NURETH14-130

DNS AND LES OF TURBULENT CHANNEL FLOWS AT VERY LOW PRANDTL NUMBER: APPLICATION TO CONVECTION IN LEAD-BISMUTH

L. Bricteux, M. Duponcheel, G. Winckelmans and Y. Bartosiewicz

Université catholique de Louvain (UCL)

Institute of Mechanics, Materials and Civil Engineering (iMMC)

Bat. Stévin, Place du Levant 2

B-1348 Louvain-la-Neuve, Belgium

Abstract

This paper presents recent developments of DNS (Direct Numerical Simulation) and LES (Large Eddy Simulation) for liquid metals with a focus on local heat transfer behavior.Three Reynolds number are considered, namely $Re_\tau = 180$, $Re_\tau = 590$, and $Re_\tau = 640$. For the two higher Reynolds hybrid LES/DNS are performed and gives satisfactory results compared to reference DNS. The analysis of wall heat transfer behavior allows to propose new best practice guidelines for RANS computations. Usual correlations for the overall wall heat transfer coefficient are also compared to the present results.

Introduction

Liquid Metal Reactors (LMR) represent a promising technology for achieving the various criteria required to be certified as a generation IV (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, for instance $Pr \approx 0.01$ for LBE and $Pr \approx 0.001$ for liquid sodium at operational conditions. This issue provides a breakdown of the usual so-called Reynolds analogy relating the momentum and the heat transport through the boundary layer. Consequently, in classical CFD approaches, which become affordable for industrial calculations, the value of the turbulent Prandtl number close to unity and the classical way of applying wall functions fail to correctly represent heat transfer in the flow and at walls . Therefore, advanced simulations such as DNS and LES are attractive to provide detailed information and the necessary basis to adapt Reynolds Averaged Navier Stokes (RANS) models for liquid metals. A good overview on the use of DNS/LES methods in nuclear applications is given in Grötzbach and Wörner [1].

At very low Prandtl and moderate, but still turbulent Reynolds numbers, the authors proposed to use a hybrid approach, where a subgrid-scale model is used for the flow dynamic while the heat transfer could be resolved without any model, providing the temperature field is fully resolved on the LES grid [2]. This is due to the fact that the smallest turbulence lengthscale of the temperature field is larger than that of the velocity field. In particular, at low Re, the heat transfer is essentially molecular. In order to capture such complex physics, high quality numerical methods are required, with negligible numerical dissipation (i.e., methods that conserve energy in absence of viscosity) and with low dispersion errors (to properly transport the turbulent structures). A fourth order energy conserving finite difference parallel code is used to satisfy these criteria. In this work, the LES of the flow is performed using the recent multiscale WALE subgrid model. The relevance of this LES approach will be evaluated for various Re and Pr numbers by comparison with existing DNS results when available, and with a new DNS simulation for some relevant cases (e.g : $Re_\tau = 590$ and $Pr = 0.01$ from Tiselj [3]). Performing such high fidelity simulations will help to collect useful data for the forced convective heat transfer in wall bounded flows of liquid metals, and allow to establish new best practice guidelines for RANS simulations used in LMR. In the first part of the paper, the flow to be studied is described. In the second part, the numerical method and the subgrid scale model are presented. The DNS and LES results for different conditions (see table 1 are then presented in a third part.

1 Description of the flow and numerical method

We perform here numerical simulations of the turbulent channel flow at several values of $Re_\tau = \frac{u_\tau \delta}{\nu}$ and at various Prandtl ($Pr = \nu/\alpha$) numbers. The friction velocity u_τ is based on the wall shear stress : $u_\tau^2 = \tau_w/\rho$, δ is the channel width and ν is the kinematic viscosity. The parameters of the studied flows are reported in Table 1. The Peclet number $Pe = Re\,.\,Pr$ is of primary importance for heat transfer with liquid metals flows. Indeed, several authors proposed heat transfer correlations which depends only on the Peclet number $Nu = f(Pe)$ instead of taking the dependence on Re and Pr separately : $Nu = f(Re, Pr)$. For instance, in the case of a uniform wall heat flux, Lubarsky and Kaufman [4] proposed the following correlation :

$$Nu = 0.625\,Pe^{0.4} = 0.625\,Re^{0.4}\,Pr^{0.4}\,. \tag{1}$$

This correlation fits fairly with various heat transfer measurements for liquid metals in the range $10^2 < Pe < 10^4$. It is interesting to remark that this correlation attributes the same importance to Re and Pr while correlations used for flows with $Pr = \mathcal{O}(1)$ (e.g. Dittus-Boelter) provides a dependence of the form : $Nu = 0.023\,Re^{0.8}\,Pr^{0.4}$, attributing more importance to the Reynolds number. Recently, an other correlation was proposed by Cheng et al. [5] for LBE and $Pe \leq 1000$:

$$Nu = 4.5 + 0.018\,Pe^{0.8}\,. \tag{2}$$

The typical Prandtl number value for lead bismuth application in GEN IV reactor is $Pr = 0.01$. The higher Reynolds number considered here is $Re = \mathcal{O}(20000)$ which is fairly high and relevant for thermal hydraulics investigations. This lead to a Peclet numer $Pe = Re \cdot Pr \approx 200$ meaning that the thermal transport is not significantly high compared to the thermal diffusion.

The channel flow problem considered here 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). The order of magnitude of the lowest tested Prandtl number matches with that of LBE. The governing equations of the flow considered are the Navier-Stokes equations for incompressible flow and constant thermophysical properties, supplemented by a SubGrid-Scale (SGS) model for LES calculation only, 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 $T = x\frac{dT_w}{dx} - \theta$, A uniform heat flux $\bar{q}_w$ is applied at the walls such that :

$$\theta = 0 \quad \text{at} \quad y = 0 \quad \text{and} \quad y = 2\delta. \tag{3}$$

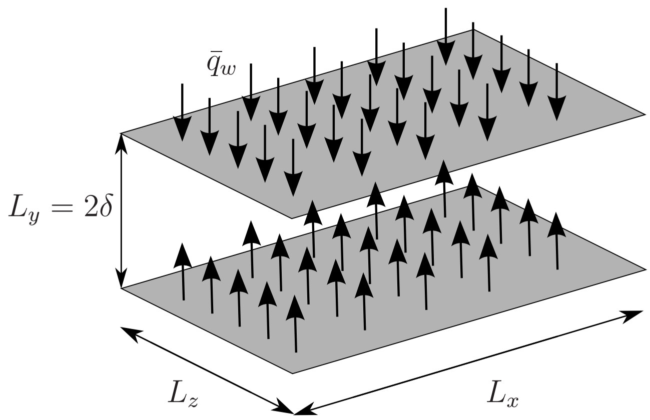

FIGURE 1 – Channel flow configuration

The wall temperature gradient forcing compensates the temperature increase in the periodic streamwise direction due to the uniform heat flux $\bar{q}_w$: $\frac{dT_w}{dx} = \frac{\bar{q}_w}{\rho\, c\, \delta \langle \overline{u}_1 \rangle}$, 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 : $S_\theta = u_1 \frac{dT_w}{dx}$. 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 constant. The Navier-Stokes equations are thus written :

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

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

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

where u_i is the LES velocity field (projected on the LES grid, $P = \frac{p}{\rho}$ is the reduced pressure (projected on the LES grid), ν is the kinematic viscosity, $\alpha = \frac{k}{\rho c}$ is the thermal diffusivity and τ^M is the SGS stress tensor model and is different from zero in the case of an LES. These equations are solved using a fractional-step method with the ≪ delta ≫ form for the pressure described by Lee et al. [6]. This form allows simple boundary conditions for the pressure and the intermediate velocity field. The convective term is integrated using a second order Adams-Bashforth scheme and the molecular diffusion term using a Crank-Nicolson scheme. 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 [7]. The stretching law used for the grid in the wall normal direction is

$$\frac{y}{\delta} = 1 + \frac{\tanh(\gamma(\zeta - 1))}{\tanh(\gamma)} \tag{7}$$

with $\zeta = y/\delta = 0$ at the lower wall and $\zeta = y/\delta = 2$ at the upper wall. The stretching parameter is chosen to ensure that the first grid point in the y direction is located such that $y^+ < 1$, as required for DNS or wall resolved LES. 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 code is implemented to run efficiently in parallel.

TABLE 1 – Parameters used for the channel flow

Re_τ	Re	Pr	L_x	L_y	L_z	Δ_x^+	Δ_{yw}^+	Δ_{yc}^+	Δ_z^+	γ
180 (DNS)	5600	1.0 / 0.1 / 0.01	$2\pi\delta$	2δ	$\pi\delta$	8.8	0.76	4.9	4.4	1.6
590 (LES)	22000	0.01	$2\pi\delta$	2δ	$\pi\delta$	38.6	0.85	52.8	19.3	2.8
640 (LES)	24428	0.025	$2\pi\delta$	2δ	$\pi\delta$	41.9	0.92	57.3	20.9	2.8

These equations involve very different physical characteristic times related either to convection or diffusion of the momentum and heat. Obviously, an explicit time integration should be able to capture those physical characteristic times in order to have a time-accurate solution. For a convective flow, and for $Pr \approx 1$, the most stringent characteristic time is usually the convective one which leads to the so-called CFL (Courant Friederichs Lewy) stability condition on the time step. However for very low Prandtl fluids, the most stringent term is that related to the diffusion of heat, which can be several order of magnitudes below the usual time-constraint depending on the Prandtl number. This constraint is obviously more pronounced along directions where heat diffusion is important, namely the wall normal direction in our case. This issue is numerically tackled by adopting an implicit time stepping (Crank-Nicolson) along the y direction.

2 Subgrid scale modeling

The SGS model is only used in the momentum equation, The heat transfer part of the problem is computed without turbulence model as it is assumed to be very well resolved on the LES grid of the flow (with $Pe = 220$). This method was already presented in [2]. The SGS model is described in [8]. The subgrid scale viscosity ν_{sgs} is computed using a high pass filtered velocity field u_i^s, which mainly contains the small resolved scales on the LES grid. The subgrid scale viscosity is thus active only when there are small scales in the velocity field. The high pass filtered strain rate tensor is defined as :

$$S_{ij}^s = \frac{1}{2}\left(\frac{\partial u_i^s}{\partial x_j} + \frac{\partial u_j^s}{\partial x_i}\right) . \tag{8}$$

In the same way, one also define the traceless symmetric part of the square of the velocity gradient tensor (see [8], [9])

$$\mathcal{T}_{ij}^s = \frac{1}{2}\left(\frac{\partial u_i^s}{\partial x_k}\frac{\partial u_k^s}{\partial x_j} + \frac{\partial u_j^s}{\partial x_k}\frac{\partial u_k^s}{\partial x_i}\right) . \tag{9}$$

This allows to build a subgrid scale viscosity using $\mathcal{T}_{ij}^{sd}$, the deviatoric part of Eq. 9 . This ensures that the SGS viscosity has the proper y^{+3} behavior in the vicinity of the wall as in [9] :

$$\nu_{sgs} = C\,\Delta^2 \frac{(\mathcal{T}_{ij}^{sd}\mathcal{T}_{ij}^{sd})^{3/2}}{(S_{ij}^s S_{ij}^s)^{5/2} + (\mathcal{T}_{ij}^{sd}\mathcal{T}_{ij}^{sd})^{5/4}} , \tag{10}$$

where $C = 1.4$ is the model coefficient previously calibrated in [8] and Δ is the LES grid length scale. The SGS model acts only on the small scale part of the LES velocity field and thus preserves the dynamics of the large scales : $\tau_{ij}^M = 2\,\nu_{sgs} S_{ij}^s$. The LES performed here is of quality, it is a wall resolved LES (first cell such that $y^+ < 1$) with fairly fine grid sizes : $\Delta x^+ = 39$ and $\Delta z^+ = 20$. The obtained results agree very well to that of the DNS of Moser et al. [10] as reported in [8]. These LES results can thus serve as reference for the considered flow.

3 Results

3.1 DNS results at $Re_\tau = 180$

The dimensionless temperature profile $\theta^+ = \frac{T_w - T}{T_\tau}$ normalized by the friction temperature $T_\tau = \frac{q_w}{\rho c u_\tau}$ is displayed in Fig. 2 for various Pr numbers. The profile obtained at $Pr = 1.0$ corresponds very well to that of the DNS of Kawamura et al. [11], which validates the numerical approach. The temperature fluctuations are reported in Fig. 3. One observes that for $Pr = 0.1$ the temperature fluctuations are much smaller to become negligible at $Pr = 0.01$. The turbulent heat diffusivity $\alpha_t = \frac{-\overline{v'\theta'}}{\frac{d\overline{\theta}}{dy}}$ is reported in Fig. 4, and its value is very small at low Prandtl numbers . This corresponds to the fact that the heat flux is dominated by its molecular part and the turbulent part becomes negligible. For the Prandtl number of LBE, and at this moderate but still turbulent Re, it is thus pointless to define a turbulent Prandtl number. Therefore, any RANS approach which would not eliminate the turbulent component of heat diffusivity at these moderate Reynolds, would fail to predict a correct heat transfer. In the case of sodium the range of Reynolds number, for which the molecular effects would dominate turbulence, would be even larger ; therefore for those moderate Reynolds, even though a turbulence model is necessary for the flow dynamic, it is then required to switch it off for the thermal field or forcing $\alpha_t = 0$. In Fig. 4, the near-wall behavior of α_t is reported and it decays as y^{+3} close to the wall as predicted by the theory. A good SGS or RANS model should mimic this asymptotic behavior.

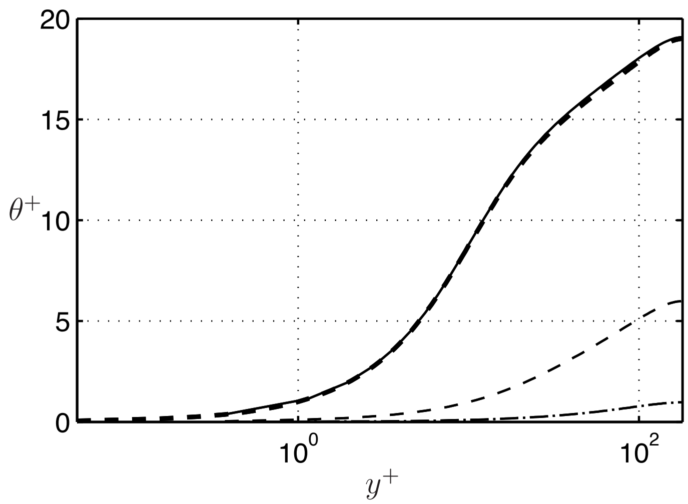

FIGURE 2 – Mean temperature profile for the turbulent channel flow at $Re_\tau = 180$. $Pr = 1.0$ (solid), $Pr = 0.1$ (dash), $Pr = 0.01$ (dash-dot). Comparison with the DNS data obtained by Kawamura et al. [11](thick dash).

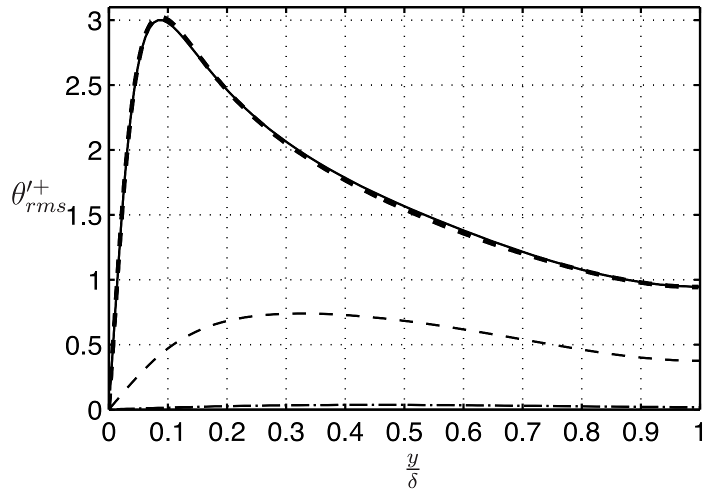

FIGURE 3 – Rms (root mean square) of the temperature fluctuations profile for the turbulent channel flow at $Re_\tau = 180$. $Pr = 1.0$ (solid), $Pr = 0.1$ (dash), $Pr = 0.01$ (dash-dot). Comparison with the DNS data obtained by Kawamura et al. [11](thick dash).

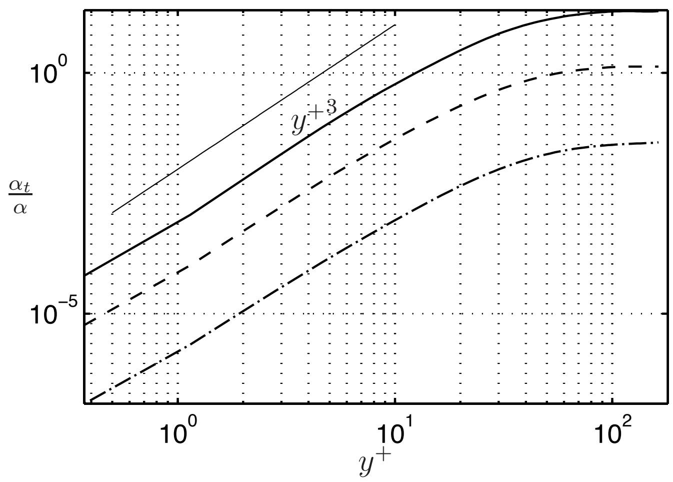

FIGURE 4 – Turbulent heat diffusivity for the turbulent channel flow at $Re_\tau = 180$. $Pr = 1.0$ (solid), $Pr = 0.1$ (dash), $Pr = 0.01$ (dash-dot). The y^{+3} near wall behavior of α_t is highlighted with the thin solid line.

3.2 LES results at $Re_\tau = 590$ and $Pr = 0.01$

The results obtained with the hybrid DNS-LES approach are compared to the DNS of Tiselj [3]. The number of grid points required for this DNS is such that $N_x \times N_y \times N_z = 384 \times 256 \times 384$. The LES has four times fewer points in each direction resulting in a 64-fold reduction in computational cost . Figs. 5 to 8 show that the agreement between the present approach and the reference DNS results is very good for both the average velocity (Fig. 5) and temperature (Fig. 6) profiles but also for the fluctuations (Fig. 7) and the heat flux components (Fig. 8). The peak in the temperature fluctuations is obtained at $y \approx 0.34\,\delta$. For near wall modeling strategy, the assumption of a linear law for the temperature is correct up to $y^+ = 50 - 60$ (Fig. 6) as it was noticed in [2]. Above this limit, a linear behavior is not valid anymore as depicted in Fig. 6. It is interesting to note that this range of validity of the linear behavior would be even broader in the case of sodium at a lower Prandtl number. In terms of best practice guideline for RANS approach, this result may have important consequences. Indeed, if the first grid point was located in this range of validity, the model would not require the knowledge of a turbulent Prandtl number for the thermal wall function. In addition, the upper bound of this y^+ does well match with the validity of the logarithm law for the velocity, which confirms that the usual Reynolds analogy is not appropriate for mapping the momentum and thermal wall functions close to the walls. The Nusselt number value obtained with the LES is $Nu = 6.02$ and $Nu = 5.88$ for the DNS of Tiselj [3] while the Equ. 1 predicts $Nu = 5.40$ (see Table 2) and that of Cheng et al. gives $Nu = 5.84$. The difference between these two results is the consequence of the difference in the mean temperature profile.

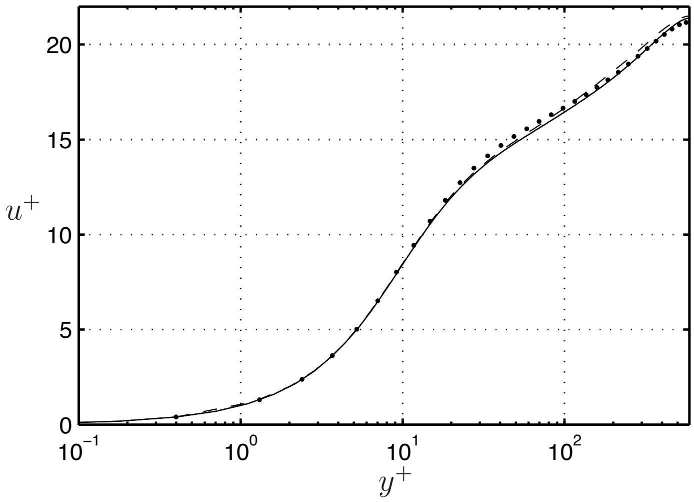

FIGURE 5 – Mean velocity profile for the turbulent channel flow at $Re_\tau = 590$. Present work DNS (dash), present work LES (dots), DNS from Tiselj [3] (solid).

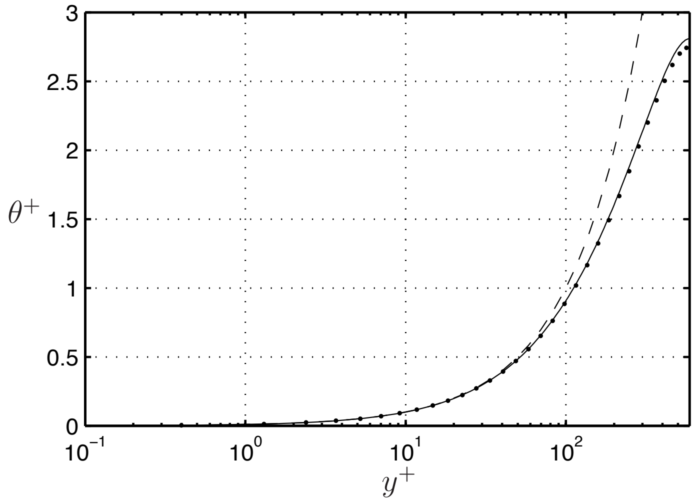

FIGURE 6 – Mean temperature profile for the turbulent channel flow at $Re_\tau = 590$ and $Pr = 0.01$. present work LES (dots), DNS from Tiselj [3](solid), theoretical near wall behaviour $\theta^+ = Pr \cdot y^+$ (dash).

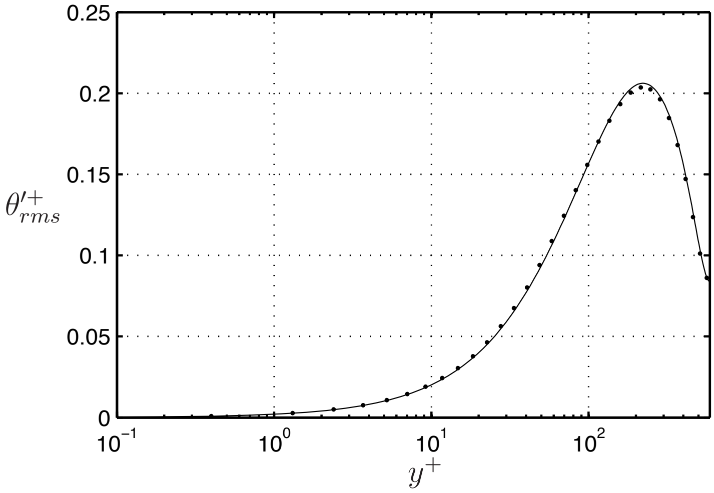

FIGURE 7 – RMS of the temperature fluctuations profile for the turbulent channel flow at $Re_\tau = 590$ and $Pr = 0.01$. present work LES (dots), DNS from Tiselj [3](solid).

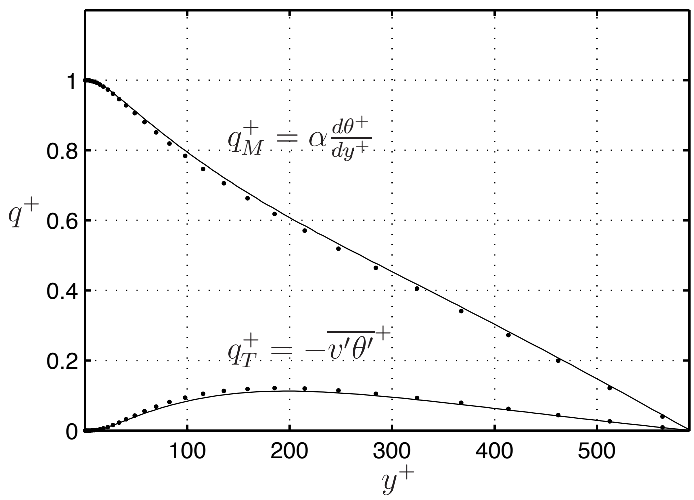

FIGURE 8 – Heat flux decomposition for the turbulent channel flow at $Re_\tau = 590$ and $Pr = 0.01$. present work LES (dots), DNS from Tiselj [3](solid).

3.3 LES results at $Re_\tau = 640$ and $Pr = 0.025$

The results are compared in this case with the DNS of Kawamura's group [12]. It is worth noting that the $Pr = 0.025$ is twice higher than the value obtained for the LBE. In this case, the thermal field is indeed more "turbulent" than in the case $Pr = 0.01$. This is highlighted on a qualitative basis in Fig. 13 where the temperature fluctuations are weaker at $Pr = 0.01$ than $Pr = 0.025$. This is the reason why the results displayed in Figs. 9 to 12 show more discrepancies than in the case at $Re_\tau = 590$ and $Pr = 0.01$. The Peclet number ($Pe = 610$) in this case is indeed three times higher. The LES results are however consistent with the DNS ones even at this lower Prandtl number which is quite high for liquid metals such as lead-bismuth or sodium at operational temperatures. This demonstrates the validity of the hybrid approach for lower Prandtl ; indeed the comparison with a DNS at this Reynolds and at $Pr = 0.01$ would provide better results. For wall modeling strategy in RANS, it can be observed that the assumption of a linear law for the temperature is correct up to $y^+ = 30 - 40$ which is consistent for this lower Prandtl number. The Nusselt number value obtained with the LES is $Nu = 8.50$ and $Nu = 7.89$ for the DNS of Kawamura's team [12] . The difference between these two results is the consequence of the difference in the mean temperature profile.

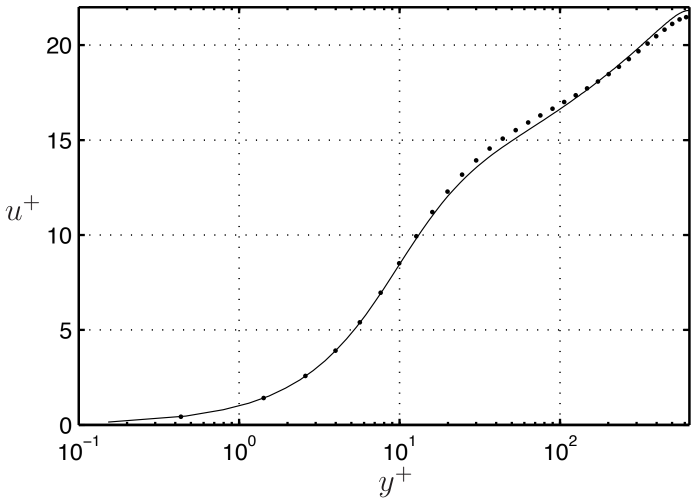

FIGURE 9 – Mean velocity profile for the turbulent channel flow at $Re_\tau = 640$ and $Pr = 0.025$. Present work LES (dots), DNS from [12] (solid).

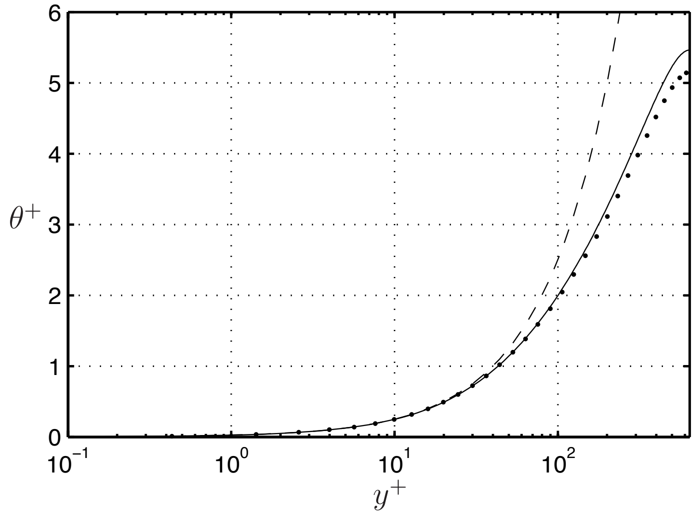

FIGURE 10 – Mean temperature profile for the turbulent channel flow at $Re_\tau = 640$ and $Pr = 0.025$. present work LES (dots), DNS from [12](solid), theoretical near wall behaviour $\theta^+ = Pr \cdot y^+$ (dash).

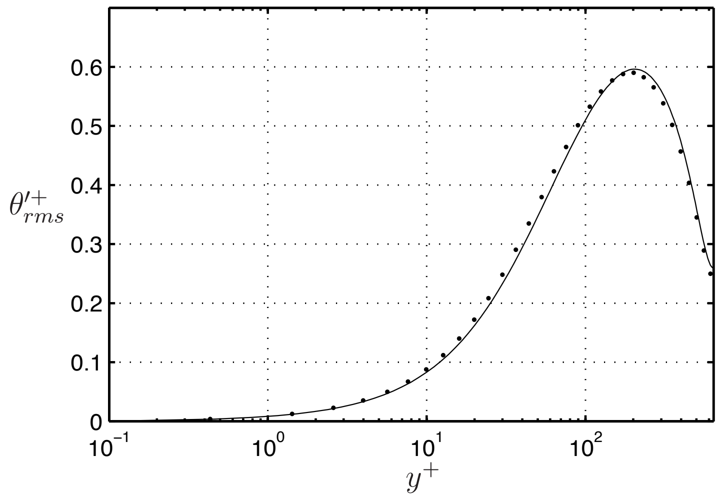

FIGURE 11 – RMS of the temperature fluctuations profile at $Re_\tau = 640$ and $Pr = 0.025$. present work LES (dots), DNS from [12](solid).

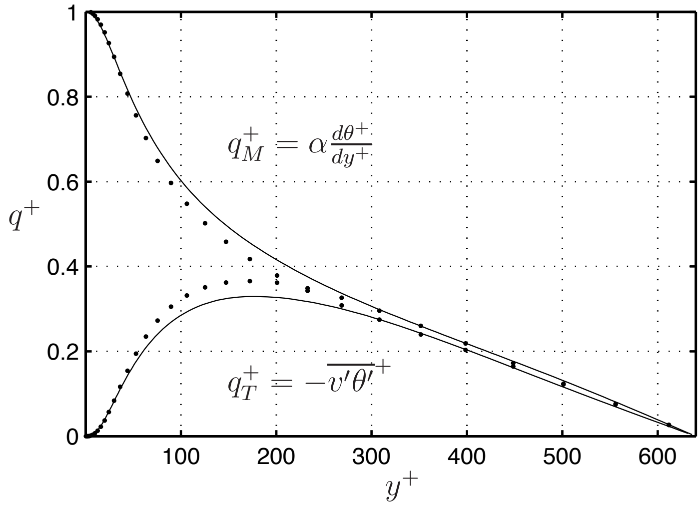

FIGURE 12 – Heat flux decomposition for the turbulent channel flow at $Re_\tau = 640$ and $Pr = 0.025$. present work LES (dots), DNS from [12](solid).

TABLE 2 – Nusselt numbers

Re_τ	Pe	Nu (LES)	Nu (DNS)	Nu (Eq. 1)	Nu (Eq. 2)
590	220	6.02	5.88	5.40	5.84
640	610	8.50	7.89	8.13	7.54

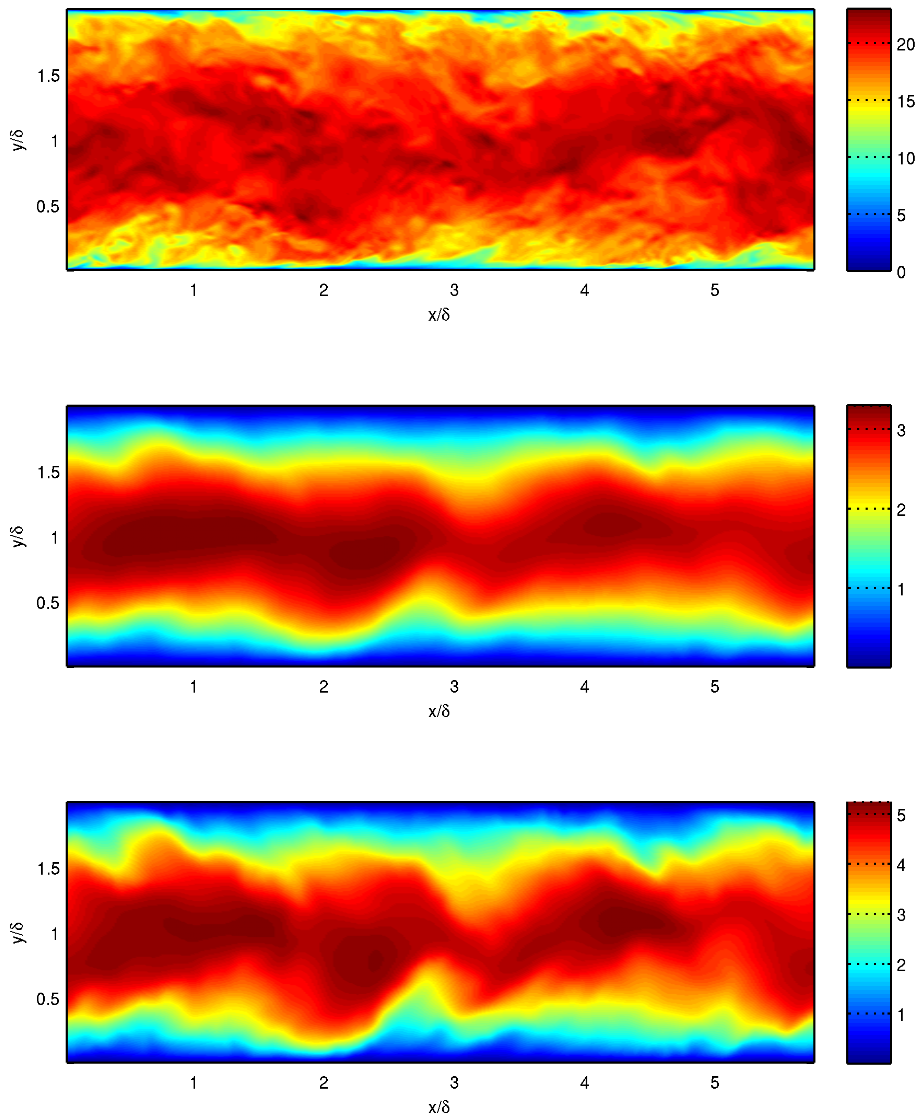

FIGURE 13 – Visualisation of a plane cut in the component u^+ of the velocity field (top) for the DNS at $Re_\tau = 590$. Visualisation of a plane cut in the temperature θ^+ of the velocity field (mid) for the DNS at $Re_\tau = 590$ and $Pr = 0.01$. Visualisation of a plane cut in the temperature θ^+ of the velocity field (bottom) for the DNS at $Re_\tau = 590$ and $Pr = 0.025$.

4 Conclusions and perspectives

In this paper we have presented an original turbulence modeling approach for very low Prandtl flows. This approach, consisting in using a state of the art LES model for the velocity field and using no turbulence model for the thermal part is validated using high quality DNS reference cases at $Re_\tau = 590$ and $Re_\tau = 640$.

As a continuation of this work, this approach should be used for higher Re flows at which no heat transfer DNS results exists (e.g : $Re_\tau = 1000$ and $Re_\tau = 2000$ with $Pr = 0.01$). At a given Prandtl number and for "challenging LES" (with more than four times less points in each direction compared to the DNS), there is a critical Re from which a model is required for the heat transfer ; in those cases, a new subgrid-scale model for the temperature, based on recent multiscale approaches will be proposed. Such a model is only active when there are small turbulent temperature scales in the flow. Finally, this paper could serve as a basis for establishing new best practice guidelines for RANS in particular to set up a consistent near wall modeling strategy and to set up a correct turbulent Prandtl number as proposed in a previous paper [2] of the authors.

ACKNOWLEDGMENTS

The simulations were done using the facilities of the Calcul Intensif et Stockage de Masse (CISM) on the UCL Lemaître cluster funded by Fond National de Recherche Scientifique (FNRS) under a FRFC grant and by UCL (Fonds Spéciaux de Recherche). This research is financially supported by the THINS research project of the Euratom 7th Framework Programme (GA number 249337). Matthieu Duponcheel is a Postdoctoral Researcher of the F.R.S.-FNRS. Dr. Iztok Tiselj from the Reactor Engineering Division of Jozef Stefan Institute is gratefully acknowledged for providing his DNS data.

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