Direct numerical simulation of turbulent flow and heat transfer in a hexagonal rod bundle

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Abstract. The aspects of numerical simulation of heat transfer in a flow along the hexagonal rod bundle are discussed in the present work. The direct numerical simulation is used to investigate the flow with Reynolds and Prandtl numbers varying in the range from 2500 to 10000 and 0.0043 to 7 correspondingly. The obtained simulation results demonstrate good agreement with available experimental data and semi-empirical correlations for the thermo-hydraulic characteristics of the channel. The empirical correlations for the Nusselt number distributions summarizing the results of the numerical simulations are proposed. The preliminary calculations have shown that the modelled time averaging interval is comparable with the initial transition time interval. This observation allows applying the approach, proposed in [7], to speed up the simulations.

1. Introduction
Heat transfer devices used in practical applications usually have a complex geometry. This fact makes almost impossible to obtain analytical solutions to predict their hydraulic and heat transfer characteristics. Rod bundle, the essential element of the nuclear reactors, is the typical example of such heat exchangers. It consists of a packed array of fuel rods, surrounded by the liquid coolant. Flow and heat structures observed in such configuration have been investigated over many years and remain an object of interest up to the present time.

Despite the intensive development of numerical methods and corresponding simulation software, a physical experiment remains the primary tool to analyze the thermo-hydraulic characteristics of rod bundles. Usually, results of the experiments are presented in the form of semi-empirical expressions, reproducing the functional dependency of the characteristics of interest on the problem parameters. Several examples of the corresponding expressions for the Prandtl numbers Pr<<1 are presented below. The correlation for the Nusselt number, valid for the range of Peclet numbers Pe<2200 and the pitch-to-diameter ratio 1.1≤χ≤1.5 was proposed in [1]:

\[
Nu = \begin{cases} 
24.151g(-8.12 + 12.76\chi - 3.65\chi^2), & Pe < 200, \\
24.151g(-8.12 + 12.756\chi - 3.65\chi^2) + \\
0.0174[1 - \exp (-6(\chi - 1))(Pe - 200)^0.9], & 200 < Pe < 2200 
\end{cases}
\]  

(1)

where Nu is the Nusselt number, non-dimensional heat transfer coefficient, defined as a ratio of convective to conductive heat transfer rates, Pe is the Peclet number, non-dimensional coefficient, which puts convective and diffusive transport phenomena in correlation, and χ is the pitch-to-diameter.
ratio, characterizing the rod geometry. The similar correlation, covering another set of experimental data for the range 150<Pe<4000 and 1.2≤χ≤2.0 was presented in [2]:

$$\text{Nu} = 0.25 + 6.2\chi + (-0.007 + 0.032\chi)\text{Pe}^{0.8-0.24\chi}.$$  \hspace{1cm} (2)

Additional correlation for Pe<4000 and 1.3≤χ≤2.0 was formulated in [3]:

$$\text{Nu} = 7.55\chi - 20\chi^{-13} + \frac{3.67}{90\chi^2}\text{Pe}^{0.56+0.19\chi}.$$  \hspace{1cm} (3)

Recently, the authors compiled in [4] several sets of experimental data and proposed the relation

$$\text{Nu} = 0.047\{1 - \exp \left[-3.8(\chi - 1)\right]\}(\text{Pe}^{0.77} + 250)$$  \hspace{1cm} (4)

as a fit for the range 1.1≤χ≤1.95 and 30<Pe<5000.

The presented semi-empirical correlations do not exhaust the list of expressions available in the literature but show the limited range of applicability for each of them. These correlations do not cover the range of low Peclet numbers (Pe~10) or provide observable deviation in the corresponding predictions. To all other, the range of low Peclet numbers is hardly achievable in the experiments due to increasing role of the sensitivity of measuring equipment. This, however, is a good example when the high-fidelity numerical methods can provide the missing data and supplement the physical experiments. The present study deals with direct numerical simulation of turbulent flow and heat transfer in a hexagonal rod bundle [5] for several liquids and liquid flow rates.

2. Computational setup

In the present paper the flow in a periodic segment of the rod bundle is investigated (figure 1). The ratio of the geometric parameters, $$\chi=S/(2R),$$ in accordance with [5] is set to 1.4. The modelling liquid is considered as Newtonian and incompressible fluid with constant properties. The flow of the corresponding liquid is described by the following system of governing equations, written in the non-dimensional form:

$$\nabla \cdot \mathbf{u} = 0,$$  \hspace{1cm} (5)

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{\text{Re}}\Delta \mathbf{u},$$  \hspace{1cm} (6)

$$\frac{\partial T_i}{\partial t} + \mathbf{u} \cdot \nabla T_i = \frac{1}{\text{Pr_i}\text{Re}}\Delta T_i,$$  \hspace{1cm} (7)

where $$p$$ is the pressure, $$T_i$$ is the temperature of i-th liquid, $$\mathbf{u}$$ is the velocity vector, Pr is the Prandtl number of i-th liquid, and $$\text{Re} = UD/\nu$$ is the Reynolds number ($$D$$ is the hydraulic diameter, $$\nu$$ is the kinematic viscosity, and $$U$$ is the bulk velocity). The corresponding calculations are performed for three Reynolds numbers 2500, 5000, and 10000, and five Prandtl numbers 0.0043, 0.0154, 0.0324, 0.71, and 7.0. With selected assumptions, heat transfer characteristics for multiple Prandtl numbers can be calculated at once, thus leading to only three different simulations with varying Reynolds numbers.

The model is supplemented with no slip boundary condition with constant heat flux on the heated walls. The periodic boundary condition with constant mass flux is preserved in the streamwise direction. The periodic conditions are also specified on the other boundaries.

The structured hexahedral grid is constructed to perform the simulations (figure 2). A grid stretching normal to the wall is used to provide the sufficient near-wall grid resolution with $$y^+<1.$$ A stretching factor normal to the wall is chosen to place several grid points into the viscous sublayer. In the third direction along the rod bundle, the homogenous grid is used. The parameters of the grids are summarized in table 1. Here, parameter $$L$$ denotes the length of the computational domain, $$N_{\text{cell}}$$ is total grid size, $$N_{\text{cyl}}$$ is the number of grid points along the cylinder arc, $$N_s$$ is the number of cells in the
longitudinal direction. The $\Delta y^+$, $\Delta \phi^+$, $\Delta z^+$ values characterize the near-wall grid step size in the directions normal to wall, along the cylinder arc and along the rod bundle correspondingly. The $\Delta z_{\text{center}}$ characterizes the maximal grid size in the center of the channel.

The range of Reynolds numbers covered in the paper includes both transient and developed turbulent flows. To model flow with the intermittency (alternation of laminar and turbulent flow region along the pipe), concerned for the lowest considered Reynolds number, the length of the computational domain is increased up to 50 hydraulic diameters.

### Table 1. Parameters of the computational models.

| Re  | $L$ | $N_{\text{cell}}$ | $\Delta y^+$ | $\Delta \phi^+$ | $\Delta z^+$ | $\Delta z_{\text{center}}$ | $N_z$ | $N_{\text{CYL}}$ |
|-----|-----|-------------------|--------------|-----------------|--------------|-----------------------------|------|----------------|
| 2500| 50  | $9.45 \times 10^6$| 0.95         | 2.02            | 3.57         | 2.02                        | 1400 | 45            |
| 5000| 20  | $11.02 \times 10^6$| 0.92         | 3.07            | 7.40         | 3.37                        | 1000 | 54            |
| 10000| 20 | $31.5 \times 10^6$| 0.95        | 4.07            | 9.05         | 4.95                        | 1500 | 75            |

3. Results

The current section presents results of preliminary investigations and validation of the simulation results with the experimental data. Despite the high impact of corresponding data in the engineering practice, the only several experiments for low Peclet numbers in the hexagonal rod geometry can be found in the literature, e.g. [5,6]. Comparison of the mean streamwise velocity profiles and profiles of the velocity pulsations with the data, presented in [6] is shown in figure 3. Results are plotted along the A-B segment, marked on figure 1. The experimental data is available in only several points and the measured and simulated data differs in the Reynolds numbers, which complicates the comparison.
However, distributions of the mean velocity and the velocity intensity generally agrees with the experimental data.

The experimental data, published in [5] includes the integral hydraulic and heat transfer characteristics, measured in the range of Reynolds numbers $10^4 - 1.3 \cdot 10^5$. Comparison of the simulation results with the series of experiments for the lowest Reynolds number is presented in table 2. The hydraulic characteristics (friction factor coefficient) demonstrate about 10% variation and the Nusselt number for the liquid with Pr=$0.0324$ shows 4% error.

![Figure 3. Comparison of the numerical results with the experimental data [6]. Left - mean velocity profiles, right - velocity intensity profiles.](image)

### Table 2. Comparison of the simulation results with the experimental data [5].

|            | Re  | FF   | Nu  |
|------------|-----|------|-----|
| Simulation | 10000 | 0.0342 | 14.51 |
| Experiment| 10200 | 0.031  | 14  |

It should be noted the semi-empirical correlations (1)-(4) underpredict the Nusselt number for the chosen model parameters. The observed variation of the experimental data with the empirical model predictions is within 9-32%. Thus, it can be concluded the results of DNS provided better correlation with the experimental data compared the widely used semi-empirical correlations.

The normalized instantaneous distributions of the streamwise velocity (figure 4), $u^* = u/U_{\text{max}}$, where $U_{\text{max}}$ is the maximum velocity value, illustrate the evolution of the spatial scales of the vortex structures with increasing the Reynolds number. It can be seen that for the lower Reynolds number the large scale vortices dominate in the flow and the flow is close to the laminar regime. For the higher Reynolds number, the scale of the vortices decreases, and the developed turbulent flow is observed.

The normalized temperature distributions, presented in the form

$$T_{i}^* = \frac{(T_i - T_{\text{imin}})}{(T_{\text{imax}} - T_{\text{imin}})}$$

where $T_{\text{imax}}$ - the maximum value of a temperature of $i$-th liquid, $T_{\text{imin}}$ - the minimum value of a temperature of $i$-th liquid, allow to compare the correlation of velocity pulsations with the corresponding pulsations of temperature fields. Indices follow the increase of Prandtl number: 0.0043 ($i=1$), 0.0154 ($i=2$), 0.0324 ($i=3$), 0.71 ($i=4$), and 7.0 ($i=5$).

The temperature distributions vary dramatically with increasing the liquid’s Prandtl number. The distributions for the low Prandtl numbers demonstrate weak sensibility to the flow perturbations: the dominating conductive heat transfer mechanism smooths out perturbations occurring as a result of convective transport. The growth of the Prandtl number increases the role of convective heat transfer. For the Pr=$0.7$ the thermal structures generally reproduce the scales of the flow structures. The further
increase in the Prandtl number decreases the scale of the thermal structures and strengthens the role of the convective heat transfer mechanism.

The averaged integral characteristics including the friction factor coefficients and the Nusselt numbers for all performed simulations are summarized in table 3. The presented results clearly show the difference for the heat transfer processes in the liquids with low and high Prandtl numbers: the fourfold increase of the Reynolds for the Pr≈0.01 leads to only 7% growth of the Nusselt number, while the same situation for the liquid with Pr≈10 leads to a fivefold heat exchange intensification. The presented results are compared with the ones predicted by the semi-empirical expressions (1)-(4). In the range of applicability of these correlations, i.e. Pr << 1, the variation of the results of numerical simulations and the corresponding predictions is within 20%. The use of these formulas for the higher range of Pr numbers, expectedly, leads to significant growth of the prediction error. Using the obtained numerical results, the following approximation can be suggested:

$$\text{Nu} = -3.55 + 0.081 \cdot \text{Pr}^{(-0.88+0.164 \cdot \text{Re}^{0.157})} \cdot \text{Re}^{(0.21+0.47 \cdot \text{Pr}^{0.114})}$$  \hspace{1cm} (9)

In the considered range of parameters, the present correlation allows to predict the Nusselt numbers within 11%.

![Figure 4. Normalized instantaneous streamwise velocity and temperature distributions in the channel cross-section. Left – Re=2500; right – Re=10000.](image)

### Table 3. Integral hydraulic and thermal characteristics obtained with help of numerical simulation.

| Re  | FF   | Pr₁  | Pr₂  | Pr₃  | Pr₄  | Pr₅  | Nu  |
|-----|------|------|------|------|------|------|-----|
| 2500| 0.0492| 12.5 | 12.5 | 12.6 | 13.1 | 18.0 |
| 5000| 0.0399| 13.2 | 13.2 | 13.4 | 21.3 | 42.9 |
| 10000| 0.0342| 13.6 | 13.8 | 14.5 | 36.5 | 88.1 |

The presented above characteristics of turbulent flows are obtained as a result of averaging in time together with spatial averaging in the homogeneous directions. The need to perform the statistical averaging of the thermal characteristics significantly increases the corresponding time averaging
interval. This aspect further increases the computational costs to perform these simulations, and the corresponding simulations take several days using tens of compute nodes.

The preliminary calculations have shown that despite the symmetry in the computational domain, the modelled time averaging interval, $T_A$, is comparable with the initial transition time interval, $T_T$, and the ratio of the intervals, $\beta = T_A/T_T$, varies in the range 1.7-12.3. This observation allows to apply the approach, proposed in [7], to speed up the simulations. The corresponding approach is based on the idea of simultaneous modelling of multiple uncorrelated turbulent flow states and combining of averaging in time together with ensemble averaging. The present problem formulation is planned to be used for further efficiency investigation of the proposed approach in the scientific and engineering applications.

4. Conclusion
Comparison of numerical results obtained from DNS for the turbulent flow in a hexagonal rod bundle for a variation of the Reynolds numbers (2500, 5000, and 10000) and Prandtl numbers (0.0043, 0.0154, 0.0324, 0.71, and 7.0) with the experimental data and semi-empirical correlations shows, that the DNS approach is capable for predicting of thermo-hydraulic characteristics of such channels. The difference for the heat transfer process in the liquids with low and high Prandtl numbers is indicated: the fourfold increase of the Reynolds for the Pr~0.01 leads to only 7% growth of the Nusselt number, while the same situation for the liquid with Pr~10 leads to a fivefold heat exchange intensification. This fact is a result of switching the dominating heat transfer mechanism and increasing the role of convective heat transfer.

The presented simulations are characterized by long time integration intervals to obtain reliable turbulent statistics, and the averaging time interval dominates over the initial transition interval performed to obtain statistically steady turbulent flow. This observation allows to apply the approach based on the idea of simultaneous modelling of multiple uncorrelated turbulent flow states and combining of averaging in time together with ensemble averaging.

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