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# Comparison between DNS and RANS approaches for liquid metal flows around a square rod bundle

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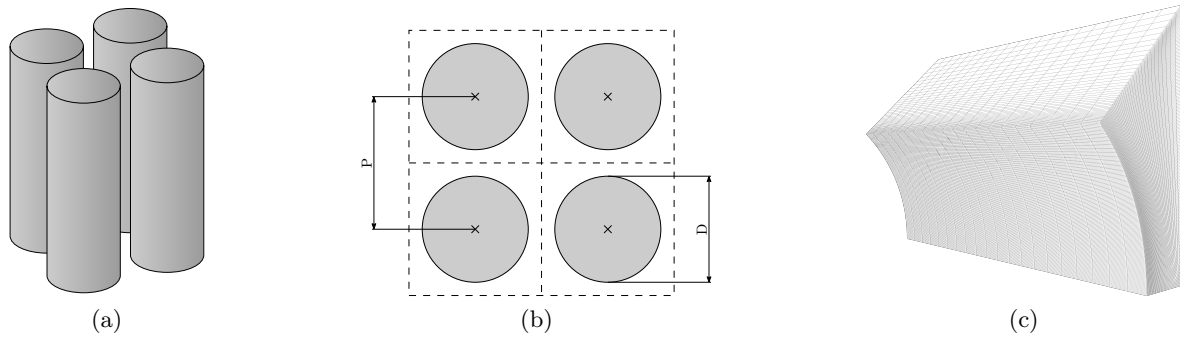
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**Abstract.** The thermal-hydraulic characteristics of liquid metal flows around rod bundles are of great interest for the research and design of fourth generation nuclear reactors. Currently, a large research effort is aimed at the development of accurate numerical models for low Prandtl number fluid flows, since the data available in the literature are quite scarce. Direct Numerical Simulation (DNS) is undoubtedly the most accurate approach, but its large requirements of computational resources and time make it less practical than other simplified methods such as the Reynolds-Average Navier Stokes (RANS) approach. The present paper provides a comparison between numerical results of a flow of liquid Lead-Bismuth Eutectic (LBE) at  $Pr=0.031$  around four vertical cylindrical rods arranged in a square lattice, obtained by DNS and RANS. Several turbulence models are considered, including the standard  $k-\varepsilon$ ,  $k-\omega$  SST, and two Reynolds stress models, namely the ones by Launder, Reece and Rodi (LRR), and Speziale, Sarkar and Gatski (SSG). The accuracy of these models is assessed by comparing the mean Nusselt number, the pressure drop, and local field distributions with those obtained by DNS.

## 1. Introduction

One of the ongoing engineering challenges in the design of IV generation nuclear power plants is the correct representation of the thermo-hydraulic behaviour of the reactor, essential to achieve high levels of safety. These reactors are distinguished by the need for greater efficiency in the use of uranium. This has led to a review of the use of common cooling liquids for nuclear cores, such as water or gas, in favour of liquid metals. Therefore, there is a growing interest in understanding the flow behaviour under both operational and accidental conditions. To achieve this aim, it is necessary to carry out and discuss the validation of turbulent heat transfer models for fluids with low Prandtl numbers. This paper discusses the initial phase of a broader study that compares the performance of various turbulence models dealing with such peculiar features. The reference database consists of some DNSs previously performed and analysed [1]. Despite the availability of high fidelity data, and the ongoing considerable efforts to develop and validate increasingly sophisticated approaches for turbulent heat transfer modeling, it is nevertheless useful to continuously assess whether models which are readily available in widespread CFD packages are able to provide reliable results. After a brief introduction to the numerical method adopted, the results section presents the data obtained by the RANS approach, comparing different turbulence models.





**Figure 1.** (a) 3D view. (b) Cross-sectional sketch. (c) 3D view of the computational mesh of one eighth of the fluid domain related to a single rod bundle.

## 2. Problem Statement

Angeli et al. [1] recently performed Direct Numerical Simulations of flow around a periodic module of 4 cylindrical rods. The rods are arranged in a square lattice, as shown in figure 1a. The rod diameter is denoted as  $D$ , while the centers are spaced by pitch  $P$ , see figure 1b. The pitch-to-diameter-ratio is fixed at  $P/D = 1.25$ . Each bar is treated as uniformly heated by a constant heat flux and the flow is considered as fully developed. Periodic conditions enforced on the velocity field and the modified pressure field  $p_m$  well delineate the physical situation. Furthermore, the temperature field needs to be normalized so that periodic boundary conditions can be set on a modified temperature-like variable  $\theta$  [2]. The chosen fluid Prandtl number is  $Pr = 0.031$  to emulate lead-bismuth eutectic, a common coolant in liquid metal cooled nuclear reactors. In the forced convection simulations, which we reproduce in this work, a friction Reynolds number of  $Re_\tau = 180$  is set.

## 3. Numerical methods

### 3.1. Direct Numerical Simulation

The reference data set is obtained through a previous analysis by means of Direct Numerical Simulation for both forced and mixed convection [1]. The solution of the differential equations relies on a Finite Volume implementation of a second order Projection Method. A second-order accurate scheme is used for the time-advancement and the spatial derivatives are implemented with a second-order accurate scheme [3] on Cartesian grids. The modeling of arbitrarily irregular cylindrical boundaries is achieved by using an original scheme developed by [4], extended to convective problems by [3]. The computational domain size is  $2.5D_h \times 2.5D_h \times 2\pi D_h$ , where  $D_h$  is the hydraulic diameter. The number of control volumes along the three directions is  $512 \times 512 \times 256$ . The grid is non-uniform on the transverse  $x - y$  plane, while a constant spacing is preferred for the streamwise direction.

### 3.2. Reynolds-Average Navier Stokes

Mean flow and temperature fields are also obtained by numerically solving the RANS equations:

$$\begin{cases} \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = \frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_i \partial x_j} - \frac{\partial \bar{r}_{ij}}{\partial x_j} + \sigma \\ \frac{\partial \bar{u}_i}{\partial x_i} = 0 \\ \frac{\partial \bar{u}_i h}{\partial x_i} + \frac{\partial \bar{u}_i |\bar{u}|^2}{2 \partial x_i} = \alpha_e \frac{\partial^2 h}{\partial x_i \partial x_j} + \frac{1}{\rho} \frac{\partial \bar{\tau}_{ij} \bar{u}_j}{\partial x_i} + \psi \end{cases} \quad (1)$$

In equation (1)  $\sigma$  is an external momentum source term that is introduced to achieve the desired flow rate through the domain. The governing equations are closed by means of several turbulence models, with the aim of comparing results. The Spalart-Allmaras [5], standard  $k-\varepsilon$  [6], and  $k-\omega$  SST [7] are considered among the eddy viscosity models. In addition, two full Reynolds stress models are used namely the Launder, Reece and Rodi (LRR) [8] and the Speziale, Sarkar and Gatski (SSG) [9]. The problem is expressed in dimensionless form by scaling the model by the diameter of the bundles. The reference bulk velocity is assumed to match that of the reference DNS, while the fluid density and thermal conductivity are set unitary, leading to the classic dimensionless forms of kinematic viscosity and specific heat:

$$\mu^* = \nu^* = \frac{1}{\text{Re}}, \quad c_p^* = \text{Re Pr}. \quad (2)$$

where Re is the Reynolds bulk number, set to match the DNS value ( $\text{Re} = 1785$ ). Periodic boundary conditions are applied at the inlet and outlet sections to achieve a fully developed flow solution. At the bundle walls no-slip conditions are enforced, and an entering heat flux is imposed. An incompressible flow solver based on the Finite Volume method, and implemented in the OpenFOAM computational toolkit [10], is used to numerically solve flow governing equations. The pressure-velocity coupling is addressed by a variant of the SIMPLE algorithm. Second-order upwind schemes are employed for advective terms, while central schemes with explicit non-orthogonality correction are used for the discretization of diffusive terms. The computational domain is reduced down to one eighth of the fluid region related to a single rod bundle, by exploiting all the possible symmetries in the geometry and mean flow; furthermore, it is discretized by means of a smoothed structured mesh which is shown in figure 1c.

### 3.3. Mesh sensitivity analysis

A mesh sensitivity study is performed, with the aim of assessing the variation of global results with varying grid size. To this end, three computational grids featuring the same topology. In table 1 the values of Nusselt number and mean dimensionless wall distance resulting from the three computational grids. Nu shows a convergent behaviour with respect to the mesh resolution, in addition, the small deviation found between the medium and fine values demonstrates that the medium mesh is of adequate resolution, thus is selected for all the numerical analyses. The fine mesh is excluded because the Nusselt number obtained differs very little from the value for the base mesh, but is more computationally intensive.

## 4. Results

Hereafter there is a selection of the outcomes obtained from the statistical analysis of the DNS compared to those of the RANS. Firstly, the contour for the average streamwise velocity field is shown in figure 2: on the left the results from the DNS show a higher value of the field at the center of the channel and it decreases moving to the subchannels. Among all the turbulence

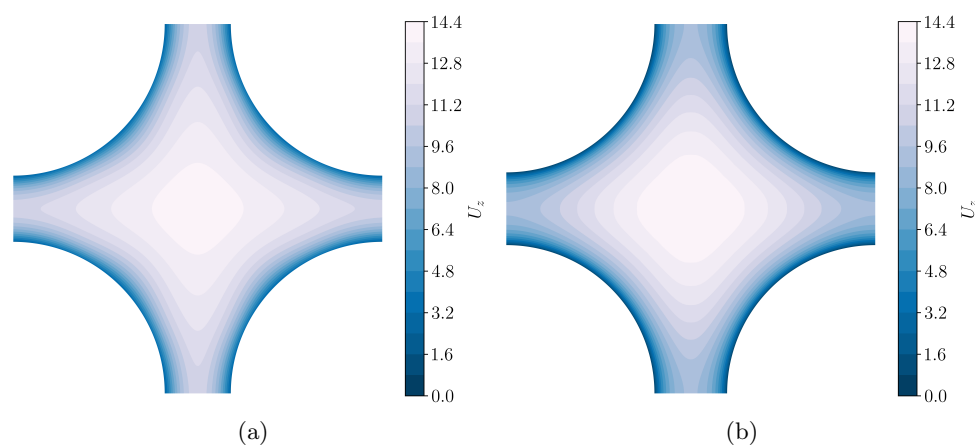
**Table 1.** Nusselt number and mean dimensionless wall distance values obtained from the coarse, medium, and fine computational meshes.

| Grid   | $\Delta^*$ | $\bar{y}^+$ | Nu    | Difference to previous grid |
|--------|------------|-------------|-------|-----------------------------|
| Coarse | 0.054      | 0.45        | 8.851 | -                           |
| Base   | 0.0041     | 0.23        | 8.880 | 0.335%                      |
| Fine   | 0.0028     | 0.12        | 8.882 | 0.007%                      |

models tested, almost the same trend is achieved with the LRR turbulence model (see figure 2b). In order to get an overview of the behaviour of all the turbulence models tested, the profiles in the narrow and large gap for the mean streamwise velocity  $U_z$  are displayed: again the model that most fits the reference data set is the Reynolds stress model LRR. It is worth noting the behaviour of the alternative Reynolds stress model tested (SSG), which confirms how well this type of models approximates the velocity field under consideration compared to eddy viscosity models,  $k-\varepsilon$  and  $k-\omega$  SST, which appear less accurate.

Continuing the discussion on velocity statistics, the behaviour of the turbulent kinetic energy is of interest: the evolution in the narrow and large gap is reported in figure 4. In general the behaviour of the RANS is consistent with the reference data as demonstrated by the lower value of  $\bar{k}$  observed in the narrow gap in figure 4a and its increase looking in the large gap in figure 4b. Some models are clearly more accurate than others and the eddy viscosity models seem to be more similar to the expected values: in particular in center of the narrow gap the  $k-\varepsilon$  model is highly accurate and also the  $k-\omega$  model exhibits comparable accuracy in the larger gap, with not only the numerical value but also the overall trend showing remarkable similarity. The Reynolds stress models are quite inaccurate in calculating the value of  $k$ , although they provide a good approximation for the  $\overline{u'_i u'_j}$  values of the Reynolds stress tensor in the presence of anisotropies [11]. It is worth noting, however, that since this is a case characterised by a low Reynolds number ( $Re = 1785$ ), the regime is weakly turbulent: this inevitably leads to greater complications for RANS models, especially if considering what happens in the narrow gap where the flow is almost laminar, and, as a consequence, some models demonstrate inaccuracies in assessing the turbulent kinetic energy. However, the study of this aspect requires more detailed investigation, which will be the subject of future studies.

Considering the thermo-hydraulic relevance of this application, it is valuable to examine the temperature field and some integral parameters. In figure 5 the results for  $\overline{\theta_w - \theta}$  are showed, where  $\theta_w$  is the value of  $\theta$  at the wall: in contrast to previous observations on the velocity field, all models describe the temperature profile quite well all over the domain, although in the large gap the models that come closest to the DNS solution are the eddy viscosity models, especially the Spalart-Allmaras one-equation model. It is worth noting that in the eddy viscosity models employed a constant turbulent Prandtl number  $Pr_t = 2.5$  has been set, according to the results of previous DNS analysis [12], which could explain the higher accuracy of the Spalart-Allmaras model. This outcome is reflected by the Nusselt number values reported in table 2: the value



**Figure 2.** (a) DNS average streamwise velocity field , (b) RANS streamwise velocity field - LRR model.

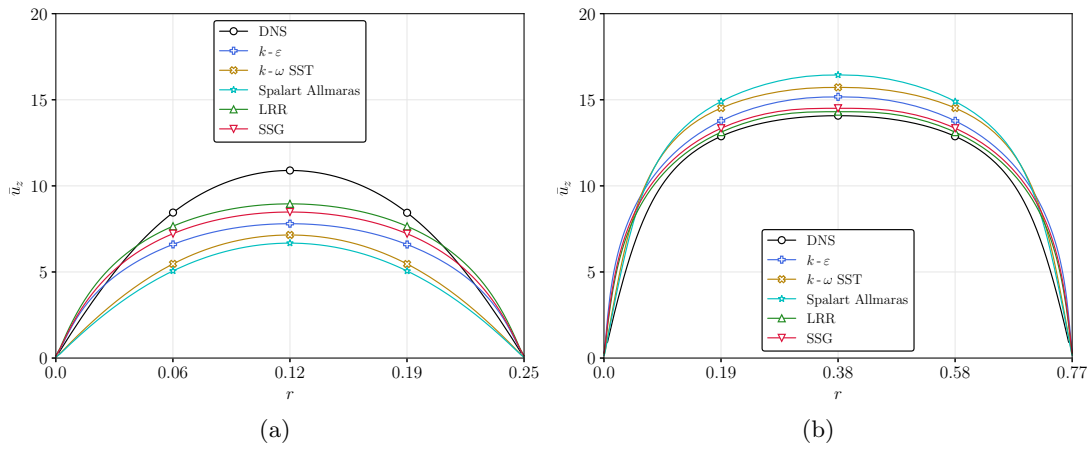


Figure 3. Profiles of  $\bar{u}_z$  for (a) narrow gap, and (b) large gap.

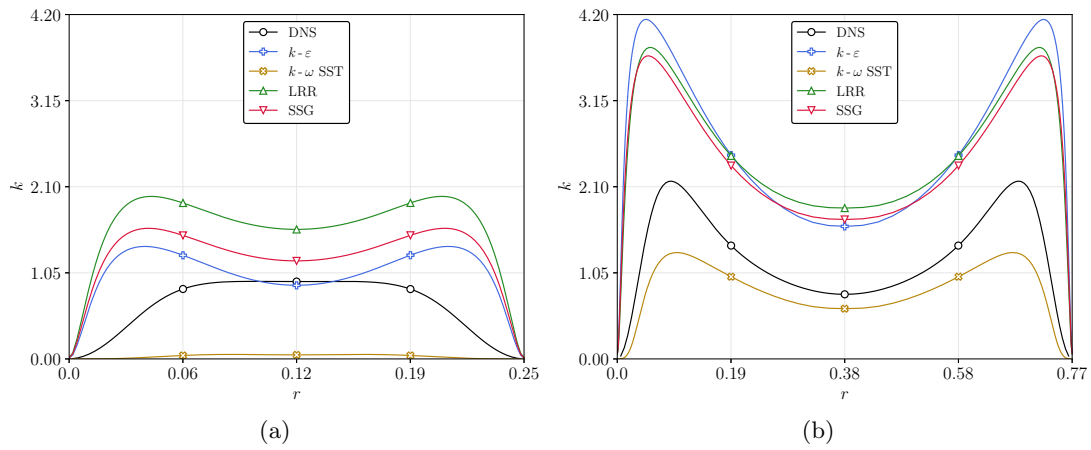


Figure 4. Profiles of  $\bar{k}$  for (a) narrow gap, and (b) large gap.

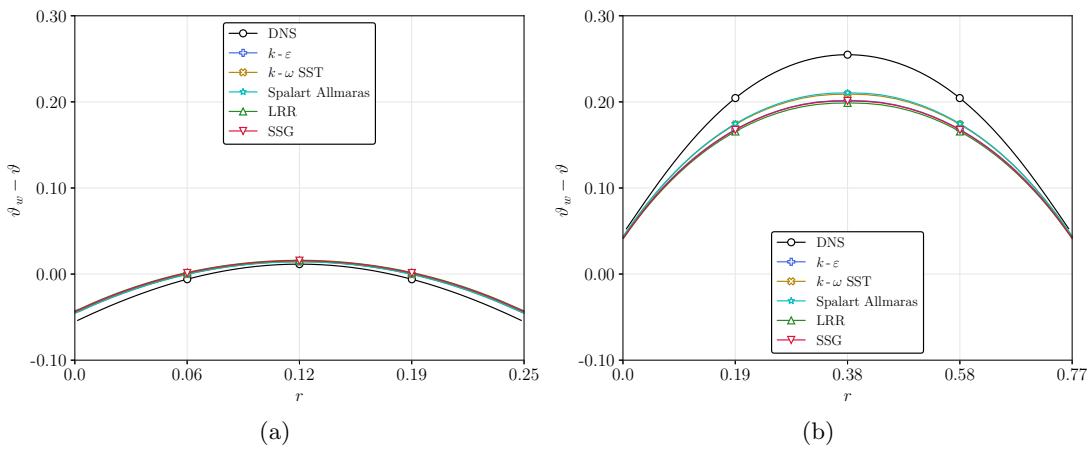


Figure 5. Profiles of  $\overline{\theta_w - \theta}$  for (a) narrow gap, and (b) large gap.

**Table 2.** Values of mean Nusselt number and external forcing.

| Numerical method | Nu   | $\sigma Re^2 / Re_\tau^2$ | $\Delta Nu\%$ | $\Delta \sigma\%$ |
|------------------|------|---------------------------|---------------|-------------------|
| DNS              | 7.60 | 4.04                      | -             | -                 |
| Spalart Allmaras | 8.11 | 3.46                      | 6.78          | -14.3             |
| $k-\varepsilon$  | 8.88 | 7.47                      | 16.8          | 85.0              |
| $k-\omega$ SST   | 8.29 | 3.73                      | 9.15          | -7.63             |
| LRR              | 9.18 | 6.87                      | 20.8          | 70.0              |
| SSG              | 9.02 | 7.15                      | 18.7          | 77.1              |

that comes closest to the reference is the Spalart-Allmaras, with a percentage variation of less than 10% compared to the DNS value. Another parameter that has been selected in the same table is the external forcing, an estimate of the constant pressure gradient due to external forcing of the flow. Even here it is evident that the Spalart-Allmaras model performs quite well, along with the  $k-\omega$  SST model. Furthermore, while the  $k-\omega$  SST model exhibits lower precision in predicting the heat transfer, it demonstrates a more evenly distributed level of accuracy compared to the Spalart-Allmaras model when considering the influence of forcing. Notably, the force term accuracy doubles, albeit at the cost of a 2% reduction in the Nusselt number accuracy.

## 5. Concluding remarks

In this work, different RANS models were applied to investigate the flow and heat transfer of liquid LBE with Prandtl number of 0.031 around vertical cylindrical rods arranged in an infinite square lattice, using DNS data as reference. A first set of conclusions can be drawn from this first brief analysis: the LRR model emerges as the most accurate to approximate the mean velocity field (in conjunction with the SSG model). This characteristic can be related to the capacity of the Reynolds stress models to represent the anisotropy of the flow, with an associated increase in computational effort (with respect to eddy viscosity models). However, when considering integral parameters, the  $k-\omega$  SST model and the Spalart-Allmaras model demonstrate the closest proximity to the reference values. One of the aspects that could help to discern between the different models could be the analysis of the turbulent kinetic energy budget and, especially, the heat fluxes budget given the thermo-hydraulic interest. In the future, the case study will be extended to the case of mixed convection, in addition to a more detailed statistical analysis.

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