Validation Of Turbulent Models As A Key Element In The Development Of CFD Methodology For Nuclear Safety And Design Applications

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Abstract – *It is an unfortunate fact that no single turbulence model is universally accepted as being superior for all classes of problems. The choice of turbulence model depends on considerations such as the physics of the flow, the established practice for a specific class of problem, the level of accuracy required, the available computational resources, and the amount of time available for the simulation. To make the most appropriate choice of model for certain application, one needs to understand the capabilities and limitations of the various options. Therefore, the validation study presented in this paper aimed to assess the capabilities of different turbulence models for the prediction of turbulent flow and heat transfer in a tightly spaced bare rod bundle. In fact, a comprehensive CFD approach toward the accurate prediction of the turbulent flow and heat transfer in a tightly spaced rod bundles was developed. Since the experimental database was not available, the numerical experiment was performed in order to generate the high fidelity reference database by means of Direct Numerical Simulations (DNS). In the first step numerical experiment was designed, later DNS was performed. Finally, the validation of lower-order turbulent models was performed. For the validation purposes six commonly used turbulent models implemented in ANSYS Fluent software were chosen. In the validation study the turbulent flow and heat transfer profiles were compared qualitatively and quantitatively against the obtained DNS results.*

Keywords: validation, RANS, DNS, rod bundle, turbulent flow

I. Introduction

In recent years, the use of Computational Fluid Dynamics (CFD) to address issues related to nuclear reactor safety has become very popular due to its higher (temporal and spatial) resolution compared to system codes. Reactor components where inherent three-dimensional phenomena are taking place are particularly suited for these computational tools. For instance, the junction of the cold leg (CL) with the reactor pressure vessel (RPV) may be subjected to thermal stresses in pressurised thermal shock (PTS) scenarios. Accurately predicting three-dimensional (3D) flows with a sufficiently fine resolution cannot be handled by lump parameter codes, nor by system codes, which makes CFD the only option **[1]**.

Despite the enormous advances in conventional CFD (which involves single-phase turbulent flows) there are still questions about the level of accuracy of these simulations, which acquires a special relevance for licensing purposes. Although in CFD simulations, the number of parameters is much lower than that of system codes, the uncertainties associated with the mesh resolution, turbulence models, boundary conditions and numerical schemes still renders the use of these advanced tools to mere "demonstrations" in the context of Nuclear Reactor Safety (NRS) **[1]**.

A proper prediction of the flow and heat transport inside the rod bundle is a challenge for the available, pragmatic turbulence models (Reynolds-Average Navier-Stokes – RANS) and these models need to be validated and improved accordingly. Although the measurement techniques are constantly getting improved, however, the CFD-grade experiments of flow mixing and heat transfer in the subchannel scale are often impossible or quite costly to be performed. In addition, lack of experimental databases makes it impossible to validate properly and/or calibrate the available RANS turbulence models for certain flow situations. In that context, Direct Numerical Simulation (DNS) can be served as a reference for model development and verification. However, despite the advancement in the super computing, performing a DNS for a realistic rod bundle at a high Reynolds number is not foreseeable in the near future. In this regard, a research program has been set-up to generate a high quality DNS database for a rod bundle configuration Hooper's hydraulic experiment **[2-5]**.

In this paper, the comprehensive approach toward the accurate prediction of turbulent flow and heat transfer in a tightly spaced bare rod bundle configuration is thoroughly presented.

The paper is laid out as follows: Section 2 describes the general idea of the validation approach toward fuel assembly level. Section 3 briefly describes the details regarding the flow configuration and the description of the adopted hydraulic experiment configuration by Hooper **[6,7]**. In Section 4, a design of a numerical experiment for a closely-spaced bare rod bundle, in order to perform a DNS, is presented. DNS of the bare rod bundle is discussed in Section 5. In Section 6, the validation study of URANS models is outlined. This is followed by a summary in Section 7.

II. Validation approach

Nuclear fuel rods in the most of existing and future nuclear reactors are grouped into fuel assemblies, where the coolant is flowing axially through the bundles. The flow area bounded by four or three fuel tubes defines a subchannel. Two adjacent subchannels are connected by a gap between two rods (see Fig. 2). This gap spacing is defined as a pitch to rod diameter ratio (p/d). The fuel rod assembly belongs to the class of compound geometries, where flow is identified by a peculiar patterns, which are not encountered in pipes or simple channels **[8-11]**. Depending on the p/d ratio, the axial coolant flow in a bare rod bundle is characterised by strong, transverse, large-scale motions across the gaps between neighbouring fuel assemblies that enhance the mixing between flows in adjacent subchannels. An appropriate term to characterize these flow patterns is the gap vortex street **[12]**, however, sometimes they are also referred as (axial) flow pulsations. The p/d ratio is the most significant geometric parameter affecting the flow structures.

CFD tools are very powerful with a great resolution, compared to system codes. However, their usage is not so straightforward to any application. The commonly used turbulence models, despite their advantages, have been developed for canonical simple geometries such as channels or pipes. Therefore, their use for other, more complex geometries must be checked and confirmed in detail beforehand (during so call validation study). This is one of the main goal of the current study.

There are different CFD approaches (as presented in Fig. 1). The most accurate and reliable CFD method is the DNS. However, this approach is extremely computational and time demanding, very costly, not applicable to daily-base nuclear industry research. Additionally, it is worth mentioning that, DNS approach is mainly limited to low Reynolds number cases, and selected computational domains are relatively small and simple.

The second approach is so-called Large Eddy Simulation (LES), which is computationally less demanding than DNS and it enables to simulate flow at relatively larger Reynolds number and a bigger/more complex geometries. In this approach the big vortexes are directly resolved and small vortexes are modelled (thus extra assumption are implemented).

The Hybrid approach, combines the LES and RANS methods at regions where they performed the best. This approach is characterised by increased accuracy (compared to RANS results) and reduced cost (compared to LES).

The last, but the most commonly and widely used approach is RANS. This method is applicable for very complex geometries, reasonable time is needed to gain the proper results, no so computationally and time costly, very attractive to the industry applications. Although those method need to be properly validated toward the specific applications.

As a first step in a validation approach toward fuel assembly level and ultimately core level modelling, a CFD methodology needs to be developed which provides accurate predictions for heat transport and turbulent unsteady flow phenomena at sub-channel level. At sub-channel level, high fidelity CFD (like DNS) can provide reference data for RANS and LES approaches. Having reference database, pragmatic RANS models could be validated and used for modelling the turbulent flow and heat transfer at fuel assembly level. The general idea of validation approach toward fuel assembly level is presented in Fig. 1.

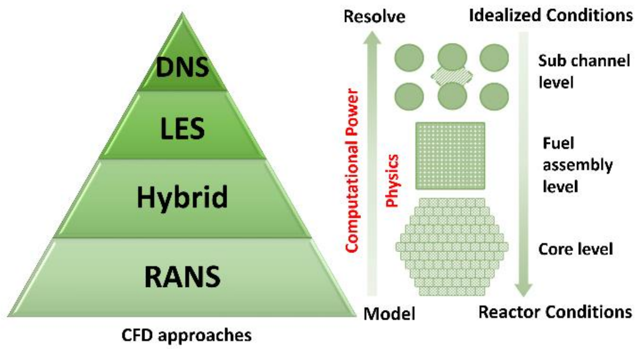

Fig. 1. Validation approach toward fuel assembly level.

III. Rod bundle case – Hooper case

Hooper's hydraulic experiment **[6,7]** is selected as a reference case. Hereafter it will be called simply Hooper case. In the experimental study a development of single phase turbulent flow through a square pitched array of rod bundles was investigated. Measurements were made for the pitch (p) to diameter (d) ratio (p/d) equal to 1.107, which indicates that rod bundle is tightly packed. The departure of the turbulent flow structure from axisymmetric pipe flow, particularly in the rod gap region, was found to depend strongly on the (p/d) ratio **[7]**.

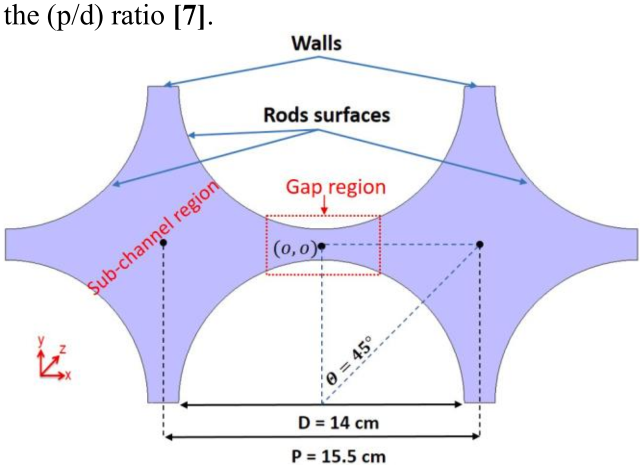

Fig. 2. Cross section of the Hooper's hydraulic experiment of a tight lattice rod bundle.

The test-section consists of six rods and its cross-section is presented in Fig 2. The rod diameter was 140 mm and the test-section length was 9.14 m, allowing 128 hydraulic diameters for flow development. Air was used as a working fluid (at normal conditions). The structural analysis of the turbulent flow were performed at Reynolds number of 49 000 corresponding to a mean axial velocity of 10.3 $\frac{m}{s}$.

IV. Design of numerical experiment

Performing a DNS of the Hooper case requires a huge amount of computational power. An initial mesh estimation of this case was performed (based on the obtained URANS results) and it would require a total of 14 billion grid points only for the flow field to perform a true DNS. Furthermore, additional constraints with respect to the simulation time-step etc. would make this DNS not feasible in the near future. Hence, a calibration of the Hooper case is performed to optimize the flow configuration in such a way that it preserves the essence of the Hooper experiment, i.e. the gap vortex street or the axial flow pulsations. Moreover, it will also allow introducing the thermal field, which was not included in the Hooper case.

In order to calibrate and optimize the Hooper case, a wide range of test cases were performed in the following three steps:

1. scaling of Reynolds number,
2. optimization of the computational domain,
3. introduction of the thermal boundary condition.

As it was already mentioned, performing a DNS of the Hooper case with original flow parameters is not feasible nor foreseeable in the near future. Thus, a scaling-down of the Reynolds number was performed in such a way that the main flow characteristics of the Hooper case were preserved and the flow field remained in the turbulent regime. Accordingly, URANS computations of ten test cases were performed by systematically decreasing the Reynolds number.

As the second step of the design procedure, the optimization of the computational domain, particularly the streamwise length of the domain, was performed. In order to do this, the axial length (L) of the computation domain was reduced to L/4, L/5 and L/6. Hence, three additional test cases were performed.

In the last step, thermal fields corresponding to different Prandtl fluids were taken into account. In this regard, thanks to the use of passive scalars, three different working fluids were selected in order to investigate the thermal behavior in the considered bare rod bundle case.

After performing the aforementioned calibration and optimization procedure, the closely-spaced bare rod bundle was finalized for the targeted DNS study. The whole calibration procedure was described in **[2,4,5]**.

V. Direct Numerical Simulations

The DNS has been carried out using the massive parallel NEK5000 code **[13]** which uses spectral element method **[14]** (SEM) to discretize the governing equations. The Gauss-Lobatto-Legendre polynomial expansion is used along each spatial direction and the same polynomial degree is adopted for the velocity and the pressure (PN-PN formulation) and as standard practice, the over-integration and filtering stabilization schemes are used **[14]**. The semi-discretized equations are then integrated in time with a third-order scheme based on the use of an implicit backward difference formula (BDF) and an explicit extrapolation scheme for the viscous and the convective terms, respectively.

As mentioned in the previous section, the Reynolds number based on the bulk velocity and the hydraulic diameter is Re = 9800, which corresponds to a friction Reynolds number Re_τ = 605. At the inlet/outlet of the computational domain, a periodic boundary condition has been imposed by means of mass flow rate. The rods are considered as no-slip walls. In total there are approximately 660 million elements of the computational mesh. A block-structured grid of macro-elements has been generated using a non-uniform wall-normal spacing in the computational domain. The spatial resolution required by the DNS simulation was estimated using Kolmogorov and Batchelor length scale predicted by Shams and Kwiatkowski **[2]** using RANS simulations. The spatial resolution in the domain ranging from a minimum of 1 (close to the wall) to the maximum of 4 in the center of the subchannel region. The obtained length scales are non-dimensionalized by using the mean friction velocity over the surface of the rod. To take into account the contribution of the polynomial refinement, the average spatial resolution is computed by assuming a uniform point distribution within each macro-element. That is, for the present case with a polynomial degree N = 7, the average spatial resolution (Δ) is obtained by dividing each macro element with eight points uniformly distributed along each spatial direction. Some of the instantaneous and mean results were presented in **[3,5]**.

VI. Validation of RANS turbulence models

As mentioned above the validation results were already published in **[5]**, however for the sake of understanding, they are recalled here. The validation study aims to assess the capabilities of different turbulence models for the prediction of turbulent flow and heat transfer in a tightly spaced bare rod bundle.

To perform the validation study, a commercial software ANSYS Fluent version R1 2022 is selected and six turbulent models are considered:

- Linear eddy viscosity models:
  - realizable $k-\varepsilon$ **[15]**, hereafter RKE
  - Shear-Stress Transport $k-\omega$ **[16]**, hereafter SST
  - Generalized $k-\omega$ **[17]**, hereafter GEKO
- Non-linear eddy viscosity models:
  - $k-\varepsilon$ based model, hereafter RG EASM
  - $k-\omega$ based model **[18]**, hereafter WJ-BSL- EARSM
- Reynolds Stress Models:
  - Stress-BSL **[19-21]**, hereafter RSM.

The Reynolds Stress Model (RSM) **[20,22]** is the most elaborate type of RANS turbulence model that ANSYS Fluent provides. Abandoning the isotropic eddy-viscosity hypothesis, the RSM closes the Reynolds-averaged Navier-Stokes equations by solving transport equations for the Reynolds stresses, together with an equation for the dissipation rate. ANSYS Fluent provides many additional options for different turbulent models, however, mainly the default options for every model have been applied in the present study. In addition for RSM and WJ-BSL-EARSM GEKO option was activated, while SST and GEKO models were run with the Corner Flow Correction option. RKE was run with Menter-Lechner Near-Wall Treatment, while RG EASM was with Enhanced Near-Wall Treatment.

It is worthwhile to mention that none of the considered turbulence models has been tuned for a particular case of a turbulent flow in a tightly spaced bare rod bundle configuration. Additionally, in the validation study a new turbulence model family called Generalize $k-\omega$ (GEKO) model with the goal of turbulence model consolidation. GEKO is a two-equation model, based on the $k-\omega$ model formulation, but with the flexibility to tune the model over a wide range of flow scenarios. The key to such a strategy is the provision of free parameters which the user can adjust for specific types of applications without a negative impact on the basic calibration of the model. In other words, instead of providing users flexibility through a multitude of different models, the current approach aims at providing one framework, using different coefficients to cover different application sectors. This approach also offers a much wider range of calibration capabilities than is currently covered by switching between existing models **[17]**. However, despite this advantage of the GEKO model, in the current study, this model was checked only with the default settings.

For the sake of comparison, two different lines are selected and are shown in Fig. 3. Line 1 (denoted as L1) is taken at the mid of the computational domain and highlights the profiles in the narrowest gap region. Whereas, Line 2 (L2) is taken in the diagonal direction to pass through the sub-channel region, where the maximum velocity field appears in the computational domain. Results obtained with different turbulence models are compared with the reference DNS results as well as among each other.

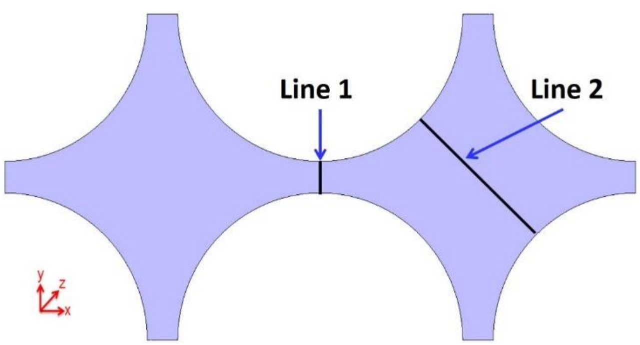

Fig. 3. Selection of the lines for the validation processing purpose.

VI.A. Wall shear stress

The proper prediction of the wall shear stress (WSS) distribution is the most crucial result for the correct prediction of a pressure drop. In bare rod bundles, wall shear stress is a non-uniform function of location with the smallest value in the gap region, and the largest value at the widest region of the sub-channel, which corresponds to the largest fluid velocity in the bulk region. Fig. 4 depicts different predictions of wall shear stress distribution along the perimeter of the bottom rod.

Clearly, all applied turbulence models usually over-predicted the wall shear stress with respect to the prediction of the DNS results. The RKE model as well as SST $k-\omega$ performed better than the other isotropic and non-isotropic models in the gap region. On the other hand, considering the sub-channel regions these models significantly over-predicted wall shear stress. The best fit in the sub-channel region was found with the WJ-BSL-EARSM model. Surprisingly, the most sophisticated model - RSM, which was tested in the validation study, did not give the best results. Those observations highlighted that for this specific application, namely flow in the tightly spaced rod bundle, there is no universal turbulence model, which could properly predict the flow behaviour in the whole domain. In general, the analysis has shown that the prediction of the wall shear stress is still the main issue for the correct reproduction of a turbulent flow in a bare rod bundle. The reason for that might be related to the fact that none of the applied turbulence models has been calibrated for this flow configuration.

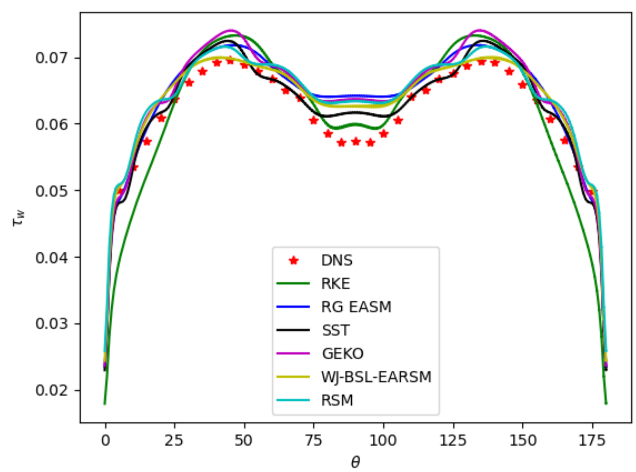

Fig. 4. Wall shear stress distribution along the rod surfaces.

VI.B. Average velocity

Fig. 5 shows a different prediction of the velocity field in the gap and sub-channel regions. The results are presented along half of the line lengths. Additionally, the length of these lines was normalized as $L^+ = L/L_{max}$, where L is the length of a certain line and L_{max} is the distance to the centers of the lines. This means $L^+ = 1$ becomes a point of line symmetry.

In the gap region (L1) all models over-predicted the velocity. The worst results along the whole length of the line L1 were obtained for the RG EASM model.

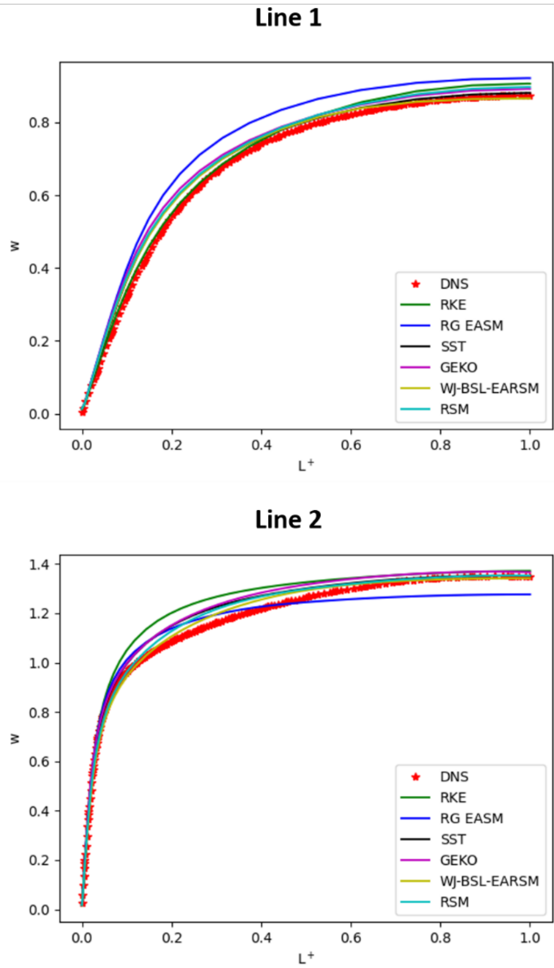

Fig. 5. Comparison of the mean velocity predicted by URANS vs DNS. Top – in the gap region. Bottom – in the sub-channel region.

This model severely overestimated the velocity in the gap region. The other models provided much better agreement. An interesting observation could be noticed, namely while moving far from the rod wall, different models are showing different responses. In the region closer to the wall ($L^+ \sim 0 - 0.3$) the best fit is obtained for the RKE model. It is worth recalling that in the validation study the realizable $k - \varepsilon$ model with the Menter-Lechner Near-Wall Treatment (NWT), adopted in the ANSYS Fluent software, was used. The Menter-Lechner NWT has been developed as an alternative formulation that is not based on the two-layer approach. It also uses a new low-Re formulation that is designed to avoid different deficiencies of existing $k - \varepsilon$ low-Re formulations. Thus, this preliminary study is showing the good potential of this approach. However, away from the rod wall ($L^+ \sim 0.5 - 1$) this model starts to deviate and in the middle of the gap is giving one of the worst agreements. While the WJ-BSL-EARSM model and SST $k - \omega$ model are giving the best fit, especially in the region close to the middle of the gap $L^+ \sim 0.8 - 1$.

In the sub-channel region (L2) all of the RANS models mostly over-predicted the velocities almost for the whole length of the line L2. RG EASM model once again deviated the most, and in turn for $L^+ > 0.4$ showed different behaviour than the other models, namely under-predicted the velocity. In turn, RSM, WJ-BSL-EARSM, and SST $k - \omega$ models for $L+ > 0.4$ gave the best agreement. These preliminary validation results evidently highlighted the need for further, more robust investigation in order to clearly define which model has the best capabilities of turbulent flow prediction in bare rod bundles. Additionally, this study is indicating that probably there is no single model which could be used in order to properly predict the flow field in the entire domain.

VI.C. Heat transfer

In the last step of the validation study presented here, the RANS models are assessed to model the turbulent heat flux. Usually, the heat transfer has been modelled assuming a simple Gradient Diffusion Hypothesis (SGDH), which has used a linear relationship between turbulent heat flux $\langle t'u'_i \rangle$ and the temperature gradient. The SGDH approach is based on the Reynolds analogy and this approach is overly simplistic and is available in all RANS-based CFD codes. Although this approach is widely used, then, it is not the best choice for predicting heat transfer, especially in liquid metal flows, as illustrated in Fig. 6-7 a).

In the present article, the results for the heat transfer of three different Prandtl fluids in combination with constant temperature boundary conditions at the walls will only be presented quantitatively.

Considering the liquid metal flow in the gap region, all the RANS models highly deviate. The presented figure indicates that for RANS models the temperature field in the gap region has almost the same value as the temperature imposed as a boundary condition on the rod walls. A similar, but not so significant trend is observed in the sub-channel region, where the temperature field is not uniform as in the gap region, which means that all the RANS models highly under-predict the temperatures.

For case with Pr = 1 presented in the Fig. 6-7 b), temperature profiles were fund in quite good agreement with the reference data. In this case the thermal and momentum boundary layer are practically equal and in fact RANS models in general are tuned for such boundary condition. For the last passive scalar, namely Pr = 2 (Fig. 6-7 c), RANS models ”loose” the prediction capabilities considering the temperature fields. It is especially visible in the gap region (L1). However, on the contrary to the case with Pr $\ll$ 1, here the RANS models over-predict the temperature fields.

These observations clearly prove that apart from the gas-cooled reactor, the usage of RANS approaches can lead to misleading results. Therefore, one should always be careful in applying the Reynolds analogy to non-unity Pr fluids, particularly to low-Pr fluids and must realize its limitations with respect to accuracy **[23,24]**.

VII. Conclusions

In the present study, a comprehensive approach toward the accurate prediction of the turbulent flow and heat transfer in a tightly spaced rod bundles is presented. The research program established for this purpose is based on three main steps, namely:

step 1 – design a numerical experiment,
step 2 – generation of a DNS database,
step 3 – validation of unsteady RANS models.

As a first step, the numerical experiment have been designed. A wide range of unsteady RANS study has been performed to calibrate and optimize the Hooper case for the targeted DNS study. This step consists of three sub-steps, i.e. (i) scaling down the Reynolds number (ii) optimizing the length of the computational domain and (iii) introducing the thermal fields.

As a second step, based on the set up configuration defined in the calibration study, the proper DNS simulation has been performed. The obtained reference database are utilized for validation purposes.

Finally, in the third step, instantaneous and mean DNS results are used to assess the prediction capabilities of different linear and non-linear RANS models. It has been found that due to a complex geometry of the rod bundle, the flow was characterized by non-uniform profiles. The validation study highlighted that no single turbulence model would universally accurately predict turbulent flow. Additionally, using RANS approaches can lead to misleading results while applying the Reynolds analogy to non-unity Pr fluids while investigating the heat transfer in tightly spaced rod bundles.

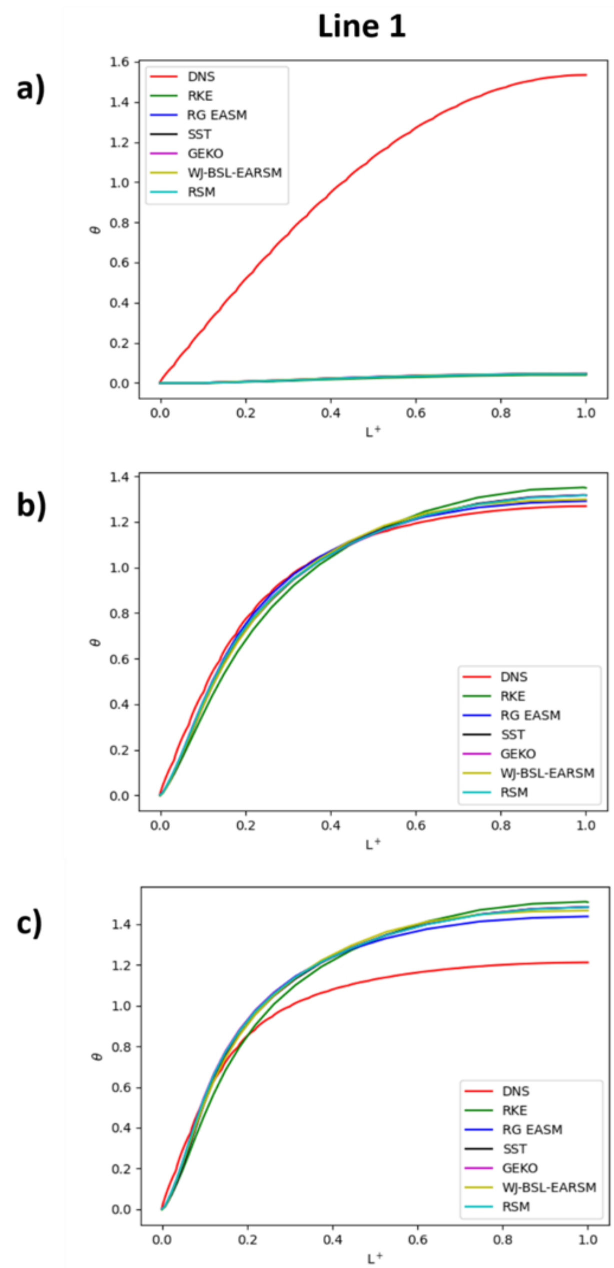

Fig. 6. Comparison of the temperature field in the gap (L1) region for: (a) liquid metal - Pr = 0.025, (b) air - Pr = 1, (c) water - Pr = 2.

Acknowledgments

The simulations presented in this paper were performed on the Świerk Computing Centre in the Department of Complex System at the National Centre for Nuclear Research, Poland. The part of work has been carried out within the framework of the

PRELUDIUM-17 project and has received funding from the National Science Center (Poland) under grant agreement No 2019/33/N/ST8/00530.

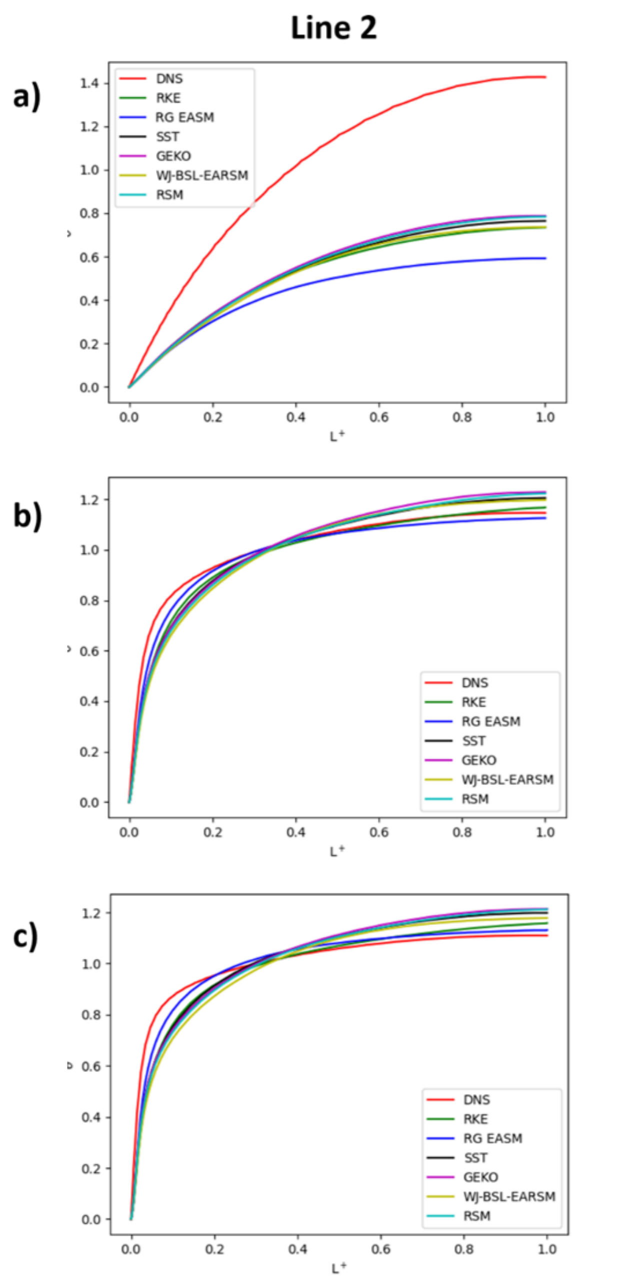

Fig. 7. Comparison of the temperature field in the sub-channel (L2) region for: (a) liquid metal - Pr = 0.025, (b) air - Pr = 1, (c) water - Pr = 2.

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