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Review of the doctoral dissertation of MSc Tomasz Kwiatkowski

„Towards the numerical prediction of flow and heat transfer in a tightly spaced rod bundle"

1. Introduction

In 2019, the European Commission published a communication on the European Green Deal, i.e. a strategy whose ambitious goal is for the EU to achieve climate neutrality by 2050. The Energy Policy of Poland until 2040 (PEP2040) sets the framework for the energy transition in Poland. It contains a strategic decision on the selection of technologies used to establish a low-emission energy system. The fifth specific objective of PEP2040 is to implement nuclear power generation in this system. This objective is combined with the strategic Polish Nuclear Power Programme. As it can be seen, this programme becomes very important in the present geopolitical situation. Therefore, any work which will help to push forward research on development of operation, safety, and efficiency of nuclear power plant and/or its components should be welcomed and supported.

There is still a limited number of research considering thermal-hydraulic aspects of whole nuclear reactor core operation, especially in Computational Fluid Dynamics (CFD) approach. The main reason for this situation comes from difficulties in handling the size of the reactor core and complexity of the transport processes. The reviewed work presents a numerical approach to the mass, momentum, and energy transfer in a flow inside of the fuel rod bundle. A good prediction of complex transfer processes occurring in such a narrow space is still a scientific challenge, especially due to a lack of reference and validation data. It should be emphasised that local transport processes determine the energy transfer in the nuclear reactor core and the safety of its operation. The Direct Numerical Simulation (DNS) database can fulfil the data gap and help to validate other methods of turbulent flow simulation. Therefore a subject of reviewed work is a part of research direction, which in the near future will be significant for the development of thermohydraulic analysis of nuclear reactor core.

2. Scope of the dissertation

The reviewed dissertation is 160 pages long and consists of Contents, List of Figures, List of Tables, Nomenclatures, PhD Candidate's contribution (list of journal articles, conference articles, other scientific publications, projects and prizes), Abstracts in English and Polish languages, 7 Chapters and References.

Chapter 1 briefly presents the most important content from the research planning point of view, which means Motivation, Thesis, and Objectives.

PhD Candidate described the issues related to the analysis of turbulent flow in the narrow fuel rod bundle and formulated the following thesis:

”The accurate prediction of turbulent flow and heat transfer phenomena inside nuclear rod bundles is very challenging for ”off-the-shelf” URANS models. Therefore this models need to be properly validated and if needed accordingly improved. This is especially important for non-unity Prandtl number (Pr) flows, particularly in the liquid metal flows.”

To confirm the thesis, the scope of the research was divided into four steps representing the objectives (general form kept as in the dissertation):

(1) to design a numerical experiment for a tight lattice bare rod bundle case using different Prandtl fluids,
(2) to generate the high fidelity database by means of Direct Numerical Simulations (DNS),
(3) to validate the pragmatic CFD turbulent models,
(4) to develop a comprehensive CFD methodology toward the accurate prediction of turbulent flow and heat transfer phenomena at sub-channel level with the set of the best practices guidelines.

This Chapter ends with an outline of the dissertation.

Chapter 2 presents a short description of turbulent flow and heat transfer in the rod bundle. PhD Candidate described the flow structure and characteristic features of flow in such geometry. He has pointed out the existence of coherent structure and generation of vortex street, and formulated one of the primary aims of the work “Development of a deep understanding of the transport by coherent structures in the core section of a nuclear reactor”.

In a subchapter, the PhD Candidate defined geometrical parameters important for conducted studies, namely P/D (pitch-to-rod diameter ratio) and also arrangement of the rods (square or triangular). He also differentiated the flow into the gap and subchanel flows. Overview of the literature that refer to the flow structure between the rods obtained experimentally and numerically could be found. The numerical part contained a description of the methods utilized in the analysis of such problems: DNS, Large Eddy Simulation (LES), Reynols Averaged Navier-Stokes in steady and unsteady approach (RANS and URANS) with examples of research results published in particular areas. At the end of this Chapter the project was presented, under which the PhD Candidate conducted his DNS investigations.

Chapter 3 contains an introduction to the RANS approach and boundary layer theory in the case of wall bounded flow. Turbulence models based on linear and nonlinear eddy viscosity hypothesis and also on the Reynolds stresses transport were presented. Then the utilized RANS turbulence models were listed. There was an information that none of the turbulence models used were adjusted to the analysed cases and that many of the options available in the commercial software (Ansys Fluent) were left as default.

Chapter 4 refers to the “design of numerical experiments for a thight lattice bare rod bundle”. In the first step, the reference case (Hooper case) was described. Then the numerical methodology was presented in following order: (1) geometry and boundary conditions, (2) solver, (3) meshing strategy. The next subchapter discusses calibration and optimization of the rod bundle process divided in three steps: (I) scaling of the Reynolds number, (II) optimization of the computational domain, and (III) introduction of the thermal field. Each step was explained in separate subchapter. On the basis of the presented contents, the Reynolds number for the analysis was selected, the computational domain and thermal boundary conditions (constant temperature and constant heat flux) were defined. The final rod bundle configuration was presented in a very short subchapter. The final part of this Chapter contains mesh estimation for DNS analysis, but it was preceded by analysis of numerical mesh for the RANS approach.

Chapter 5 summes up the DNS analysis of Hooper case, starting with description of DNS setup and the applied numerical method. Meshing strategy was described in detail and was based on the Kolmogorov and Batchelor turbulence scales. PhD Candidate presented the strategy to reduce calculation time, when changing the Courant number after achieving convergence of the flow. This consideration was followed by a determination of the statistical steady state and temporal integration of instantaneous fields of friction velocity and wall heat flux. The results exhibited lack of steadiness in the cases of constant heat flux boundary conditions, therefore further analyses were presented only for constant temperature ones. Then the procedure of temporal and spatial averaging was discussed. The final part of this Chapter presents the results of DNS analysis for the reference case, which can be divided into two groups – results referring to the velocity field, its turbulence characteristics and to the instantaneous/average temperature field.

Chapter 6 contains validation of RANS models, listed in Chapter 3. At the beginning, the numerical settings (initial and boundary conditions, solver settings) were briefly summarized. Then the PhD Candidate presented mesh sensitivity studies for one component of velocity vector and two parameters characterising turbulence: kinetic energy of turbulence and one component of Reynolds stress tensor. The results were presented in the form of comparison between the RANS and DNS approaches for various variables (wall shear stress, averaged streamwise component of velocity, turbulence kinetic energy and temperature field).

Chapter 7 presents a summary of the research. It is followed by the References Chapter, which contains a list of 100 publications.

3. Achievements

- The subject of the research and dissertation is very important not only for general mass, momentum and energy transfer in turbulent flow analysis, but also for design of the nuclear reactor core and safety systems.
- The state-of-the-art presents an analysis of past and present studies referring to the experimental and numerical contributions in the analysis of turbulent flow in narrow gaps.
- The procedure of numerical DNS experiment design was presented. Emphasis was placed on the selection of computational domain and meshing strategy. PhD Candidate presented examples of best practices helping to obtain the results in finite (shorter) time.
- The most important achievement was to conduct the DNS experiment and construct the database of DNS Hooper case. The results will be a source of valuable data for the validation of other numerical models for many future works. The turbulence characteristics can help to understand local transport phenomena in all scales. It is a significant achievement for all processes involving turbulent flow in narrow spaces and can bring great scientific development in many disciplines.

- Comparison of commonly applied RANS turbulence models and DNS results can be treated as a first step toward their validation. It is extremely important process and step, because in analysis of real systems, for example a nuclear reactor core, such models are/will be utilized. Therefore, validation with DNS results will answer the questions related to their accuracy and limitations.
- The suggestions for future works are valuable for continuation of presented research and also research conducted by other scientific groups. These suggestions can help to extend the present state, especially in the range of adaptation of RANS turbulence models.
- The dissertation was written with use of LaTeX software.

The achievements exhibit a wide approach to analysis of turbulent flow in narrow gap between rods covering RANS and DNS analysis, which opens a window for their prediction in the future. The realization of declared objectives was proved. The design of the numerical analysis, its conduction, and the discussion of the results confirmed the formulated thesis.

4. Critical comments

The comments are written in order of issue appearance in the dissertation.

- There is no definition of hydraulic diameter for the analyzed system and also Hooper reference case.
- Page 25 – The expression "Prandtl number flows" is not correct, the Prandtl number is a feature of the fluid, not the flow.
- Page 34 and Page 35 – There is no information on what kind of contribution to the field development was presented in publications 38-41, 44-53, 54-58, etc. This remark is of general meaning: state-of-the-art is not properly presented, since many of the reported aspects were not mentioned, such as geometrical parameters, flow regimes or analysed fluids. There is no information on what the difference is between the cited DNS studies and the studies undertaken by a PhD Candidate.
- Page 40 – the dimension of ε should be m^2s^{-3}.
- Page 43 – Navier-Stokes equation represents only the momentum conservation law, it should not be considered as a group of equations based also on the mass and energy conservation laws.
- Page 44, Eq. 3.15 – The α is the thermal diffusivity, not the thermal expansion coefficient.
- Page 46, Eqs. 3.24 and 3.25 – I suppose that in the first terms the gradient of mean velocity should be listed. In Eq. 3.25 The tensor notation has been changed to the vector one, which causes misunderstanding.
- Page 47 – The expression 'viscous velocity scale' probably should be 'friction velocity scale'.
- Page 47, Eq. 3.27 – The length scale should be written without the plus symbol.
- Page 47 – The y^+ it is dimensionless wall distance.
- Page 48, Fig. 6 – The meaning of red line is not mentioned.
- Page 49, Table 1 – The boundary layer regions are not listed in any order.

- Page 49, Eq. 3.32 – In the first term on the right, the kinematic viscosity should be written instead of dynamic one.
- Page 54 – Selection of RANS turbulence models and also usage of default options were not justified.
- Page 58 – 'Classical inlet-outlet boundary conditions' are not explained.
- Page 59, Eq. 4.1 – The CFL condition is presented for the 1D system but it should be in 3D.
- Page 63, Fig. 12 – The average velocity value (URANS) is compared with the measured turbulent-velocity component. In my opinion, such a comparison should not be made. The average velocity is compared with one of the velocity vector components, moreover, in different time scales.
- Page 67 – There is no information how the bulk velocity was calculated.
- Page 68 – The information about other velocity components is missed.
- Figs. 18, 19, 20 – They present the results only at line L1, the results at other lines (L2, L3) are not presented.
- Page 73, Table 4 – It presents the list of test cases considered to optimize the streamwise length, but the goal function was not defined nor the procedure of optmisation.
- Figs. 25 and 28 – The iso-contours suggest two different situations (heating and cooling). Lack of clear explanation is confusing. Moreover, usage of dimensional and dimensionless values causes misunderstanding.
- Page 79, Fig. 27 and page 81 Fig. 29 – In the caption the temperature profile should be mentioned, not a thermal boundary layer. The results at L3 are not presented.
- Page 82, Table 6 – Fluid temperature is missed.
- Page 88, Figs. 38, 39, Page 89, Figs. 40 – In some cases, the profiles of non-dimensional length scales are not reaching values 0 and 1, moreover, the parameters L, L1, L3 are not defined.
- Page 93 – In which region was the creeping flow found?
- Page 93, Eq. 5.3 – The presence of a pressure gradient in the energy equation was not justified.
- Page 110, Fig. 56 – It represents velocity fluctuation instead of mean velocity distribution. Similarly, pages 112 and Fig. 58 show the averaging of velocity fluctuation.
- Page 123 – The sentence 'Moreover, the heat transfer characteristics become very complex' is too general. There should be some explanation as to what kind of parameters from the heat transfer characteristics were in mind and what does it mean that it is complex.
- There is no information on how the value of turbulent Prandtl number (equal to 0.9) was determined?
- It would be better to consider less RANS turbulence models but with adaptation to the system.
- It would be of great benefit to show more DNS results referring to various turbulence statistics as listed in subchapter 5.4.11.

5. Comments requiring explanations

(1) When scaling the pulsatile/oscillatory flow, the Strouhal number should be taken into account. Why wasn't it considered at the stage of numerical experiment design?
(2) What was the effect of the walls closing the gap on the structure and stability of flow?
(3) Fig. 4, The PSD results for the L/5 length system exhibit different behavior at higher frequency values. How can it be explained?
(4) Fig. 10 and other referring to the mesh structure – What does happen with the flow structure in the places where orthogonality was of poor quality?
(5) Figure 11 is an example on which the nonsymmetrical flow can be observed (at least the nonsymetrical distribution of some parameter). How could the symmetrical distributions shown later be explained? Similar situation occures in Fig. 26 and further.
(6) I do not understand the comment on Fig. 26 (Page 78). Are the fluids at different temperature values? I could not directly find information about fluid temperature.
(7) PhD Candidate mentioned the intensive mass flow between the sub-channels through the gap. To visualize this mass flow, the distribution of the velocity vector field and particular velocity components should be shown. Moreover, when talking about vortex street, the vorticity distribution should be shown, especially that the PhD Candidate sometimes mentioned vortex street in the gap, sometimes on its both sides.
(8) Was the analyzed Reynolds number sufficiently high to compare the results with Kolmogorov law?
(9) The input velocity profile has a significant influence on the turbulent flow in the case of RANS approach. When various velocity profiles are used in the analysis even without conducting the computation, we can be sure that the results will be different. Were the velocity profiles, developed with the validated RANS models, compared with each other?
(10) Page 97, Fig. 46, Comparison of Kolmogorov length scales by RANS and UDNS are shown. The scale representing the UDNS results exhibits the maximum value equal to 4.8, but much higher value 11.89 is also shown in figure. Could it be explained? Could the areas of appearance of much higher value be identified?
(11) Page 99, Fig. 48, The spatial resolution for fully resolved DNS is shown. It looks like the spatial resolution for thermal calculation is above π value. How does this fact influence the results? An additional question is raised by the general view of spatial resolution distribution, on which the influence of mesh is clearly visible. Does it affect the results?
(12) Page 112, Table 8, in general the errors take a high value, especially covu and covv for all cases, but also for other quantities too. What could be the reason?
(13) Pages 127-128 – the sentence "However, once the correlation between conductivity and viscosity break down, the profile becomes much different." is not clear.
(14) Page 138, the following part requires explanation: Proper prediction of the wall shear stress (WSS) distribution is the most crucial 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 subchannel,** which corresponds to the largest fluid velocity in the bulk region.

6. Editorial comments

In my opinion, the reviewed dissertation could be prepared in a batter manner from an editorial point of view. There are numerous lingwistic, grammar, style and jargon mistakes. The main jargon expressions can be mentioned:

- turbulent kinetic energy should be turbulence kinetic energy,
  - turbulence viscosity should be turbulent viscosity,
  - thermal field should be temperature field,
  - x velocity, streamwise velocity, etc. should be x, streamwise, etc. velocity component,
  - the radial temperature should be temperature values in the radial direction or something similar,
  - Prandtl fluid! – there is no Prandtl fluid. There should be fluid of particular Prandtl number value,
  - the expression 'turbulence modellers' is not proper,
  - the following sentence "The influence of Pr number was observed, namely Pr number influencing/changing the scales of motion within the energy equation". Prandtl number cannot do anything, it only represents some fluid properties and abilities. Moreover, the part "change of scales of motion within the energy equation" is not clear at all.
- The Nomenclature section does not contain all used symbols (e.g. δm, δt) or acronyms (KLS, UDNS, EDM, etc.). Some symbols describe more than one variables (τ shear stress and time scale, λ wavelength, thermal conductivity, k turbulence kinetic energy wavelength, etc.) and also two symbols describing the same variable (λ and k wavelength).
- In general, there is no information from which publication the equations are taken from. It is important, because in the dissertation there is no consistency in used symbols and tensor or vector notations. It is a good habit to mark the source of information whether it is an equation, a formula, or any other data.
- Page 37 – The literature citation suggests that Pope is the author of both publications, but in fact he is the author of only one [61].
- Page 100, Fig. 49 – The maximal values of Kolmogorov and Batchelor time scales are 3.785 and 1.893 respectively. In the text, other values are found.
- Page 112 - The abbreviations in Table 8 are not explained.
- Page 115 – Figure 60 was not recalled in the text.
- Page 117, Fig. 62 – The legend does not agree with the description in the caption.
- Page 118 – Figures 63 and 64 have the same captions.
- Pages 122 and 123, Figs. 66 and 67 – Temperature scales are missed.
- Page 126 – There should be in Fig. 70 and in Fig. 71 instead of 72 and 73.
- Page 141, Fig. 79 – The scale is missed.
- Page 153 – Bibliographical data for position [45] is missing.

PhD Candidate should put more efforts in the dissertation preparation process, however, all the comments referring to the editorial part do not lower the presented scientific contents. They only make it difficult to follow.

7. Summary

PhD Candidate posses knowledge, competences and skills to prepare very good dissertation, but in some parts it does not represent high quality scientific publication. Therefore, many remarks were prepared to point out the shortcomings, which should be avoided in future work and publications. Besides the comments, which were formulated on a mentioned purpose, I am convinced that PhD Candidate was deeply involved in conduction of the presented numerical experiment, which required a lot of work and time. He represents a profile of mature researcher, which is able to conduct advanced investigations on his own.

The content of the dissertation exhibits the knowledge of the PhD Candidate's about turbulence as a complex phenomenon present everywhere. The approach to the numerical analysis of turbulent flows, especially in a narrow rod bundle, confirms the competencies and skills of the PhD candidate in the usage of RANS turbulence models and the commercial software Ansys Fluent and what is more important the DNS analysis and the NEK5000 code. The analysis of results demonstrates critical thinking that leads to finding problems for further studies and new research directions.

I confirm that the doctoral dissertation of MSc Tomasz Kwiatkowski meets the requirements set out in Art. 186 paragraph l point 5 (Act of 20 July 2018 - Law on Higher Education and Science) and I am applying for admission of the PhD Candidate to the next steps of the doctoral procedure.