

New subgrid-scale models for large-eddy simulation of Rayleigh-Bénard convection

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Abstract. At the crossroad between flow topology analysis and the theory of turbulence, a new eddy-viscosity model for Large-eddy simulation has been recently proposed by Trias *et al* [PoF, 27, 065103 (2015)]. The S3PQR-model has the proper cubic near-wall behaviour and no intrinsic limitations for statistically inhomogeneous flows. In this work, the new model has been tested for an air turbulent Rayleigh-Bénard convection in a rectangular cell of aspect ratio unity and π span-wise open-ended distance. To do so, direct numerical simulation has been carried out at two Rayleigh numbers $Ra = 10^8$ and 10^{10} , to assess the model performance and investigate *a priori* the effect of the turbulent Prandtl number. Using an approximate formula based on the Taylor series expansion, the turbulent Prandtl number has been calculated and revealed a constant and Ra -independent value across the bulk region equals to 0.55. It is found that the turbulent components of eddy-viscosity and eddy-diffusivity are positively prevalent to maintain a turbulent wind essentially driven by the mean buoyant force at the sidewalls. On the other hand, the new eddy-viscosity model is preliminary tested for the case of $Ra = 10^8$ and showed overestimation of heat flux within the boundary layer but fairly good prediction of turbulent kinetics at this moderate turbulent flow.

1. Introduction

Buoyancy-driven flow has normally been an important subject of scientific studies regard its numerous applications in environment and technology. When thermal buoyancy forms the pure mechanism of developing the turbulent flow more complexity inherits to the heat transport system. This happens in Rayleigh-Bénard convection (RBC), characterized by a fluid layer heated from below and cooled from above. It constitutes a canonical flow that approaches many natural and industrial processes as ventilation of indoor spaces, cooling of electronic devices, convection in the solar plants and dominant circulations in oceans and atmosphere. Although extensive experimental and numerical works have enlightened many turbulent dynamics and heat transport mechanisms in RBC [1], there are still clashes between different studied configurations in respect to the heat transfer scaling, particularly at the ultimate regime (high Rayleigh number $Ra > 10^{14}$ [2]). Nowadays, direct numerical simulation (DNS) is the most used tool that can clarify the experimental differences and provide a fully controlled picture in details about the problem [1]. However, at high Ra numbers, DNS is not feasible since many smaller scales will be produced with high kinetic and thermal dissipations coupled and diversely distributed between the bulk and boundary layer (BL) regions [3]. Hence, in the foreseeable future, numerical



simulations of turbulent RBC will have to resort to models of the small scales. In this sense, large-eddy simulation (LES) have proposed itself to be a reliable tool for investigating thermal turbulent flows at much higher Ra numbers. In LES the contribution of the large-scale energy containing flow is computed directly and only the small-scale effects that are supposed to be isotropic and universal, are modeled. The key feature therein depends on how properly approaching the unresolved subgrid-scale (SGS) of stresses and heat flux evolved in the filtered governing equations (defined in Section 3). To do so, the eddy-viscosity assumption is by far the most used closure model. Examples thereof in RBC, are the well-known Smagorinsky model extended for buoyancy effects by Edison [4] and afterwards the work of Peng *et al.* [5] who used the dynamic Smagorinsky model where the SGS heat flux was treated similarly employing the gradient diffusion hypothesis. They tested their models in horizontally open-ended RBC domain with periodic conditions at Ra numbers up to 10^9 [5], and found a fairly agreement with DNS. However, dynamic strict limitations as known are imposed in respect to the instability and the periodic-direction averaging procedure which make them less amenable in geometrically complex flow. Recently, Foroozani *et al.* [6] has utilized the dynamic Smagorinsky model in Lagrangian technique applied in a cubic cell at Ra numbers up to 10^{10} , and found a good agreement with the analogous experiments. Therein, the previous limitations are overcome but the models require high complexity and significant computational cost, as well substantial deviations of turbulence features from that in cylindrical cells, are observed. In this work, the new subgrid-scale eddy viscosity models proposed recently by Trias *et al.* [7] are tested in RBC. The S3PQR-model [7] has the proper cubic near-wall behaviour, no intrinsic limitations for statistically inhomogeneous flows and has already been successfully tested for several flows as decaying isotropic turbulence and turbulent channel flow. In order to assess its performance, DNS study has been carried out [8] and used to investigate the turbulent Prandtl number Pr_t . In the LES, the SGS heat flux are treated following the gradient transport hypothesis and the turbulent diffusivity κ_t is deduced from the eddy viscosity ν_t with a constant Pr_t . Such studies as Chumakov [9] in homogeneous isotropic turbulence, has shown the strong correlation of the SGS scalar flux with the SGS stress and consequently derive to the reasonable validation of Daly and Harlow [10] assumption that approaches κ_t in terms of the SGS stress tensor. Therefore we think that the constant turbulent Prandtl number is a viable option where the κ_t will rely on how quality ν_t is calculated.

2. Direct numerical simulation

We consider an air-flow (Prandtl number $Pr = 0.7$) in a rectangular cell of aspect ratio unity (square cross-section) and π longitudinal distance (see Figure 1). The fluid is heated from below and cooled from above by two isothermal walls while the lateral sidewalls are adiabatic. No-slip condition is applied on all the four solid walls whereas periodic one is imposed in the longitudinal direction. Under these assumptions, the mechanism of RBC is developed and described by the governing equations of Navier-Stokes (NS) and the thermal energy. They read, in non-dimensional form, as follows

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + (Pr/Ra)^{1/2} \nabla^2 \mathbf{u} + \mathbf{f}, \quad \nabla \cdot \mathbf{u} = 0, \quad (1)$$

$$\partial_t T + (\mathbf{u} \cdot \nabla) T = (RaPr)^{-1/2} \nabla^2 T, \quad (2)$$

where $\mathbf{u} = (u, v, w)$ is the velocity vector in $\mathbf{x} = (x, y, z)$ Cartesian coordinates, p is the pressure field and $\mathbf{f} = (0, 0, T)$ is the body force vector with the temperature field T . Two Ra numbers have been considered $Ra \in \{10^8, 10^{10}\}$ in a spatial finite volume staggered discretization using fourth-order symmetry preserving scheme and a second-order explicit one-leg scheme regard the temporal discretization (references in [8]). The grids are constructed following refinement approaches that satisfy the DNS requirements [11] with an accurate solution and

low computational cost. For details about DNS procedures and references quantities of the governing equations the reader is referred to [8]. Here the main simulation parameters with the Nusselt number (Nu) results are outlined in Table 1, that correspond very well with the results of recent DNS as Scheel *et al* . [12].

Table 1: Summary of simulation parameters where N_{BL} is the number of grid points within the thermal BL and t_{avg} is the averaging time in free-fall time units (TU).

Case	Ra	$N_x \times N_y \times N_z$	N_{BL}	$t_{avg}[TU]$	Nu
DNS1	10^8	$400 \times 208 \times 208$	9	500	30.9
DNS2	10^{10}	$1024 \times 768 \times 768$	12	200	128.1

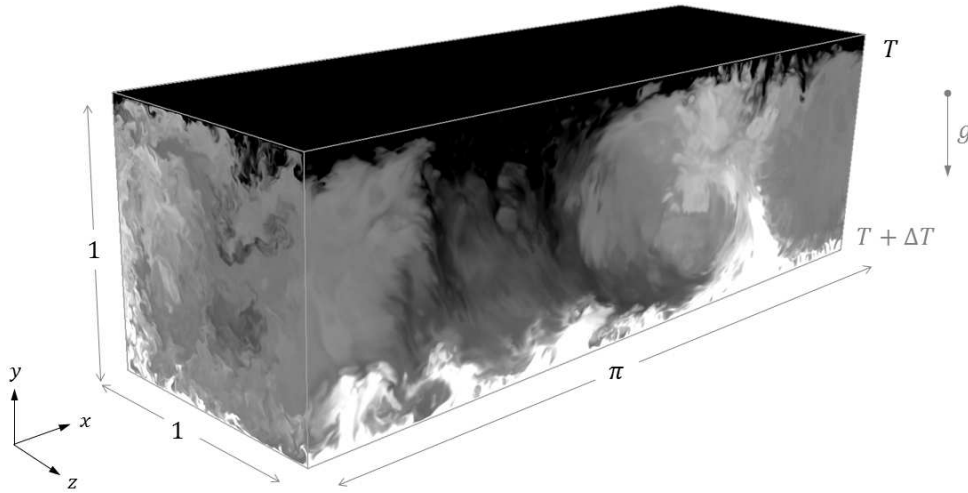


Figure 1: DNS temperature snapshot in the studied RB configurations at $Ra = 10^{10}$.

3. Large-eddy simulation

We consider hereafter the most popular Large-eddy simulation (LES) in the framework of the new eddy-viscosity models proposed by Trias *et al* . [7], for the case of RBC problem. Shortly, LES equations result from applying a spatial filter, with filter length Δ , under which the (small) scales of motion are modeled. The large scales that are more energetic and boundary conditions dependent, are resolved directly without modeling, in contrary to the Reynolds averaged Navier-Stokes (RANS) methods that model all the scales. Following the governing equations (Eqs 1 and 2), LES filtered equations are given as

$$\partial_t \bar{\mathbf{u}} + (\bar{\mathbf{u}} \cdot \nabla) \bar{\mathbf{u}} = -\nabla \bar{p} + (Pr/Ra)^{1/2} \nabla^2 \bar{\mathbf{u}} + \bar{\mathbf{f}} - \nabla \cdot \tau(\bar{\mathbf{u}}), \quad \nabla \cdot \bar{\mathbf{u}} = 0, \quad (3)$$

$$\partial_t \bar{T} + (\bar{\mathbf{u}} \cdot \nabla) \bar{T} = (RaPr)^{-1/2} \nabla^2 \bar{T} - \nabla \cdot q(\bar{\mathbf{u}}, \bar{T}), \quad (4)$$

where $\bar{\mathbf{u}}$, \bar{T} and \bar{p} are respectively the filtered velocity, temperature and pressure. The SGS stress tensor $\tau(\bar{\mathbf{u}})$ and the SGS heat flux vector $q(\bar{\mathbf{u}}, \bar{T})$, approximate the effect of the under-resolved scales as

$$\tau(\bar{\mathbf{u}}) \approx \overline{\mathbf{u} \otimes \mathbf{u}} - \bar{\mathbf{u}} \otimes \bar{\mathbf{u}}, \quad (5)$$

$$q(\bar{\mathbf{u}}, \bar{T}) \approx \overline{\mathbf{u} T} - \bar{\mathbf{u}} \bar{T}, \quad (6)$$

and they need to be modeled in order to close the system. The most popular assumptions thereof, are the eddy-viscosity models where the SGS stress tensor is approached as

$$\tau(\bar{\mathbf{u}}) \approx -2\nu_t \mathbf{S}(\bar{\mathbf{u}}). \quad (7)$$

where $\mathbf{S}(\bar{\mathbf{u}}) = 1/2(\nabla \bar{\mathbf{u}} + \nabla \bar{\mathbf{u}}^t)$ is the rate-of-strain tensor. Similarly, the SGS heat flux is approximated employing the gradient-diffusion hypothesis and given by

$$q(\bar{\mathbf{u}}, \bar{T}) \approx -\kappa_t \nabla \bar{T}. \quad (8)$$

By applying the Reynolds analogy *i.e.* the assumption of that the heat flux in a turbulent system is analogous to momentum flux, which suggests that its ratio must be constant for all horizontal positions. Hence, the eddy-diffusivity κ_t is derived from the eddy-viscosity ν_t by a constant turbulent Prandtl number Pr_t as

$$\kappa_t = \nu_t / Pr_t. \quad (9)$$

The effect of Pr_t is investigated in the next Section 4, while ν_t is calculated following the S3PQR-model recently proposed by Trias *et al.* [7] where the eddy-viscosity is based on the first $P_{\mathbf{GG}^t}$, second $Q_{\mathbf{GG}^t}$ and the third $R_{\mathbf{GG}^t}$ invariants of \mathbf{GG}^t tensor with $\mathbf{G} \equiv \nabla \bar{\mathbf{u}}$, the gradient of the resolved velocity field. They read as follows

$$\nu_t^{S3PQ} = (C_{s3pq} \Delta)^2 P_{\mathbf{GG}^t}^{-5/2} Q_{\mathbf{GG}^t}^{3/2}, \quad (10)$$

$$\nu_t^{S3PR} = (C_{s3pr} \Delta)^2 P_{\mathbf{GG}^t}^{-1} Q_{\mathbf{GG}^t}^{1/2}, \quad (11)$$

$$\nu_t^{S3QR} = (C_{s3qr} \Delta)^2 Q_{\mathbf{GG}^t}^{-1} R_{\mathbf{GG}^t}^{5/6}, \quad (12)$$

where C is the model constant and Δ is the subgrid characteristic length. They have the proper cubic near-wall behaviour with a guarantee to locality, numerical stability, no intrinsic limitations for stability inhomogeneous flows (complex geometrically flows) and low computational cost. The S3QR-model (Eq. 12) is used here with a model constant equals to $C_{s3qr} = 0.762$, where more details about the three new models are available in the corresponding work [7].

4. Turbulent Prandtl number Pr_t

Turbulent Prandtl number is defined as the ratio between ν_t and κ_t , ($Pr_t = \nu_t / \kappa_t$) indicating the link between the subgrid effects of thermals and kinetics in a turbulent system. It is an extremely difficult quantity to measure by experiments and depends intimately on the molecular fluid properties and the flow parameters [13]. For example, in the scope of the most used Reynolds analogy in considering a constant value of Pr_t , Kim and Moin [14] gave a range of the turbulent Prandtl number equals to 0.4 in the center and 1 near the walls of a forced convection heat transfer air channel flow. Pallares and Davidson [15] clarified that just a simple value $Pr_t = 0.4$ agrees well with the DNS and experimental results. However these results were restricted for air flow ($Pr \sim 1$). In RBC, Eidson [4] suggested a value of 0.4 in his model that included the SGS buoyant production contribution in evaluating ν_t . In summary, different values can be found in the literature ranging from 0.1 to 1.0 [16] in addition to the dynamic procedures and temperature dependence Pr_t models. The majority are sharing the behaviour of flat profile of Pr_t in the bulk and increased maximum values near the wall in stratified and buoyancy effects flows. In the present work, the Pr_t has been evaluated *a priori* using the DNS dataset. To do so, the left-hand-sides of Eqs. 7 and 8 have been approximated by the leading term of the Taylor series expansion, *i.e.* $\tau(\bar{\mathbf{u}}) \approx (\Delta^2/12)\mathbf{AA}^t$ and $q(\bar{\mathbf{u}}, \bar{T}) \approx (\Delta^2/12)\mathbf{A}\nabla T$. Then, the values of ν_t and κ_t

are obtained using a least square minimization combined with an ensemble temporal average $\langle \cdot \rangle$, as following

$$\nu_t \approx - \left\langle \frac{\mathbf{A}\mathbf{A}^t : \mathbf{S}(\mathbf{u})}{2\mathbf{S}(\mathbf{u}) : \mathbf{S}(\mathbf{u})} \right\rangle, \quad (13)$$

$$\kappa_t \approx - \left\langle \frac{\mathbf{A}\nabla T \cdot \nabla T}{\nabla T \cdot \nabla T} \right\rangle, \quad (14)$$

where $\mathbf{A} \equiv \nabla \mathbf{u}$. This can evolve to a dynamical model of Pr_t , however the averaging (locally or temporally) procedure would be necessary since it can produce effective negative diffusion (or eddy-viscosity) which potentially leads to a blowup in calculations [17, 18]. The resultant profiles of averaged in time and the horizontal (x, z) plane for Pr_t , ν_t and κ_t , have been presented in Figure 2, where ν_t and κ_t are normalized by their maximum values. In consistent with the literature, the Pr_t reveals a similar behaviour in taking a constant value in the bulk region $Pr_t \approx 0.55$ that increases near the walls till numbers bigger than 1. The interesting result is the fact that the value of Pr_t in the bulk of turbulent RBC seems to be universal *i.e.* it is independent of Ra number and in fairly good correspondence with the most popular used value of 0.4. The

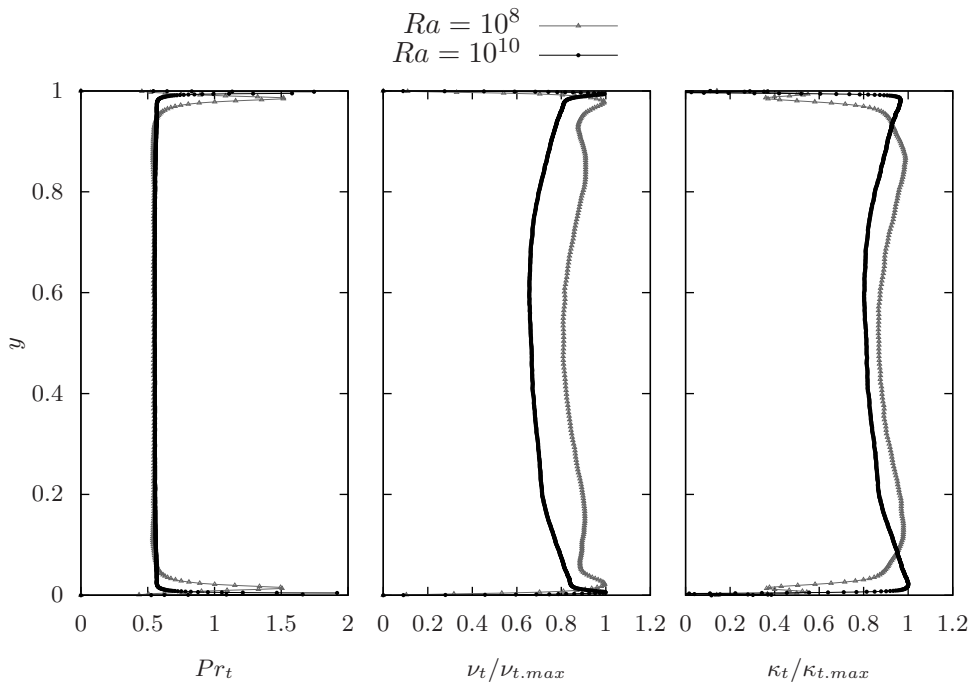


Figure 2: Vertical profiles of the averaged time and (x, z) plane of Pr_t , $\nu_t/\nu_{t.max}$ and $\kappa_t/\kappa_{t.max}$ evaluated from Eqs. 13 and 14.

profiles of the turbulent viscosity and diffusivity are positively skewed in average near the walls where the emission of thermals take a place and arise by buoyancy. This emphasize the findings of Burr *et al.* [19], that the mean flow is driven by the mean buoyant forces and not by the Reynolds stresses and the turbulent energy production is positive *i.e.* positive eddy-viscosity. However, it is well-known the phenomena of counter-gradient turbulent transport of momentum in RBC *i.e.* negative eddy-viscosity [20], when the kinetic energy moves in the opposite direction - from the fluctuations to the mean flow. It is mainly explained as almost all the thermal plumes rising from the heated bottom or falling from the cooled top that convey the most portion of kinetic and thermal coupled fluctuations, are accumulating and tilted away to contribute to the

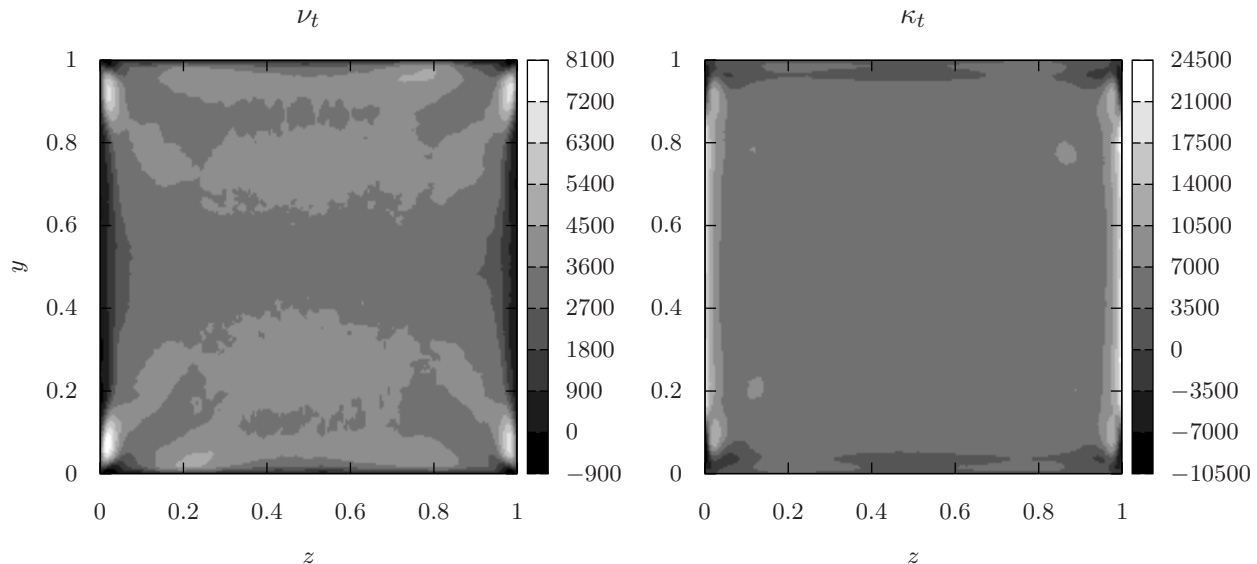


Figure 3: Averaged time and periodic x -direction planes of ν_t and κ_t , evaluated from Eqs. 13 and 14.

momentum transport in the mean flow. In order to gain more insight, the averaged time and periodic x -direction planes of ν_t and κ_t , are plotted in Figure 3 in the case of $Ra = 10^8$. Both terms reveal negative values limited in the corners of the lateral adiabatic sidewalls. The highest positive values of κ_t correspond with the plumes traveling in the vicinities of the sidewalls where the values of ν_t are so small (almost zero). While, next to the thermal BLs, ν_t presents high positive magnitudes in regions of the out impinging flow (mixing action or the opposite-side plumes) to concentrate with four ν_t peaks in the four corners (see Figure 3, left). This leads to a turbulent wind driven by the mean buoyant force at the sidewalls with a positive eddy-viscosity domination.

5. Preliminary results

Since no significant difference was reported in the literature regarding the change of Pr_t value over the number 0.4 (ranging from 0.1 to 1), the value found from the DNS assumption 0.55 is used in Eq. 9. The obtained results of the overall Nu number in Table 2, and profiles of the averaged (time and periodic direction) turbulent features in Figure 4, are presented for the case of $Ra = 10^8$. It can be noted that the model can predict well the turbulent kinetic statistics both in the BL and bulk regions of RBC where the turbulence is comparable statistically to isotropic nature far enough from the solid walls. Regard the turbulent heat flux, the model capture its evolution in the bulk even at coarser grids with significant improved behaviour in comparison with the no-model case, however it overestimates the fluctuated thermals within the BL where the Pr_t takes its highest values essentially associated with the number of Ra . This could emphasize on the outstanding importance of the dynamical coupling between kinetic and thermals that occurs in the BLs and the constant modeling should take it in account. In other words, the impacts of the buoyant production particularly in the thermal plumes born region (thermal BL) are critical and have to be included in assuming the model constants as C_{s3qr}

Table 2: Obtained results of the overall averaged Nu number at DNS and LES grids.

Mesh	DNS1	Mesh A		Mesh B	
	$400 \times 208 \times 208$	$120 \times 80 \times 80$	No model S3QR	$168 \times 110 \times 110$	No model S3QR
Nu	30.86	39.2	38.0	35.6	35.0

and Pr_t at this moderate turbulent case. These impacts become reduced with increasing the Ra number because the BL tends to be diminished and the flow becomes bulk dominated for instance in the ultimate regime. Therefore, it can be said that there is strong trend of the new models to be the key ingredient in turbulent natural convection models type RBC at very high Ra numbers, since they predict well the flow behaviour through the bulk.

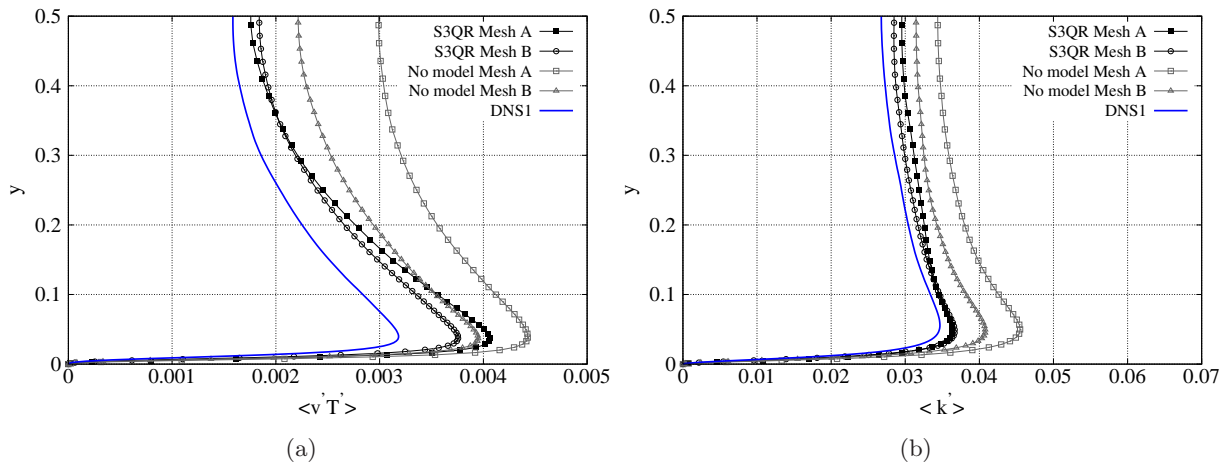


Figure 4: Vertical profiles of turbulent heat flux $\langle v'T' \rangle$ (a) and the turbulent kinetic energy $\langle k' \rangle$ (b), taken along the mid-width $z = 0.5$ line from the averaged time and periodic x -direction plane. Regard the symmetry, the profiles are closer viewed in range of $y = [0, 0.5]$.

6. Concluding remarks

The new eddy-viscosity models proposed by Trias *et al.* [7] have been tested for an air turbulent RBC within a rectangular cell of aspect ratio unity and π span-wise open-ended distance. To do so, DNS study is considered at two Ra numbers 10^8 and 10^{10} in order to judge the model performance and investigate the effect of the turbulent Prandtl number Pr_t . Using an approximate formula based on the Taylor series expansion with the least square technique, the eddy-viscosity ν_t and the turbulent diffusivity κ_t have been calculated from the DNS dataset and revealed a positive mean prevailing within RBC. These have supported the fact that the wind turbulent is mainly driven by the buoyant force at the sidewalls and not by the Reynolds stresses and the turbulent energy production is positive. Applying their ratio in $Pr_t = \nu_t / \kappa_t$, the turbulent Prandtl number has displayed a constant value of 0.55 across the bulk, independent of Ra number which consists very well with the values in literature. Afterwards, the S3QR-model [7] has preliminary used in LES frame modeling at $Ra = 10^8$. Therein, the subgrid under-resolved terms have been approached following the gradient-diffusion and turbulent-viscosity

hypotheses where ν_t is based on the Q_{GG^t} and R_{GG^t} invariants of the resolved GG^t tensor and κ_t is derived from ν_t with a constant Pr_t . The results have revealed an overestimation of Nu number and turbulent heat flux within the BL where an important dynamical kinetic/thermal coupling should be taken in account in the constants of the model at this number of Ra . However, the bulk turbulent features, in particular the kinetics through both the BL and bulk, are fairly good predicted in comparison with the no-model case, the issues that strongly encourage the new model trends to be key ingredient in turbulent RBC models at very high Ra number.

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