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Numerical prediction of turbulent heat transfer at low Prandtl number.

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Abstract. This paper is concerned with comparing different approaches for the numerical prediction of heat transfer in a turbulent channel flow at very low Prandtl number and high Reynolds number. Results obtained with a Reynolds Averaged Navier Stokes (RANS) approach at relevant Reynolds numbers for the liquid metal reactor problematic ($Re_\tau = 590, Re_\tau = 1020$), are presented and discussed. Original results obtained with a wall resolved Large Eddy Simulations (LES) at $Re_\tau = 2000$ are provided. The velocity profile agrees very well with that of a reference Direct Numerical simulation (DNS). The obtained temperature profile can serve as a reference as the energy equation is computed without any Subgrid Scale (SGS) model at this low Pr.

1. Introduction

Liquid Metal Reactors (LMR) represent a promising technology for achieving the various criteria required to be certified as a GEN-IV concept. For those reactors, two coolants are envisaged: the sodium and a lead-bismuth eutectic (LBE). The Prandtl number of such fluids is very low, typically in the order of magnitude of $Pr \approx 0.01$. At this Prandtl, the temperature field is much smoother than the velocity field, and for moderate Reynolds the heat transfer at the wall could be essentially molecular while the flow is fully turbulent. The classical Reynolds analogy, which is the base of the turbulent Prandtl concept and the wall function approach, fails to correctly predict the local heat transfer when the usual best practice guidelines are followed. Indeed, it was observed in [1] that the heat transfer for a low Prandtl number fluid could be molecular even though the flow is turbulent, making the usual Reynolds analogy inappropriate.

A first issue concerns the location of the first grid point; if this one is placed in the lower bound of the possible range where the logarithmic law is valid for the velocity profile, namely $y^+ \approx 60$, then the linear law should be used for the temperature profile of liquid metals with $Pr \leq 0.01$, which encompasses the LBE for certain temperatures and the sodium in general. Indeed, as it was showed by [1], the laminar sublayer extends up to $y^+ \approx 60$. For higher Prandtl numbers or for a less stringent first grid point placement, a law for the buffer region should be established which requires to know the eventual logarithmic law in order to use a blending function.

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A second issue is the determination of the turbulent heat diffusivity in the core flow. This is usually achieved in RANS through the use of a turbulent Prandtl number. It was found that the case at $Re_\tau = 590$ presented a well defined plateau at $Pr_t \approx 2$ (see [1]), which was not in agreement with available correlations. The first part of the paper is focused on classical RANS methodologies with an improved best practice guideline derived from the obtained DNS/LES results. In this part, different RANS approaches for evaluating the turbulent Prandtl number are compared and their performance are assessed against DNS data. This paper also presents new results obtained from a LES at $Re_\tau = 2000$ and $Pr = 0.01$ ($Re \approx 90000$, leading to $Pe \approx 900$), which is very close to operational conditions in LMR cores. In these LES, the mesh is considered fine enough to fully resolve the temperature field, while a sub-grid scale model is necessary for the momentum equation. Some conclusions are drawn concerning the choice of RANS approaches for heat transfer prediction in this kind of flow.

2. Channel flow setup

The physical case of interest in this paper is the developed turbulent flow of a low Prandtl number fluid through a uniformly heated channel. It is numerically tackled by the computation of a time-developing flow between two plates with periodic boundary conditions in the streamwise and spanwise directions (Fig. 1) and which reaches statistical equilibrium.

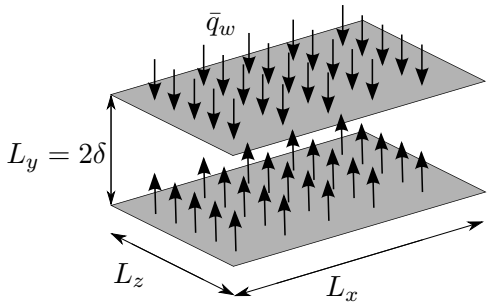


Figure 1. Channel flow configuration

The governing equations are the Navier-Stokes equations for incompressible flow and constant thermophysical properties, supplemented by a turbulence model, and the energy conservation equation for the temperature T. In order to handle periodic boundary conditions, it is required to use a modified temperature $\theta(x, y, z, t)$ variable such that

$$T = x\frac{dT_w}{dx} - \theta, \tag{1}$$

where the wall temperature gradient forcing compensates the temperature increase in the periodic streamwise direction due to the uniform heat flux $\bar{q}_w$:

$$\frac{dT_w}{dx} = \frac{\bar{q}_w}{\rho\, c\, \delta\, \langle \overline{u}_1 \rangle}\,, \tag{2}$$

where $\langle \overline{u}_1 \rangle$ is the streamwise time and space averaged velocity. This leads to a modified energy equation for θ with the following source term:

$$S_\theta = u_1 \frac{dT_w}{dx}\,. \tag{3}$$

The flow is driven by a streamwise pressure gradient forcing defined by $F_x = -\frac{dP_f}{dx}$. This pressure gradient is adapted in time so that the mass flux is kept constant. The Navier-Stokes equations are thus written:

$$\frac{\partial u_i}{\partial x_i} = 0, \tag{4}$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + F_i + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + \frac{\partial \tau_{ij}^M}{\partial x_j}, \tag{5}$$

$$\frac{\partial \theta}{\partial t} + u_j \frac{\partial \theta}{\partial x_j} = S_\theta + \alpha \frac{\partial^2 \theta}{\partial x_j \partial x_j} - \frac{\partial q_j^M}{\partial x_j}, \tag{6}$$

where $P = \frac{p}{\rho}$ is the reduced pressure, $\nu = \mu/\rho$ is the kinematic viscosity, $\alpha = \frac{k}{\rho c}$ is the thermal diffusivity and τ^M is the turbulence stress tensor model. The turbulent heat flux model is q_j^M. These equations involve very different physical characteristic times related either to convection or diffusion of momentum and heat.

3. Wall-resolved RANS simulations

The results presented in this section concern wall-resolved RANS simulations of the channel flow at $Re_\tau = 590$ and $Re_\tau = 1020$. The simulation parameters were chosen in order to allow their validation against DNS data available from literature [2, 3].

3.1. Investigated models

The flow solver used for these investigation is the finite volume based solver OpenFoam. Three models are investigated, namely the $k-\epsilon$ Launder and Sharma [4] model, the $k-\omega$ SST model of Menter [5] and the $k-\epsilon$ model of Chien [6]. These models provide only the turbulent viscosity ν_t, the turbulent heat diffusivity α_t is determined considering a turbulent Prandtl number $Pr_t = \frac{\nu_t}{\alpha_t}$. The classical approach consists in choosing a constant turbulent Prandtl: $Pr_t \approx 0.85$. This value is not appropriate as showed in [1]. In this work, other correlations are also investigated. The correlation of Reynolds [7] provides values for Pr_t as a function of the Peclet number ($Pe = Re\,Pr$):

$$Pr_t = \left(1 + 100\,Pe^{-1/2}\right)\left(\frac{1}{1 + 120\,Re^{-1/2}}\right). \tag{7}$$

The correlation of Kays [8] depends on both the the Prandtl number and $\frac{\nu_t}{\nu}$:

$$Pr_t = 0.85 + \frac{0.7}{\frac{\nu_t}{\nu}\,Pr}. \tag{8}$$

Finally, a third correlation proposed by Weigand et al. [9, 10] was also used in the present analysis. It provides Pr_t as a function of a turbulent Peclet number $Pe_t = Pr\,\frac{\nu_t}{\nu}$:

$$\frac{1}{Pr_t} = \frac{1}{2\,Pr_{t\infty}} + CPe_t\sqrt{\frac{1}{Pr_{t\infty}}} - (CPe_t)^2\left[1 - exp\left(-\frac{1}{CPe_t\sqrt{Pr_{t\infty}}}\right)\right], \tag{9}$$

where $C = 0.3$. The appropriate value for $Pr_{t\infty}$ away from the wall is given by

$$Pr_{t\infty} = 0.85 + \frac{100}{Pr\,Re^{0.888}}. \tag{10}$$

3.2. RANS flow results

The calculation of the channel flow at $Re_\tau = 590$ has been performed using a wall-resolved approach applying different turbulence models. The RANS equations are solved for a two-dimensional domain with periodic boundary conditions. In the direction normal to the wall, mesh stretching has been applied ensuring that the first grid point is located well below $y^+ = 1$. Fig. 2 illustrates the velocity profiles in a channel at $Re_\tau = 590$. The RANS results fairly agree with the DNS data in the linear region of the boundary layer. In the log-region of the boundary layer and in the wake region at the centre of the channel, an overestimation of the velocity is observed for the Launder Sharma and the Chien turbulence models. On the contrary, the $k-\omega$ SST model provides a good approximation of the velocity profile in the log-region while it underestimates the velocity at the centre of the channel. Taking DNS data of [2] as a reference, discrepancies of 5.5%, 3.1% and 1.8% on the bulk velocity are calculated for respectively the Launder Sharma, the Chien and the $k-\omega$ SST turbulence models. For $Re_\tau = 2000$ (see Fig. 6), the differences appear to be smaller. Indeed, using the DNS data of Hoyas et al. [11] as a reference, discrepancies of 3.7%, 1.4% and 1.2% on the bulk velocity are calculated for respectively the Launder Sharma, the Chien and the $k-\omega$ SST turbulence models.

In Fig. 2, the velocity profile normalised by the centerline velocity u_c is also provided. This figure compares the DNS velocity profile for $Re_\tau = 590$ with the velocity profile obtained using the Chien turbulence model. Clearly, the RANS velocity profile is flatter than that of the DNS [2], meaning that the Chien turbulence model overestimates the importance of turbulent momentum diffusivity.

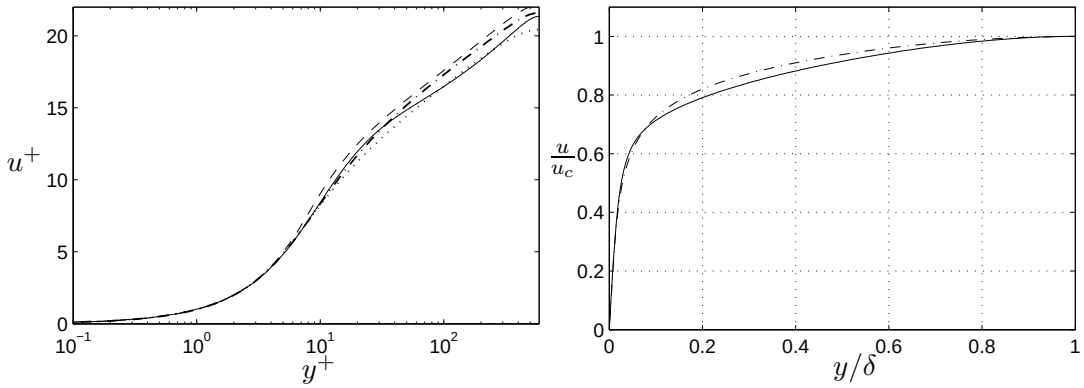


Figure 2. Mean velocity profile for the turbulent channel flow at $Re_\tau = 590$ in wall coordinates (left) and outer coordinates (right); DNS [2] (solid); RANS with Chien model (dash-dot); RANS with the $k-\omega$ SST model (dot); RANS with the Launder-Sharma model (dash).

3.3. RANS thermal results

For the channel flow, the simplified energy equation (Eq. 6) is

$$\frac{u_1}{\langle \overline{u}_1 \rangle} \frac{\overline{q}_w}{\rho c \delta} + \frac{\partial}{\partial y}\left((\alpha + \alpha_t) \frac{\partial \theta}{\partial y} \right) = 0\,, \tag{11}$$

where α is the molecular heat diffusivity and α_t is the turbulent heat diffusivity. Notice that the source term is function of the velocity profile through the $\frac{u_1}{\langle \overline{u}_1 \rangle}$ ratio which appears, according to previous conclusions, too diffusive compared to DNS data. For the first case at $Re_\tau = 590$ and $Pr = 0.01$, the evaluation of the turbulent Prandtl number was done using the Kays [8] and Reynolds [7] models. The evolution of Pr_t over the channel height according to both models

is compared with DNS data in Fig. 3. The following remarks can be made regarding this comparison:

- The Reynolds model doesn't take into account the y variations of Pr_t;
- The Kays model is more accurate in predicting the turbulent Prandtl number except in near wall region;
- Both models predict values of Pr_t significantly higher than 0.85 which is in agreement with the DNS data;
- In the core flow, an overestimates of the turbulent Prandtl number is observed compared to the DNS data.

The calculated fully developed temperature profiles along the channel height for $Pr = 0.01$, $Re_\tau = 590$ are shown in Fig. 4. On the one hand, application of the classical approach $Pr_t = 0.85$ clearly underestimates the temperature over the channel height compared with the DNS data [2] due to an overestimation of the turbulent heat diffusivity α_t. On the other hand, accurate prediction of the temperature profile is provided by RANS simulation when the Reynolds and Kays models are used. However, these results are obtained despite the overestimation of the turbulent Prandtl number. One can argue that thanks to the overestimation of Pr_t over the channel height, the excess of momentum diffusivity introduced by the turbulence models is compensated, since $\alpha_t = \frac{\nu_t}{Pr_t}$.

Concerning the flow at $Pr = 0.025$ and $Re_\tau = 1020$, similar conclusions can be drawn as for the previous case regarding the estimation of the turbulent momentum diffusivity and the accuracy of models to predict the turbulent Prandtl number. The temperature profiles are shown in Fig. 5 including the DNS data of Abe et al. [3]. In the present case, three models have been investigated to estimate the turbulent Prandtl number: the models of Kays, Weigand et al. and Reynolds. While the two first models provide an underestimation of the maximum temperature difference over the channel, an overestimation is observed when the Reynolds model is applied. Using the DNS data of Abe et al. [3] as a reference, the deviation on the maximum temperature difference over the channel equals 3.6%, 3.9% and 9.2% when using respectively the Kays model, the Weigand model and the Reynolds model to predict Pr_t.

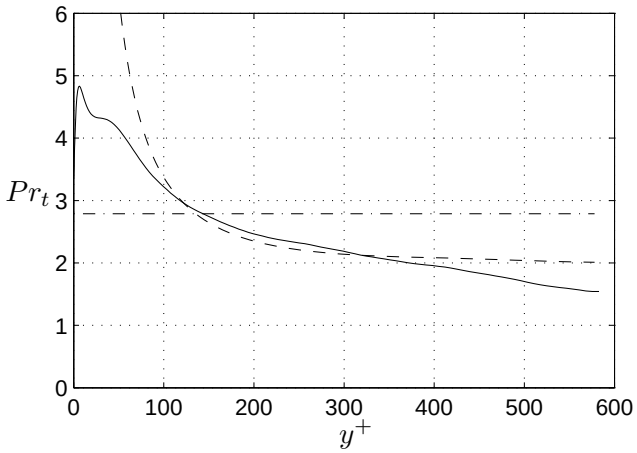


Figure 3. Turbulent Prandtl numbers at $Re_\tau = 590$; DNS [2] (solid); Kays correlation (dash); Reynolds correlation (dash-dot).

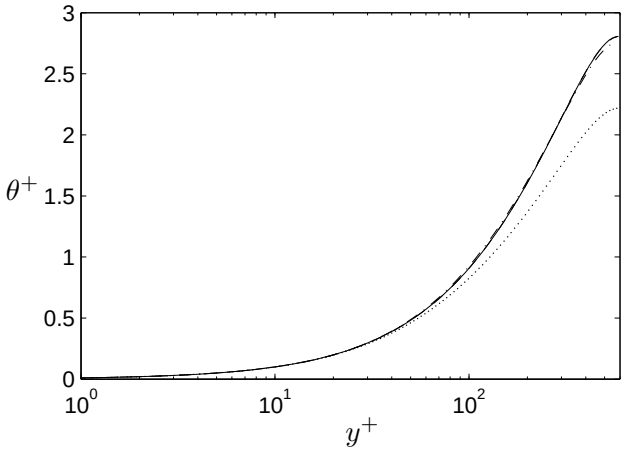


Figure 4. Mean temperature profile for the turbulent channel flow using the Chien model at $Re_\tau = 590$ and $Pr = 0.01$. DNS [2] (solid); Constant Pr_t (dots); Kays correlation (dash-dot); Reynolds correlation (dash).

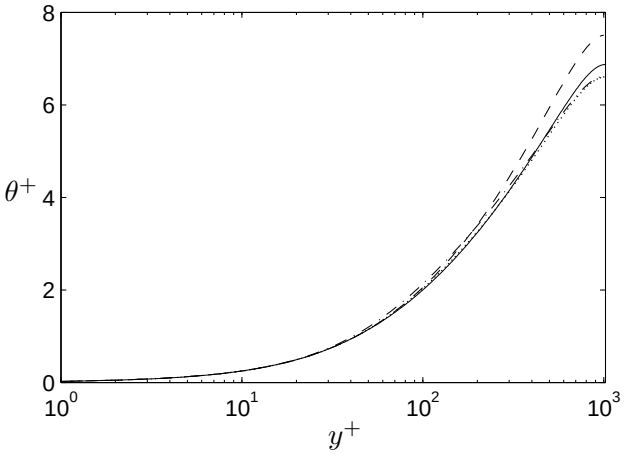


Figure 5. Mean temperature profile for the turbulent channel flow using the Chien model at $Re_\tau = 1020$ and $Pr = 0.025$. DNS [3] (solid); correlation of Weygand et al. (dots); Kays correlation (dash-dot); Reynolds correlation (dash).

4. LES results at $Re_\tau = 2000$

In order to simulate flows at Reynolds number that are closer to real conditions in LMR, DNS approaches are clearly out of reach in complex geometries. It was showed in [1] that a hybrid LES-DNS (SGS modeling applied only for the momentum equation) approach is appropriate to perform simulations of this kind of flows at high Re at a more reasonable cost than DNS. Those LES results can also be used to assess quality of RANS models.

In this section a set of preliminary LES results obtained for the turbulent heat transfer in channel flow at a much higher Reynolds number ($Re_\tau = 2000$, $Re \approx 90000$, leading to $Pe \approx 900$) are presented. The reference DNS for the velocity field is that of Hoyas et al. [11]. This flow regime is the highest attained for a channel flow DNS to date, thus the LES of the base flow already constitutes a challenge. Eq. 6 are solved using a fractional-step method with the "delta" form for the pressure described by Lee et al. [12]. This form allows simple boundary conditions for the pressure and the intermediate velocity field. The convective term is integrated using a

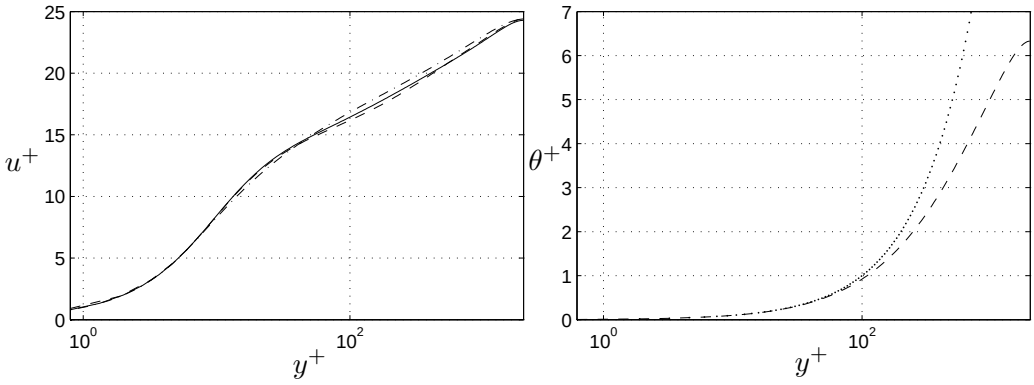


Figure 6. Mean velocity (left) and temperature (right) profile for the turbulent channel flow at $Re_\tau = 2000$ and $Pr = 0.01$. DNS [11] (solid); LES (dash); RANS with Chien model (dash-dot); $\theta^+ = Pr\, y^+$ (dots).

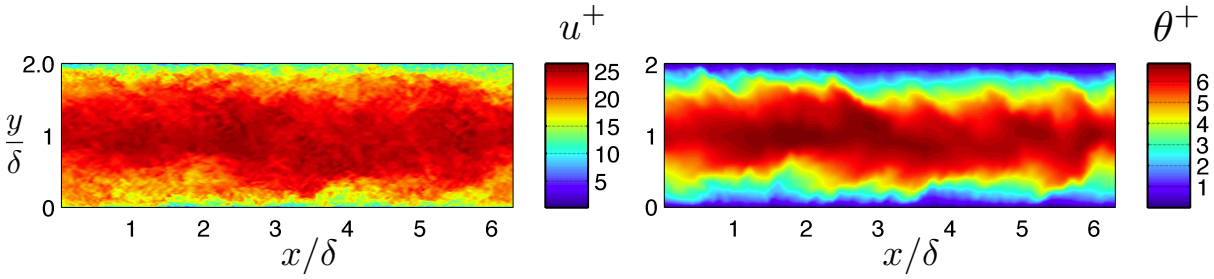


Figure 7. Colormaps of the LES results at $Re_\tau = 2000$ and $Pr = 0.01$. The slice are taken in an arbitrary $x - y$ plane.

second order Adams-Bashforth scheme and the molecular diffusion term is integrated using a Crank-Nicolson scheme. The subgrid scale model is the regularized variational multiscale version of the WALE model as defined in [13]. The SGS model term is integrated explicitly, also using the Adams-Bashforth scheme. The equations are discretized in space using the fourth order finite difference scheme of Vasilyev [14]. The discretization of the convective term conserves energy on cartesian stretched meshes and is therefore particularly suited for direct or large-eddy simulations of turbulent flows. The Poisson equation for the pressure is solved using a multigrid solver with a line Gauss-Seidel smoother. The parameter of the computational box are $L_x \times L_y \times L_z = 2\pi\delta \times 2\delta \times \pi\delta$, the grid is stretched in the y direction in order to perform a wall resolved LES. The grid sizes are $N_x \times N_y \times N_z = 384 \times 256 \times 384$ leading to a total of about 38 million grid points.

The mean velocity profile, reported in Fig. 6, is in very good agreement with that of the DNS. Moreover it can be observed that the model of Chien provides reliable prediction. The topology of the velocity field and temperature field are compared in Fig. 7. Even at this high Re, one observes that the temperature field is much smoother than the velocity field. This enforces the validity of the approach proposed here: performing a LES for the flow and use no SGS model for the temperature fields. This approach allows to obtain the temperature profile also reported in Fig. 6. It is interesting to note that the temperature profile agrees well with the linear law $\theta^+ = Pr\, y^+$ up to $y^+ \approx 60$ as already observed at $Re_\tau = 590$ and $Re_\tau = 180$ in [1]. Still no log layer can be observed on the temperature profile.

5. Conclusions and perspectives

In this study, state of the art results concerning the numerical prediction of turbulent heat transfer at low Prandtl number are presented. On one hand, RANS investigations allowed to conclude that for the range of Reynolds numbers envisaged the Chien model stands-out to be the most appropriate. It was also showed that the correlation of Kays allows to obtain reliable prediction of the temperature profile. On the other hand, original LES results at $Re_\tau = 2000$ were presented. The velocity statistics are in good agreement with that of the DNS. The hybrid approach (LES for the flow and DNS for the thermal part) allows to obtain temperature profile and fluctuations on which one can rely. This is of primary importance in the framework of GEN-IV LMR. The perspectives are wide: it is indeed interesting to go towards more complex geometries, for instance a sub-channel configuration with fuel pins. Moreover assessing the validity of the RANS approach at higher Reynolds number $Re_\tau = 2000$ by comparison with the LES results obtained is ongoing work. Investigating wall function approaches for the temperature is also relevant if one goes to even higher Re and more complex geometries.

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