyhedral mesh with an offset layer near the wall region in order to capture well the high gradient flow. This gives a total of around 0.3 M grid points for a RANS simulation of a single cubic domain. As mentioned earlier two different types of computational domains are considered here in order to calibrate the numerical tools to perform DNS. Hence it is important to avoid the numerical dependent error during the RANS study. As a result, a similar mesh of single cubic domain is projected for eight cubic domain and gives a total of 2.4 M grid points and is sufficient to predict the overall flow topology. It is worthwhile to mention here that, an independent grid sensitivity study (not shown here) for eight cubic domain was performed for four different mesh configurations, i.e. 0.15, 0.36, 0.71 and 2.4 M grid points. The results suggested that the selected mesh resolution (~ 2.4 M) is appropriate to reproduce overall flow topology.

2.3 Turbulence Modelling and Numerical Methods

All numerical simulations presented in this paper are performed by using the commercially available Star-CCM+ code [19]. Selection of the turbulence model is quite important for such types of complex flow, which includes flow separation, reattachment and stagnation regions. Reynolds stress models or anisotropic type models could provide a better numerical solution but pose a severe limitation due to convergence issues and reverse flow, as observed in [14]. However, in the present study we deal with the calibration of a computational domain for a DNS study and involve a wide range of RANS calculations. Therefore, anisotropic and RSM type models, being computationally quite expensive, were not considered. Hence, a standard k-epsilon model has been selected here, which has also been used by In et al. [9] and which provided reasonable numerical solutions. For all RANS simulations, a second order upwind scheme has been used. However, for the DNS, a second order central scheme with 5% boundedness in combination with second order implicit scheme for time integration is selected. For more details, see User Manual Star-CCM+ [19].

2.4 Flow Parameters

Following a real pebble bed reactor configuration, which is PBMR-250MWth in this study, Helium is considered as a working fluid. All other flow parameters are given in Table 1. By keeping the same velocity scales based on the specification given in Table 1, mass flow rates have been calibrated for single and eight cubic domain and are 0.1124 and 0.4496 kg/s, respectively. This gives the Reynolds number of 21614 based on the pebble diameter.

3. Pebble-Bed Domain Considerations

Although the increasing computing power has made the DNS of relatively moderate Reynolds number channel flows possible, the computer resources are not yet sufficient to perform DNS for a pebble bed reactor core. Nonetheless, an effort has been made here in order to find an optimized computational domain which should be well suited for the available computing resources. For this very reason, two computational domains are selected, i.e. single and eight cubic. A RANS study has been performed to check the influence of the computational domain on the flow physics. A wide range of RANS studies has been performed, and for the sake of simplicity has been given respective nomenclatures (see Table 2). Among them, the first case (CASE1) is related to the eight cubic configuration with simple inlet (mass flow rate) outlet (pressure outlet) conditions along with symmetry on four side of the computational domain.

Thermal Power	**250**	**MWth**
Core Height / Diameter	9.0 / 3.7	m
Helium Inlet / Outlet Temperature	500 / 900	°C
Total inlet mass flow rate	120	kg/s
Primary System Pressure	8.5	MPa
Number of Fuel Pebble	380,000	-
Helium gas density	5.36	kg/m^3
Helium gas Viscosity	$3.69 * 10^{-5}$	$N.s/m^2$
Helium Thermal Conductivity	0.3047	W/m.K
Helium Specific Heat	5441.6	J/kg.K

Table 1: Specification of PBMR-250MWth [6]

Test Cases	**M (kg/s)/ Q (W/m^2)**	**Domain**	**Boundary conditions**
CASE1	0.4496 / 0	8 cubic	In/out, symmetry
CASE2	0.4496 / 0	8 cubic	Periodic/symmetry
CASE3	0.4496 / 0	8 cubic	All periodic
CASE4	0.1124 / 0	1 cubic	Periodic/symmetry
CASE5	0.02248 / 0	1 cubic	Periodic
CASE6	0.01605 / 0	1 cubic	Periodic
CASE7	0.01124 / 0	1 cubic	Periodic
CASE8	0.01605 / 58220	1 cubic	Periodic
CASE9	0.01605 / 8317	1 cubic	Periodic
CASE10	DNS, $Re_\tau = 180$	Pipe	Periodic

Table 2: List of test cases performed

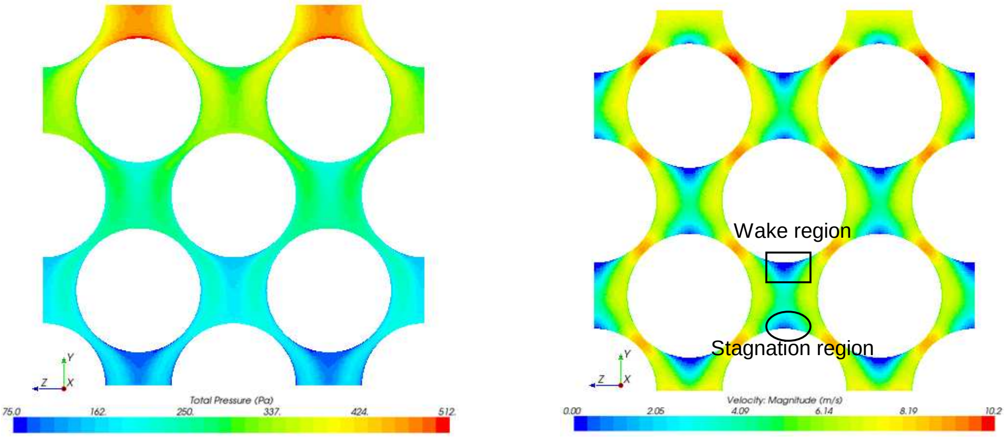

Figure 2: Iso-contours (Left) CASE1: pressure and (Right) CASE1: velocity magnitude along the cross-sectional plane at the mid of computational domain.

Figure 2, displays the iso-contours of pressure and velocity along the mid cross-section of the domain. One can notice a typical pressure drop from top to bottom along with the flow direction. By looking at Figure 2 (right), high velocity regions are noticeable in the narrow regions of 5mm between the pebbles followed by flow separation on the spherical surface of a pebble. Downstream of each pebble, a low velocity region appears which indicates a wake region. Furthermore, a relatively high velocity stream hits the pebble at the top and produces a stagnation region, shown by another low velocity region. In order to obtain an optimized computational domain, a qualitative and quantitative comparison has been made for eight (CASE2) and single cubic (CASE4) domain by using periodic boundary conditions instead of in/out flow condition. Iso-contours of velocity across the mid cross-section for CASE4 are displayed in Figure 3 (left), and show no apparent difference in flow physics in comparison with the eight cubic domain.

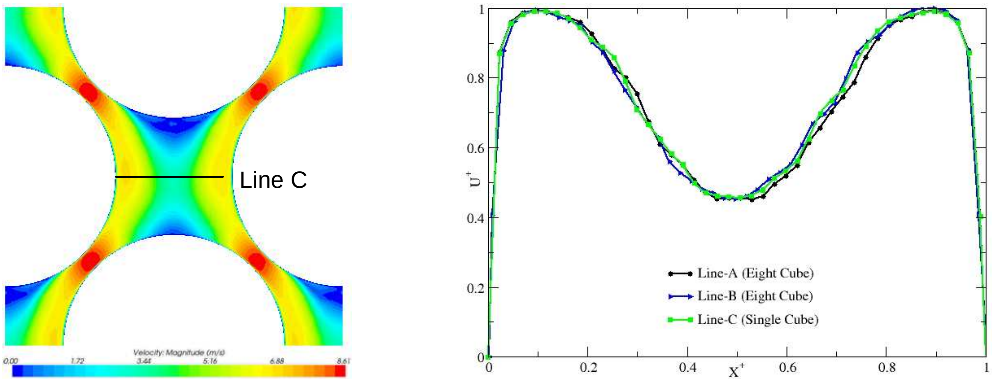

Figure 3: (Left) CASE4: Iso-contours of velocity field and (Right) CASE2, 4: comparison of velocity profiles across sub-channel for line A, B and C of CASE2 (Fig. 4) & 4 (Fig. 3), respectively.

In addition a quantitative comparison of the velocity scales has been made in the sub-channel region between the pebbles, see Figure 3 (right). Non-dimensionlized velocity profiles ($U^+=U/U_{max}$) of different sub-channel regions are compared and indicate no significant influence of the computational domain on the overall flow topology. The obtained results support the assumption of application of a single cubic domain for the performance of DNS.

4. Boundary Conditions Calibration

4.1 Periodicity for the Cross Flow

In addition to the computational domain calibration, several other parameters need to be checked and boundary conditions are among one of them. In order to sustain turbulence in DNS, it is preferred to use periodic boundary conditions via mass flow rate or pressure drop along the principle flow direction.

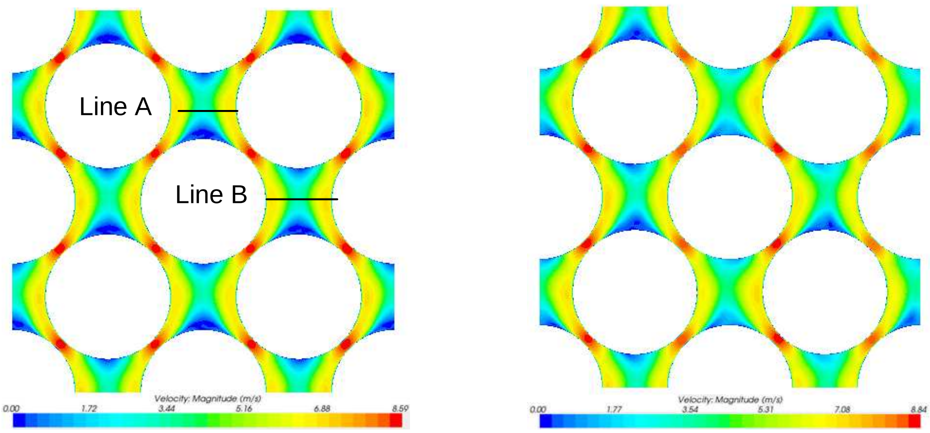

Figure 4: Iso-contours of velocity field across the mid cross section of the domain for (Left) CASE2: and (Right) CASE3.

This has been successfully performed and shown in the previous section for both single and eight cubic domains. However, this periodicity has been used in combination with symmetry on four sides of the domain, which destroys swirl flow and/or three-dimensional flow which may appear in the low velocity regions. To avoid this issue, periodic boundary conditions (CASE3) are used instead of symmetry and the obtained numerical solution is shown in Figure 4. Although the overall flow topology remains the same, a difference in the velocity scale has been observed. One may argue the prediction capability of RANS for three-dimensional effects, but even using RANS, the obtained results indicate the importance of using periodic boundary conditions over symmetry, which destroys the flow three-dimensionality.

4.2 Calibration of Mass Flow Rate

Aforementioned results based on RANS analyses indicate a single cubic domain as a feasible choice for DNS. Furthermore, to meet DNS requirements, an estimate has been made for the number of grid points, which provided an order of 73 M grid points. Considering the available computational resources and the need of long time integration for the original flow parameters make this considered DNS very expensive. To cope with this issue, again a number of RANS calculations have been performed by scaling the mass flow rate, provided that the main flow characteristics are preserved.

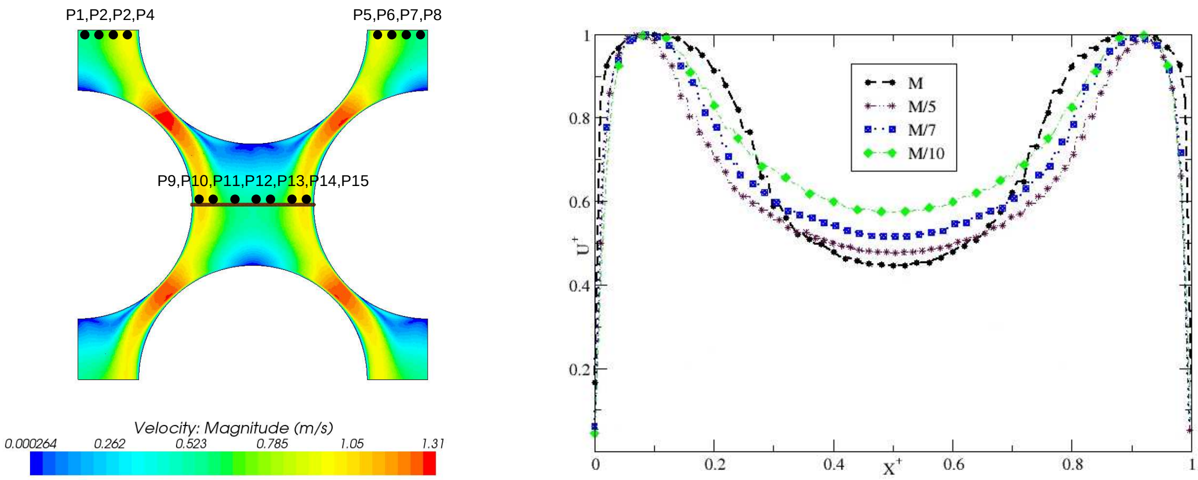

Figure 5: (Left) CASE6: Iso-contours of velocity field across the mid cross section of the domain and (Right) comparison of velocity profiles across sub-channel for different mass flow rates.

Non-dimensionalized velocity profiles in a sub-channel region for original mass flow and its scaling by 5 (CASE5), 7 (CASE6) and 10 (CASE7) times are compared in Figure 5. Results show an apparent decrease in the boundary layer thickness for the scaled mass flow rate cases. The velocity scales in the centre core region for M5 and M7 are close to M, however, this gap seems relatively big for M10 and could lead to flow laminarization. Furthermore, M7 ($1/7^{th}$ of original mass flow rate) seem to reproduce high gradients near wall region, as also shown by M5 and the original mass flow rate case. In addition, Figure 5 displays the overall flow topology produced in the case of M7, and one can clearly notice the stagnation regions and the relatively low velocity region in the centre of sub-channel region. But the important consideration which leads to the selection of the mass flow rate is related to the mesh requirements. Based on the scaled mass flow rate, i.e. M7, an estimate was made for the DNS mesh requirements which gave around 12.5 M grid points. This seems feasible keeping in mind the available computing resources. Obviously, the mesh requirements will be less challenging for the M10 case, but to avoid the possible risk of laminarization, M7 has been selected for DNS. Further discussion regarding the meshing issues for this selected DNS domain is given in detail in section 5.

4.3 Calibration of Heat Input

All the previous RANS studies and their respective discussion were focussed on iso-thermal flow analysis of pebble-bed geometry. However, the main purpose of this work is to understand the flow physics including heat transfer and to identify and understand the physics of hot spots. To this respect, the important question arises whether this heat input into this computational domain can be considered as an active or passive scalar and how the boundary conditions for an infinite pebble bed can be calibrated. In this context, the first test (CASE8) considered heat input based on the original configuration following the PBMR-250 MWth specification, i.e. heat flux (Q) per pebble = 58,220 W/m^2. Figure 6 displays the iso-contours of temperature distribution on the pebble surfaces for CASE8. The results show a wide range of temperature difference of around 172 K on a pebble surface with an average temperature of 843 K.

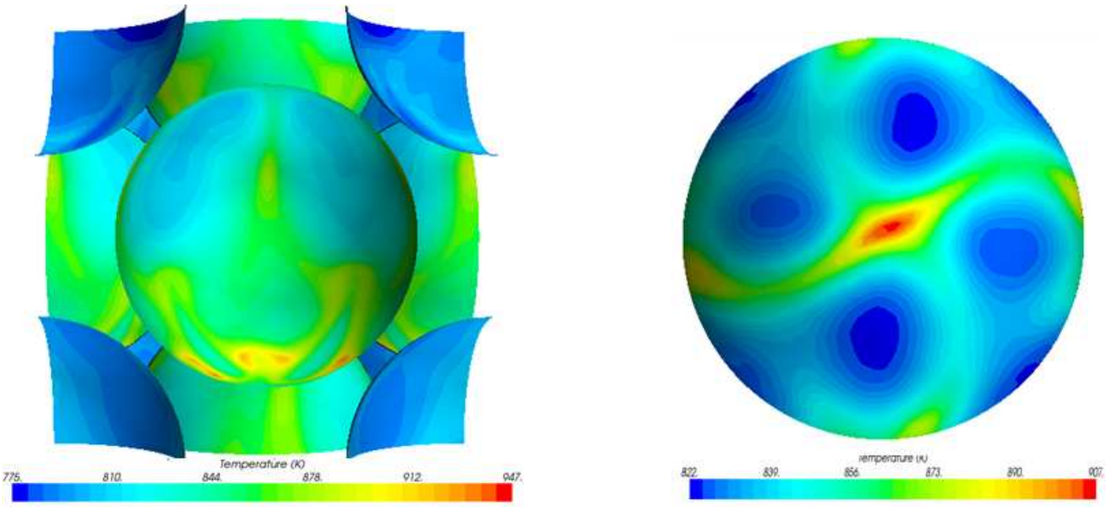

Figure 6: CASE8: Temperature distribution on (Left) all pebbles (Right) bottom half pebble with Q=58,220 W/m^2 and M7.

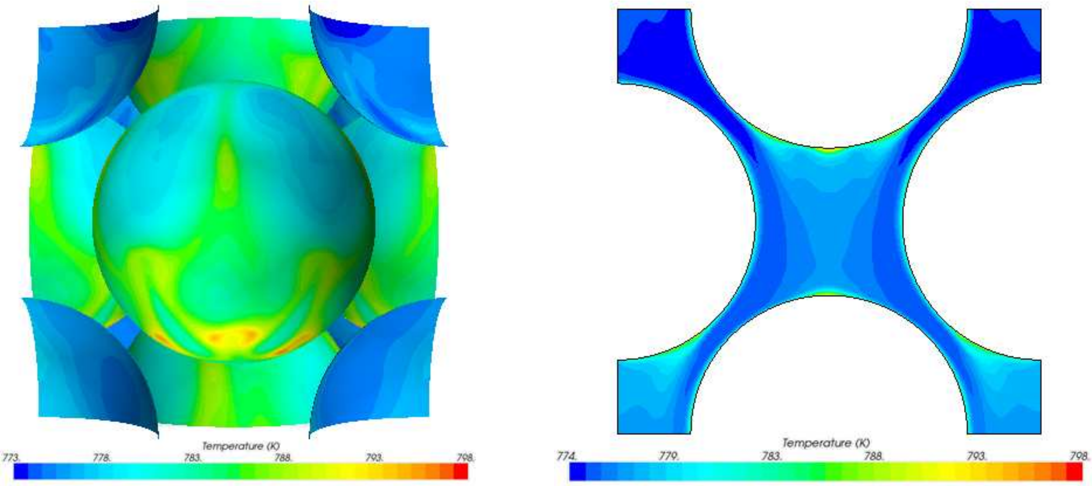

Figure 7: CASE9: Temperature distribution on (Left) all pebbles (Right) mid cross-section of the domain with Q=8,317 W/m^2 and M7.

Temperature distribution on the bottom half pebble is shown in Figure 6 (right), and seems symmetric which is expected as we have considered and arranged pebble bed distribution. A high temperature region at the centre of the pebble indicates a hot-spot, which corresponds to the stagnation region. On the contrary, low temperature distribution appears adjacent to the high velocity region. Nevertheless, this temperature distribution corresponds to the scaled mass flow-rate which may not reflect the real pebble bed reactor configuration. Hence it is decided to scale the heat input corresponding to the scaled mass flow rate, i.e. $Q_{scaled} = Q/7 = 8317\ W/m^2$. Figure 7 displays the temperature distribution along the pebbles and shows a similar temperature distribution as for original heat flux input shown in Figure 6. In addition, the overall temperature difference appearing in the domain is around 24 K, with an average pebble temperature of 783 K. As there is no big change in the properties of Helium for this temperature variation, it was concluded to consider the scaled heat input as a passive scalar.

5. Mesh Generation for DNS Study

Based on all previously mentioned RANS studies, a single cubic domain was selected in order to perform DNS. A very important issue that arises in making a setup for DNS is to generate a mesh within the DNS requirements along with the choice of numerical schemes, which allow as little as possible dissipative and dispersive error. In usual practice, a smooth or structured type mesh is preferred for a DNS study. However, this type of meshing strategy seems not possible for such a pebble bed configuration. A number of techniques regarding mesh have been tested and finally thanks to the versatile meshing capability within Star-CCM+, a polyhedral mesh along with a polyhedral off-set layer has been generated and is shown in Figure 8. This grid consists of around 13.5 M points with a dimensionless mesh size of smaller than 1 in wall normal, around 5 in azimuthal and 5-7 in the cross-sectional directions, respectively.

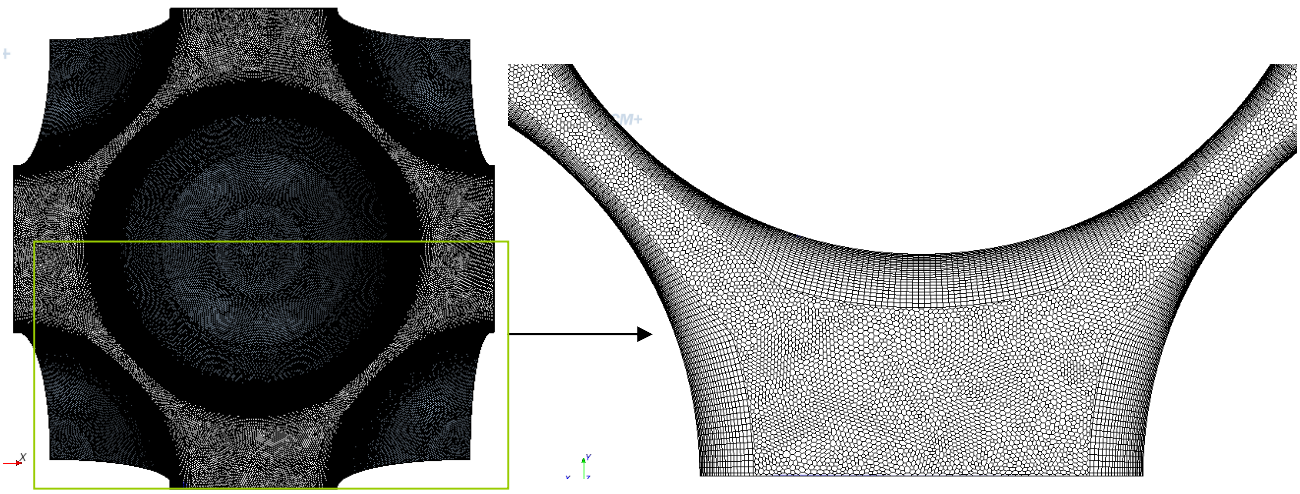

Figure 8: Polyhedral mesh with prism off-set layer for DNS (Left) front view and (Right) its zoom.

Although this mesh seems sufficiently fine to get a resolved solution, the integrity and fidelity of this type of meshing strategy in combination with the available numerical schemes in Star-CCM+ was checked. In order to check the capability of aforementioned mesh within Star-CCM+ to perform DNS, an additional DNS (CASE10) of a pipe flow at $Re_\tau=180$ has been performed. The same type of meshing strategy, i.e. polyhedral with polyhedral off-set layer (see Figure 9), has been adopted for a pipe (radius=1 m, length ~ 6 m), with a total of 3.7 M grid points and dimensionless sizes of Δr^+~0.4-11, Δz^+ ~ 7-8 and $\Delta\theta^+$ ~ 5. It is important to mention here that for DNS, a second order central scheme with 5% boundedness for space discretization has been used along with second order implicit scheme for temporal discretization.

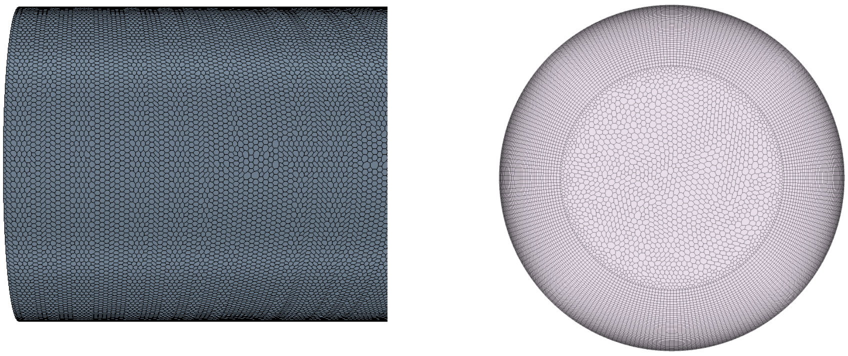

Figure 9: Polyhedral mesh of a pipe with prism off-set layer (Left) zoom of wall near inlet and (Right) inlet section.

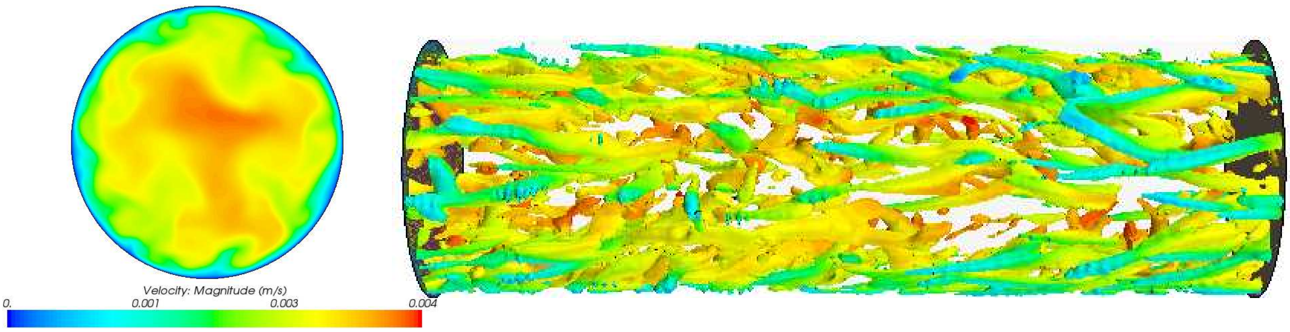

Figure 10: (Left) Iso-contours of velocity field at the mid cross-section of pipe (Right) Iso-surfaces of Q-criterion coloured with velocity magnitude.

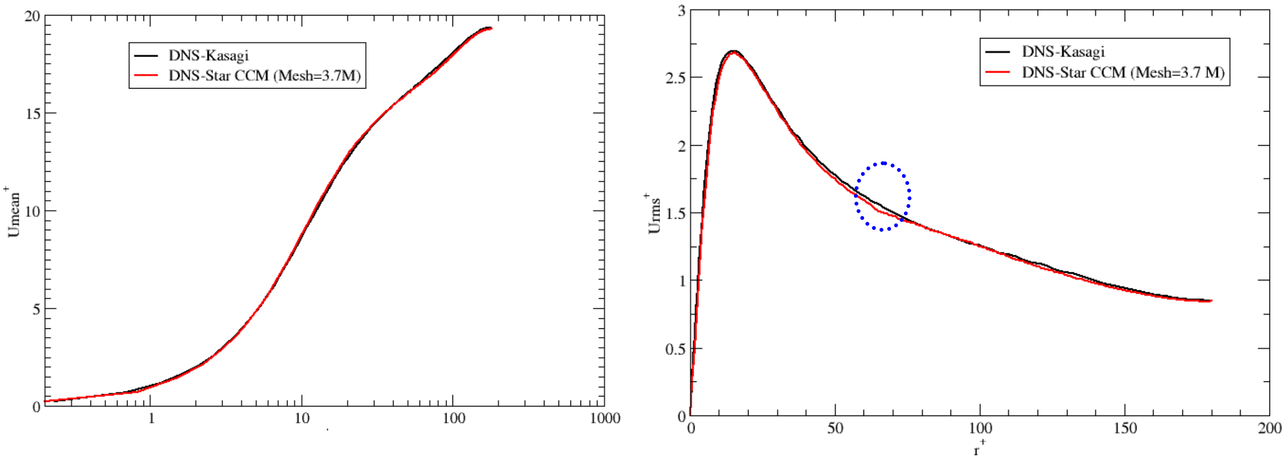

Figure 11: Evolution of (Left) velocity component and (Right) its fluctuation in the principle direction.

Figure 10 displays the velocity contours across the centre of the pipe and shows the intermittency of high and low velocity region which leads to strong mixing zone. This mixing of flow structures can be clearly observed with the help of iso-surfaces of Q-criterion coloured with velocity and also indicates the signature of hair pin vortices along the flow direction from left to right. On the quantitative basis, mean velocity profiles and their fluctuations in the principle directions are compared with Kasagi's DNS database [20] and are given in Figure 11. The obtained results from Star-CCM+ show good comparison and support the capability of mentioned numerical tools to perform DNS. In addition to this, special care has been taken to see the behaviour of flow properties near the mesh transition (polyhedral off-set to full polyhedral in the wall normal direction). One can clearly notice a slight under-prediction in the velocity fluctuations in that very region, highlighted by dotted blue circle in Figure 11. This is mainly due to the jump in the cells near that transition interface. Keeping this issue in mind, the original mesh configuration for the pebble bed DNS was revisited and further improvements to the mesh were made in order to get a smooth increase in the cell size across this transition region. As a result, a mesh was created with ~15 M grid points and improved mesh quality as shown in Figure 12.

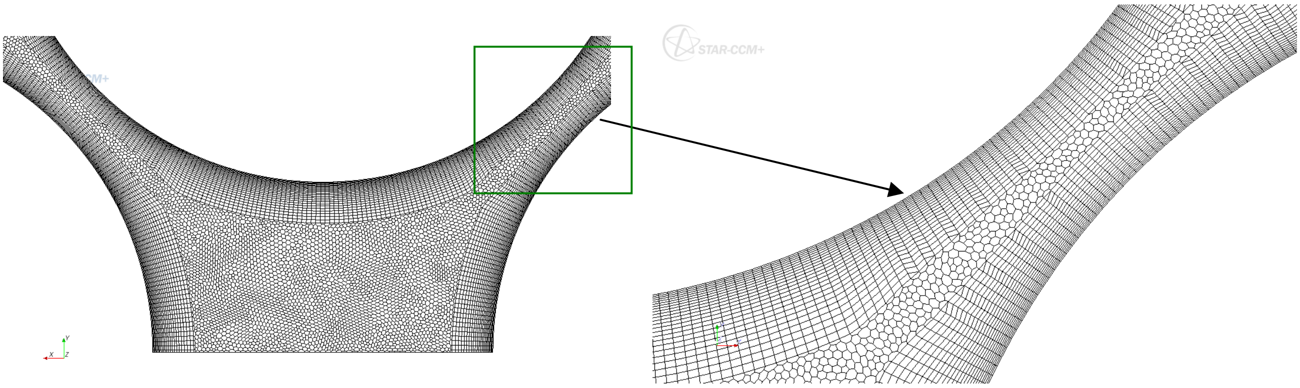

Figure 12: Polyhedral mesh for DNS (Left) zoom of front view without pebbles (Left) zoom near 5 mm gap between the pebbles.

5.1 Computational Domain Check via On-going DNS

In order to reproduce an infinite computational domain, periodic boundary conditions are used. However, the size of the domain should be long enough in order not to be influenced by inflow conditions, which may lead to a misleading solution. The best practice is to do a two point correlation analysis along the domain to check whether the domain is sufficiently large to un-correlate the influence of inflow conditions [21]. Although it might be expected from the selected single cubic domain that the flow is uncorrelated, it cannot be ruled out that the modelled gap of 5mm between the pebbles may pose a problem in this respect. Therefore, a cross correlation of the velocity signals from several probes located (see Figure 5) at the inlet of the domain and in the sub-channel region has been performed and is shown along with the wide frequency range in Figure 13. These velocity signals are obtained from the ongoing DNS for a single cube pebble geometry. Iso-surfaces of Q-criterion (coloured with velocity magnitude) through-out this single cubic domain are also given in Figure 13, which clearly indicate the appearance of small scale turbulence structures covering the entire computational domain. The aforementioned velocity signals contain around 20,000 samples with a small Δt of $5 \cdot 10^{-5}$ s and were extracted after the turbulence level through-out the domain was sustained. Two point cross-correlations of these velocity signals are computed and are shown in the Figure 13. The frequency range is given in logarithmic scale. One can notice that the value of cross-correlations is close to zero for the shown wide range of frequencies. A slight increase in the correlations for the frequency ranges < 100 Hz is observed but remains less than 0.5 which suggests a weak correlation. More importantly the high frequency range, where the value of correlation is almost zero, represents the small scale turbulence and is dominated in the whole computational domain. This justifies the fact that the selected domain has no apparent influence of inflow conditions.

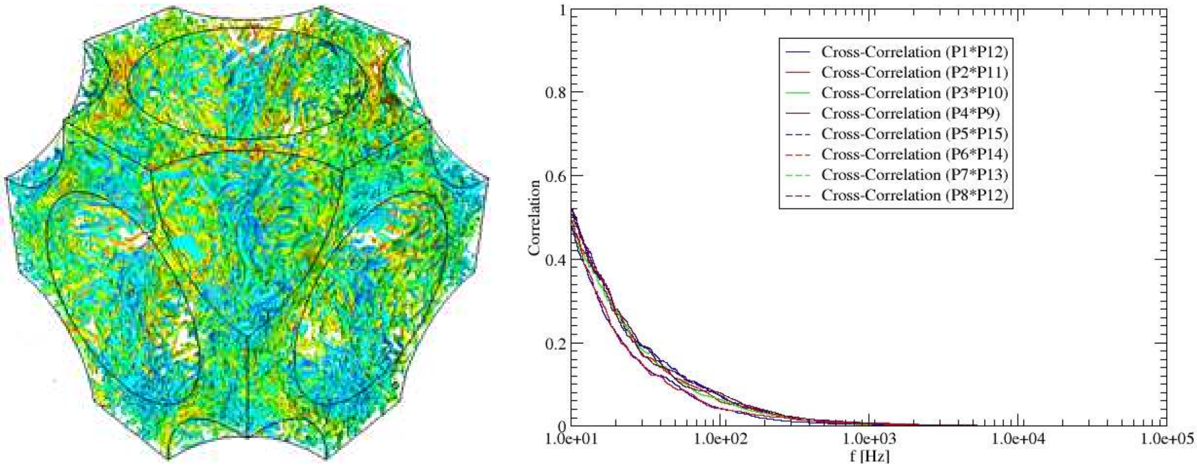

Figure 13: (Left) Iso-surfaces of Q-criterion coloured with velocity scale and (Right) evolution of two point correlation with the corresponding frequencies, see also Figure 5.

6. Summary

A wide range of RANS studies has been performed to calibrate a pebble bed configuration for DNS. Extensive comparison, on qualitative and quantitative basis, of a single and eight face cubic centered domain has been made and no apparent difference has been found in the flow topology. As a result, a single cubic domain was selected and calibrated for periodic boundary conditions to produce sustained turbulence for an infinite pebble bed domain. The size of the single cubic domain was further checked with the help of a two point correlation and was found to be sufficient to un-correlate the influence of inflow conditions. Furthermore, mass flow rate and heat flux were scaled to $1/7^{th}$ of the original flow parameters, and were successfully calibrated to obtain a mesh requirement in a feasible range of available computational resources. Finally, in order to check the fidelity and integrity of the mesh and the Star-CCM+ computational tool, a DNS of a pipe flow was performed which showed good results and supported the assumption that the planned numerical strategy is able to meet DNS requirements.

7. Acknowledgements

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