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On a proper tensor-diffusivity model for large-eddy simulation of buoyancy-driven turbulence

F.X. Trias · F. Dabbagh · A. Gorobets ·
C. Olier

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Abstract In this work, we aim to shed light to the following research question: *can we find a nonlinear tensorial subgrid-scale (SGS) heat flux model with good physical and numerical properties, such that we can obtain satisfactory predictions for buoyancy-driven turbulent flows?* This is motivated by our findings showing that the classical (linear) eddy-diffusivity assumption, $\mathbf{q}^{eddy} \propto \nabla \overline{T}$, fails to provide a reasonable approximation for the actual SGS heat flux, $\mathbf{q} = \overline{\mathbf{u}T} - \overline{\mathbf{u}}\overline{T}$: namely, *a priori* analysis for air-filled Rayleigh-Bénard convection (RBC) clearly shows a strong misalignment. In the quest for more accurate models, we firstly study and confirm the suitability of the eddy-viscosity assumption for RBC carrying out *a posteriori* tests for different models at very low Prandtl numbers (liquid sodium, $Pr = 0.005$) where no heat flux SGS activity is expected. Then, different (nonlinear) tensor-diffusivity SGS heat flux models are studied *a priori* using DNS data of air-filled ($Pr = 0.7$) RBC at Rayleigh numbers up to 10^{11} . Apart from having good alignment trends with the actual SGS heat flux, we also restrict ourselves to models that are numerically stable *per se* and have the proper cubic near-wall behavior. This analysis leads to a new family of SGS heat flux models based on the symmetric positive semi-definite tensor $\mathbf{G}\mathbf{G}^T$ where $\mathbf{G} \equiv \nabla \overline{\mathbf{u}}$, *i.e.* $\mathbf{q} \propto \mathbf{G}\mathbf{G}^T \nabla \overline{T}$, and the invariants of the $\mathbf{G}\mathbf{G}^T$ tensor.

Keywords LES · subgrid-scale models · buoyancy-driven flows · turbulence · tensor-diffusivity

F.X. Trias (corresponding author) · F. Dabbagh · C. Olier
Heat and Mass Transfer Technological Center (CTTC), Technical University of Catalonia,
C/Colom 11, 08222 Terrassa (Barcelona) E-mail: xavi@cttc.upc.edu

F. Dabbagh
Christian Doppler Laboratory for Multi-Scale Modeling of Multiphase Processes, Johannes
Kepler University, Altenbergerstraße 69, 4040 Linz, Austria

A. Gorobets
Keldysh Institute of Applied Mathematics of Russian Academy of Sciences, 4A, Miusskaya
Sq., Moscow 125047, Russia

1 Introduction

Turbulent flows driven by thermal buoyancy are present in many scientific and technological applications, such as solar thermal power plants, indoor space heating and cooling, flows in nuclear reactors, electronic devices, and convection in the atmosphere, oceans and the deep mantle. The self-sustained cycle of plumes produces alternative nonequilibriums between the buoyant production and the viscous dissipation, which are mainly compensated by the pressure transport mechanisms [1]. Therefore, predicting the complex coherent dynamics in a turbulent buoyancy-driven flow is a great challenge. In this regard, direct numerical simulations (DNS) have provided a fruitful knowledge about the problem in the fields of coherent dynamics and turbulence physics [2, 3]. Apart from overcoming the uncertainties pertaining to experimental studies, in the last decade DNS has allowed to investigate and resolve many queries in Rayleigh-Bénard convection (RBC) at relatively high Rayleigh, Ra , numbers [4–9]. However, DNS of the buoyancy-driven flows is limited to relatively low Rayleigh numbers because the convective term produces far too many relevant scales of motion. Therefore, in the foreseeable future, numerical simulations of turbulent flows will have to resort to models of the subgrid-scales (SGS). We, therefore, turn to large-eddy simulation (LES) to predict the large-scale behavior of incompressible turbulent flows driven by buoyancy. In LES, the large-scale motions are explicitly computed, whereas the effects of small-scale motions are modeled. Since the advent of computational fluid dynamics, many SGS models have been proposed and successfully applied to a wide range of flows (see, for instance, the encyclopedic works of Sagaut [10] and Berselli *et al.* [11]). Eddy-viscosity models for LES is probably the most popular example thereof. Then, the SGS heat flux is usually modeled using the (linear) eddy-diffusivity assumption. However, this type of model systematically fails to provide a reasonable approximation of the actual SGS heat flux because they are strongly misaligned [12]. This was clearly shown in our previous work [13] where SGS features were studied *a priori* for a RBC at Ra -number up to 10^{10} . This leads to the conclusion that nonlinear (or tensorial) models are necessary to provide a good approximation of the actual SGS heat flux. In this regard, the nonlinear Leonard model [14], which is the leading term of the Taylor series expansion of the SGS heat flux, provides very accurate *a priori* approximation. However, the local dissipation introduced by the model can take negative values; therefore, the Leonard model cannot be used as a standalone SGS heat flux model, since it produces a finite-time blow-up. A similar problem is encountered with the nonlinear tensorial model proposed by Peng and Davidson [15]. An attempt to overcome these instability issues is the so-called mixed model [12], where the Leonard model is combined with an eddy-diffusivity model.

In this context, we plan to shed light to the following research question: *can we find a nonlinear subgrid-scale heat flux model with good physical and numerical properties, such that we can obtain satisfactory predictions for buoyancy-*

driven turbulent flows? To that end, we consider nonlinear SGS heat flux models that can adequately represent the dynamics of the smallest (unresolved) scales, overcoming the above-mentioned inherent limitations of the eddy-diffusivity models [13]. The specific SGS models that we consider consist of a linear eddy-viscosity term for momentum supplemented by a nonlinear model for the SGS heat flux. The model terms are designed to preserve important mathematical and physical properties, such as symmetries of the Navier-Stokes equations, and the near-wall scaling and the dissipative nature of the SGS. The desired features are already included in existing models for the SGS stresses. Examples of eddy-viscosity models that exhibit the proper near-wall behavior are the WALE model [16], the σ -model [17], and the S3PQR model proposed in our previous work [18]. Therefore, the present work focuses on the development of a nonlinear SGS heat flux that, among other features, is numerically stable *per se* and provides a good representation of the actual SGS heat flux both in the bulk and near-wall regions. Note that preliminary stages of this work were already presented in the 7th ECCOMAS-CFD conference [19], the ICCFD10 conference [20], the DLES12 conference [21] and the ETC17 conference [22].

The rest of the paper is organized as follows. In the next section, the theoretical background of LES simulation of buoyancy-driven flows is presented together with an *a priori* analysis of the SGS features of existing SGS heat flux models. Then, in Section 3 the suitability of the eddy-viscosity assumption to model the SGS stresses is assessed carrying out RBC simulations at a very low Prandtl number (liquid sodium, $Pr = 0.005$). In this case, only SGS stresses need to be modeled for the momentum equation since no heat flux SGS activity is expected at such a low Pr number. Then, in Section 4, different aspects of nonlinear SGS heat flux models are studied. This analysis leads to a new family of nonlinear SGS heat flux models: apart from being numerically stable *per se*, they show a good representation of the SGS heat flux both in the bulk and the near-wall region. Finally, relevant results are summarized and conclusions are given.

2 Background

2.1 Large-eddy simulation of buoyancy-driven turbulent flows

In LES, a coarse-graining or spatial filtering operation is applied to distinguish between large and small scales of motion. This operation is denoted by an over-bar in what follows, $\overline{(\cdot)}$. Then, the governing equations are the filtered

Fig. 1 Schema of the Rayleigh-Bénard configuration studied displayed together with the instantaneous temperature field corresponding to the air-filled ($Pr = 0.7$) DNS at $Ra = 10^{10}$ [3, 13]

Navier-Stokes (NS) and the thermal energy equations

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + (\bar{\mathbf{u}} \cdot \nabla) \bar{\mathbf{u}} = \sqrt{\frac{Pr}{Ra}} \nabla^2 \bar{\mathbf{u}} - \nabla \bar{p} + \bar{\mathbf{f}} - \nabla \cdot \bar{\boldsymbol{\tau}}; \quad \nabla \cdot \bar{\mathbf{u}} = 0, \quad (1)$$

$$\frac{\partial \bar{T}}{\partial t} + (\bar{\mathbf{u}} \cdot \nabla) \bar{T} = \frac{1}{\sqrt{RaPr}} \nabla^2 \bar{T} - \nabla \cdot \bar{\mathbf{q}}, \quad (2)$$

where $\bar{p}$ is the filtered pressure, $\bar{T}$ is the filtered temperature and $\bar{\mathbf{u}} = (\bar{u}, \bar{v}, \bar{w})$ is the filtered velocity field in Cartesian coordinates $\mathbf{x} = (x, y, z)$. The reference length, temperature and velocity used for the dimensionless form are respectively the cavity height, H , the temperature difference between the upper and lower walls, $\Delta\theta$, and the buoyant velocity, $\sqrt{\alpha g H \Delta\theta}$. The Boussinesq approximation is used to model the buoyancy forces, *i.e.* $\bar{\mathbf{f}} = (0, \bar{T}, 0)$. The studied configuration is displayed in Figure 1; namely, a squared cross section with a longitudinal span-wise open-ended distance of π . The cavity is subjected to a temperature difference between the horizontal isothermal walls whereas the vertical walls are adiabatic. No-slip boundary condition is imposed for velocity at the four solid walls. Periodic boundary conditions are applied in the span-wise direction for all quantities. Hence, the system only depends on the Rayleigh number based on the cavity height $Ra = (\alpha g \Delta\theta H^3)/(\nu\kappa)$, and the Prandtl number $Pr = \nu/\kappa$, where α is the volumetric thermal expansion coefficient, g is the gravitational acceleration, ν is the kinematic viscosity and κ is the thermal diffusivity. The global response of the system is measured via the average Nusselt number, Nu , given by

$$Nu = \sqrt{RaPr} \langle vT \rangle_A - \frac{\partial \langle T \rangle_A}{\partial y}, \quad (3)$$

where the brackets operator, $\langle \cdot \rangle$, denotes the temporal average and the subscript A refers to the average over an horizontal $x - z$ plane at a given y -position. Finally, the SGS stress tensor, τ , and the SGS heat flux vector, $\mathbf{q}$, represents the effect of the unresolved scales,

$$\tau = \overline{\mathbf{u} \otimes \mathbf{u}} - \overline{\mathbf{u}} \otimes \overline{\mathbf{u}}, \quad (4)$$

$$\mathbf{q} = \overline{\mathbf{u}T} - \overline{\mathbf{u}}\overline{T}, \quad (5)$$

and they need to be modeled to close the system. In this regard, the most common approach is the eddy-viscosity assumption: *i.e.* the SGS stress tensor and the rate-of-strain tensor, $\mathbf{S} = 1/2(\nabla\overline{\mathbf{u}} + \nabla\overline{\mathbf{u}}^T)$, are aligned

$$\tau \approx -2\nu_e \mathbf{S}(\overline{\mathbf{u}}), \quad (6)$$

where ν_e is the eddy-viscosity. Similarly, the SGS heat flux is often approximated employing the gradient-diffusion hypothesis (linear model), given by

$$\mathbf{q} \approx -\kappa_t \nabla \overline{T} \quad (\equiv \mathbf{q}^{eddy}). \quad (7)$$

Then, the Reynolds analogy assumption is usually applied to evaluate the eddy-diffusivity, κ_t . In this case, the eddy-diffusivity, κ_t , is computed from the eddy-viscosity, ν_e , using a constant turbulent Prandtl number, Pr_t , independently of the instantaneous flow topology, *i.e.* $\kappa_t = \nu_e/Pr_t$. These assumptions were shown to be erroneous to provide accurate predictions of the SGS heat flux [12, 13, 23]. Namely, *a priori* analysis shows that the eddy-diffusivity assumption, $\mathbf{q}^{eddy}$ (Eq. 7), is completely misaligned with the actual SGS heat flux, $\mathbf{q}$ (see Figure 2, top left). To explain this, it can be argued that the rotational geometries are prevalent in the bulk region over the strain slots, *i.e.* $|\Omega| > |\mathbf{S}|$ (see Refs [3, 13]). Then, the dominant skew-symmetric rate-of-rotation tensor, Ω , rotates the thermal gradient vector, $\nabla\overline{T}$, to be almost perpendicular to $\mathbf{q}^{eddy}$ (see Eqs.7 and 9). Here, $\mathbf{G}$ represents the gradient of the resolved velocity field, *i.e.* $\mathbf{G} \equiv \nabla\overline{\mathbf{u}}$. Then, the rate-of-strain, $\mathbf{S}$, and the rate-of-rotation, Ω , tensors are respectively given by the symmetric and skew-symmetric parts of $\mathbf{G}$,

$$\mathbf{S} = \frac{1}{2}(\mathbf{G} + \mathbf{G}^T) \quad \Omega = \frac{1}{2}(\mathbf{G} - \mathbf{G}^T). \quad (8)$$

Therefore, the eddy-diffusivity paradigm is only applicable in the not-so-frequent strain-dominated areas. This matches with the findings of Chumakov [24], who performed *a priori* study of the SGS flux of a passive scalar in isotropic homogeneous turbulence.

In contrast, the tensor diffusivity (nonlinear) Leonard model [14], which is actually the leading term of the Taylor series expansion of $\mathbf{q}$,

$$\mathbf{q} \approx \frac{\delta^2}{12} \mathbf{G} \nabla \overline{T} \quad (\equiv \mathbf{q}^{nl}), \quad (9)$$

provides a much more accurate *a priori* representation of $\mathbf{q}$ (see Figure 2, top left).

Fig. 2 Joint probability distribution functions (PDF) of the angles (α, β) defined in the top right figure and plotted on a half unit sphere to show the orientation trends in the space of the mixed model. The PDF of γ is shown along the bottom strip of each chart. Alignment trends of the actual SGS heat flux, $\mathbf{q}$ (top, left), the Daly and Harlow [25] model (see $\mathbf{q}^{DH}$ in Eq. 12) (bottom, left) and the Peng and Davidson model [15] (see $\mathbf{q}^{PD}$ in Eq. 10) (bottom, right). For comparative and simplicity reasons, the JPDF and the PDF magnitudes are normalized by its maximal. For further details, the reader is referred to our paper [13].

2.2 Nonlinear SGS heat flux models for large-eddy simulation

Since the eddy-diffusivity, $\mathbf{q}^{eddy}$, cannot provide an accurate representation of the SGS heat flux, we turn our attention to nonlinear tensorial models. As mentioned above, the Leonard model [14] given in Eq.(9) can provide a very accurate *a priori* representation of the SGS heat flux (see Figure 2, top left). However, the local dissipation (in the L2-norm sense) is proportional to $\nabla T \cdot \mathbf{G} \nabla T = \nabla T \cdot \mathbf{S} \nabla T + \nabla T \cdot \mathbf{\Omega} \nabla T = \nabla T \cdot \mathbf{S} \nabla T$ (recall that $\mathbf{\Omega}$ is a skew-symmetric tensor). Since the velocity field is divergence-free, $\lambda_1^S + \lambda_2^S + \lambda_3^S = \text{tr}(\mathbf{S}) = \nabla \cdot \bar{\mathbf{u}} = 0$, where λ_i^S represents the eigenvalues of the rate-of-strain tensor $\mathbf{S}$. Then, the eigensystem can be ordered $\lambda_1^S \geq \lambda_2^S \geq \lambda_3^S$ with $\lambda_1^S \geq 0$ (extensive eigendirection) and $\lambda_3^S \leq 0$ (compressive eigendirection), and λ_2^S is either positive or negative. Hence, the local dissipation introduced by the model can take negative values; therefore, the Leonard model cannot be used

as a standalone SGS heat flux model, since it produces a finite-time blow-up. The same problem is encountered with the nonlinear tensorial model proposed by Peng and Davidson [15],

$$\mathbf{q} \approx C_t \delta^2 \mathbf{S} \nabla \bar{T} \quad (\equiv \mathbf{q}^{PD}), \quad (10)$$

which actually has exactly the same dissipation (in the L2-norm sense) as the Leonard model. An attempt to overcome these instability issues is the so-called mixed model [12], where the Leonard model (Eq. 9) is linearly combined with an eddy-diffusivity model (Eq. 7),

$$\mathbf{q} \approx \frac{\delta^2}{12} (\mathbf{G} \nabla \bar{T} - \Lambda |\mathbf{S}| \nabla \bar{T}) \quad (\equiv \mathbf{q}^{mix}), \quad (11)$$

where Λ is the ratio of the corresponding model coefficients. Another interesting nonlinear model was proposed by Daly and Harlow [25] for modeling the SGS heat flux for RANS,

$$\mathbf{q} \approx -\mathcal{T}_{SGS} \tau \nabla \bar{T} = -\frac{1}{|\mathbf{S}|} \frac{\delta^2}{12} \mathbf{G} \mathbf{G}^T \nabla \bar{T} \quad (\equiv \mathbf{q}^{DH}), \quad (12)$$

where $\mathcal{T}_{SGS} = 1/|\mathbf{S}|$ is an appropriate SGS timescale [24] and the SGS stress tensor, τ , is approximated with the gradient model [26], *i.e.* $\tau \approx (\delta^2/12) \mathbf{G} \mathbf{G}^T$. Notice that the model proposed by Peng and Davidson (Eq. 10) can be viewed in the same framework if the SGS stress tensor is estimated by an eddy-viscosity model, *i.e.* $\tau \approx -2\nu_e \mathbf{S}$ and $\mathcal{T}_{SGS} \propto \delta^2/\nu_e$. These two models have shown a much better *a priori* alignment with the actual SGS heat flux (see Figure 2, bottom) than the eddy-diffusivity model.

3 Assessment of eddy-viscosity models for buoyancy-driven turbulent flows

As mentioned above, we focus on finding a nonlinear SGS heat flux model with good physical and mathematical properties, that provides an accurate approximation of the actual SGS heat flux, $\mathbf{q}$. In particular, the specific SGS models that we consider consist of a linear eddy-viscosity term for momentum (see Eq. 6) supplemented by a nonlinear model for the SGS heat flux. However, since momentum and thermal energy equations are coupled (see Eqs. 1 and 2), results in *a posteriori* tests will depend on both models. Therefore, before investigating any new SGS heat flux model, the suitability of the eddy-viscosity assumption for buoyancy-driven turbulent flows must be assessed. To do so, we consider an RBC at very low Prandtl number (liquid sodium with $Pr = 0.005$). In this case, the molecular thermal diffusivity is much larger than the molecular viscosity. Looking at the relation between the so-called Obukhov-Corrsin scale, η_T , and the Kolmogorov length scale, η_K ,

$$\eta_T = \left(\frac{1}{Pr} \right)^{3/4} \eta_K, \quad (13)$$

it is clear that the cutoff length for temperature, η_T , is much larger than the cutoff length for the kinetic energy, η_K (see Refs. [27] and Chapter 15 in [10]). In our particular case, η_T is $(1/0.005)^{3/4} \approx 53.2$ times larger than η_K . This is clearly depicted in Figure 3 where temperature and velocity fields corresponding to a DNS simulation of a liquid sodium RBC at $Ra = 7.14 \times 10^7$ are shown. This large scale separation implies that there is a wide range of cutoff wavenumbers to carry out an LES simulation for the velocity field while doing a DNS for temperature. This opens the possibility to test *a posteriori* a SGS stress model while resolving all the scales for the temperature field.

Despite that many relevant turbulent thermal convection phenomena in nature (*e.g.* Earth mantle, turbulent convection in the Sun) and technology (*e.g.* liquid-metal batteries, nuclear engineering) are ruled by very low Pr -number fluids, numerical simulations and experiments are very scarce compared with those in air or water. Both laboratory experiments and numerical simulations are challenging. Namely, the thermal and velocity boundary layers become respectively thicker and thinner as Pr -number decreases. Combined with the above-mentioned separation of cutoff scales between temperature and velocity, it implies much more stringent mesh resolution requirements for the same heat transfer. Apart from this, unlike the cases with $Pr \sim 1$, explicit time-integration schemes are not suitable to solve the thermal energy equation. Instead, an implicit treatment of the thermal diffusivity term is necessary to avoid having too small time-steps. For a recent review of turbulent convection at low Pr -numbers the reader is referred to [8].

Because of its simplicity and robustness, the eddy-viscosity assumption is the most common closure model for the SGS stress tensor (see Eq. 6). Then, following the same notation as in Ref. [17], most of the existing eddy-viscosity models can be expressed as

$$\nu_e = (C_m \delta)^2 D_m(\bar{\mathbf{u}}), \quad (14)$$

where ν_e is denotes the eddy-viscosity, C_m is the model constant, δ is the sub-grid characteristic length, and $D(\bar{\mathbf{u}})$ is the differential operator with units of frequency associated with the model. No summation over m is implied here. Research was initially focused on overcoming the intrinsic limitations of the classical Smagorinsky model [28]; namely, its differential operator, $D(\bar{\mathbf{u}}) = |\mathbf{S}(\bar{\mathbf{u}})|$, does not vanish near solid walls. First attempts made use of wall functions [29,30]. Later, Germano *et al.* [31] proposed the dynamic procedure where the constant C_m is computed using the Jacobi identity. Nevertheless, this approach requires averaging (usually in the homogeneous directions) and *ad hoc* clipping for negative values of ν_e . Attempts to overcome these limitations are the dynamic localization model [32], the Lagrangian dynamic model [33], and the different global dynamic approaches [34, 35]. Alternatively, it is possible to build models that vanish in the near-wall region. Examples thereof are the WALE model [16], the Vreman model [36], the QR model [37], the σ -model [17], the S3PQR model proposed in our previous work [18] and the

vortex-stretching-based model [38]. Hereafter, all the LES simulations have been carried out with the S3QR model given by

$$\nu_e = (C_{s3qr}\delta)^2 Q_{\mathbf{GG}^T}^{-1} R_{\mathbf{GG}^T}^{5/6}, \quad (15)$$

where the model constant is given by $C_{s3qr} = 0.762$ and, $Q_{\mathbf{GG}^T}$ and $R_{\mathbf{GG}^T}$ are respectively the second and third invariants of the symmetric second-order tensor $\mathbf{GG}^T$. Similarly to the Vreman model [36], the S3QR model is based on the invariants of $\mathbf{GG}^T$ too. Nevertheless, unlike the Vreman model it has the correct cubic near-wall behavior [39], *i.e.* $\nu_e = \mathcal{O}(y^3)$. Apart from this, it is designed to fulfill a list of desirable physical and numerical properties; namely, positiveness ($\nu_e \geq 0$), Galilean invariance, locality, and it automatically switches off for laminar, 2D, and axisymmetric flows. Moreover, it has no limitations for statistically inhomogeneous flows and has a low computational cost. For further details about this model, the reader is referred to our work [18].

Numerical simulations have been carried out using the STG in-house code: it is based on a symmetry-preserving finite-volume discretization [40] of the incompressible NS equations on structured staggered grids. Regarding the time-integration, a second-order self-adaptive explicit scheme [41] is used for momentum, whereas the diffusive term in the thermal transport equation is treated implicitly. Then, the pressure-velocity coupling is solved using a fractional step projection method [42]. For details about the numerical algorithms, the Poisson solver, and the verification of the code, the reader is referred to [43]. Finally, the approach proposed in [44] is used for the spatial discretization of the eddy-viscosity models. It is worth mentioning that, in our opinion, using symmetry-preserving discretizations is an excellent starting point for LES simulations. Namely, for coarse grids, the energy of the resolved scales of motion is convected in a stable manner: that is, the discrete convective operator transports energy from a resolved scale of motion to other resolved scales without dissipating any energy, as it should do from a physical point-of-view. Hence, stable simulations without SGS model can be carried out even on extremely coarse grids. This allows showing the contribution of the SGS model neatly. Therefore, we think that it forms a solid basis for testing SGS scale models. The interested reader is referred to Refs. [40] and [45].

Figures 4 and 5 show the performance of different eddy-viscosity models for a liquid sodium ($Pr = 0.005$) RBC at $Ra = 7.14 \times 10^6$ and $Ra = 7.14 \times 10^7$ using the configuration displayed in Figure 1. Results are compared with the DNS solutions obtained using a mesh of $488 \times 488 \times 1280 \approx 305M$ ($Ra = 7.14 \times 10^6$) and $996 \times 996 \times 2048 \approx 1911M$ ($Ra = 7.14 \times 10^7$) grid points, respectively. All simulations have been carried out for 500 non-dimensional time-units $[TU]$ with an averaging period of $250[TU]$, except for the DNS simulation at $Ra = 7.14 \times 10^7$, for which only $100[TU]$ have been computed. The grid points are uniformly distributed in the span-wise direction whereas

Fig. 3 Visualization of the separation between scales for temperature (left) and velocity (right) for a DNS simulation of a liquid sodium ($Pr = 0.005$) RBC at $Ra = 7.14 \times 10^7$ carried out using a mesh of $996 \times 996 \times 2048 \approx 1911M$. Instantaneous temperature field (left) and magnitude of the velocity field (right) with a sequence of zooms. See the movie in the paper database [46].

the wall-normal points are distributed using a hyperbolic tangent function,

$$y_j = \frac{L_y}{2} \left(1 + \frac{\tanh \{ \gamma_y (2(j-1)/N_y - 1) \}}{\tanh \gamma_y} \right), \quad j = 1, \dots, N_y + 1 \quad (16)$$

where N_y denotes the number of grid points in the y -direction. The stretching parameter for the DNS simulation is taken equal to $\gamma_y = \gamma_z = 0.75$ ($Ra = 7.14 \times 10^6$) and $\gamma_y = \gamma_z = 0.7$ ($Ra = 7.14 \times 10^7$), respectively. This distribution of grid points has been determined following the boundary layer resolution requirements proposed by Shishkina *et al.* [47] in conjunction with the Grötzbach criterion [48] for the bulk region. For more details about the mesh refinement criteria, the reader is referred to our previous works [3, 13]. Furthermore, the exact grid point distribution can be found in [46], where these DNS results are publicly available. For LES and no-model simulations, $\gamma_z = 1$ whereas the stretching parameter in the vertical direction, γ_y , is chosen to keep the first off-wall grid point at double distance than the one used in the DNS, *i.e.* $\Delta y_{wall}^{LES} = 2\Delta y_{wall}^{DNS}$. This corresponds to $\Delta y_{wall}^{LES} = 2.89 \times 10^{-3}$ ($Ra = 7.14 \times 10^6$) and $\Delta y_{wall}^{LES} = 1.52 \times 10^{-3}$ ($Ra = 7.14 \times 10^7$), respectively. In these cases, the subgrid characteristic length is computed as the cube root of the cell volume, *i.e.* $\delta = (\Delta x \Delta y \Delta z)^{1/3}$. Averages over the four statistically invariant transformations (time, span-wise and, horizontal and vertical planes of symmetry) are carried out for all the fields. The standard notation $\langle \cdot \rangle$ is used to denote this averaging procedure. The least to be expected from numerical simulations of turbulence is a good prediction of the mean global quantities. Figure 4 shows the average Nusselt number for a set of meshes and eddy-viscosity models: namely, the S3QR model [18], the WALE model [16], the Vreman model [36] and the QR model [37]. To illustrate the contribution

Fig. 4 Results for the average Nusselt number obtained for a liquid sodium ($Pr = 0.005$) RBC at $Ra = 7.14 \times 10^6$ (top) and $Ra = 7.14 \times 10^7$ (bottom) using different meshes. Comparison between LES results obtained with the S3QR model [18], the WALE model [16], the Vreman model [36], the QR model [37] and results obtained without model. Solid square represents the DNS solution carried out using a mesh of $488 \times 488 \times 1280 \approx 305M$ (top) and $966 \times 966 \times 2048 \approx 1911M$ (bottom) grid points, respectively. The top horizontal axis represents the computational cost measured in CPU core-hour at the MareNostrum 4 supercomputer.

of the eddy-viscosity models to improve the quality of the solution, the results obtained without model, *i.e.* $\nu_e = 0$, are also shown. It is remarkable that, in general, LES solutions are in good agreement with the DNS even for the coarsest meshes ($48 \times 26 \times 26$ for $Ra = 7.14 \times 10^6$ and $96 \times 52 \times 52$ for $Ra = 7.14 \times 10^7$), conversely, only the finest meshes ($128 \times 72 \times 72$ and $192 \times 104 \times 104$ at $Ra = 7.14 \times 10^6$ and $512 \times 288 \times 288$ at $Ra = 7.14 \times 10^7$)

Fig. 5 Results for the average turbulent kinetic energy, $\langle k \rangle$, temperature variance, $\langle T'T' \rangle$ and turbulent heat flux, $\langle v'T' \rangle$, for a liquid sodium ($Pr = 0.005$) RBC at $Ra = 7.14 \times 10^6$ with two different meshes of $64 \times 36 \times 36$ (left) and $96 \times 52 \times 52$ (right) grid points. Comparison between LES results obtained with the S3QR model [18], the WALE model [16] and results obtained without model at the vertical mid-plane, $z = 0.5$. Solid line represents the DNS solution carried out using a mesh of $488 \times 488 \times 1280 \approx 305M$ grid points.

are able to provide reasonable results when the model is switched off. Notice that even for the coarsest mesh $\Delta x^{LES}/\Delta x^{DNS} < \eta_T/\eta_K = Pr^{-3/4} \approx 53.2$ (see Eq. 13); therefore, no heat flux SGS activity is expected. A closer inspection reveals that slightly better results are obtained with the S3QR and WALE models, especially for the lowest Ra -number. These two models have the proper cubic near-wall behavior, *i.e.* $\nu_e = \mathcal{O}(y^3)$, whereas for the other two models (Vreman and QR) the eddy-viscosity vanishes as $\nu_e = \mathcal{O}(y^1)$. The additional dissipation introduced in the near-wall region by these two models may negatively affect the results (see Ref. [18], for a detailed explanation). To emphasize the benefits of LES modeling, the approximate computational

cost of the simulations is displayed in the top horizontal axis of Figure 4. It has been measured on the MareNostrum 4 supercomputer and corresponds to the above-mentioned total integration period of $500[TU]$. As mentioned above, only $100[TU]$ have been computed for the DNS simulation at $Ra = 7.14 \times 10^7$, which actually suffices to have a good enough estimation of the Nusselt number. In this case, and for the sake of comparison, the computational cost has been re-scaled to $500[TU]$. It is worth mentioning that for both cases, the gap between the DNS and the coarsest (finest) LES meshes is approximately five orders (more than two orders) of magnitude. Typical RAM requirements for these simulations are approximately 2 GB per million grid points, which corresponds to ≈ 268 double-precision numbers per grid point. This leads to $\approx 3.7\text{ TB}$ of RAM for the DNS simulation at $Ra = 7.14 \times 10^7$ which has been carried out using 3872 CPU-cores on the MareNostrum 4 supercomputer, *i.e.* $\approx 1\text{ GB}$ per CPU-core. Of course, these memory requirements will depend on the order of accuracy of the numerical schemes and the Poisson solver configuration [43].

Finally, to see the effect of the eddy-viscosity models in more detail, results for the average turbulent kinetic energy, $\langle k \rangle$, the temperature variance, $\langle T'T' \rangle$ and the turbulent heat flux, $\langle v'T' \rangle$, at the vertical mid-plane ($z = 0.5$) are displayed in Figure 5 for two meshes ($64 \times 36 \times 36$ and $96 \times 52 \times 52$). In this case, only the lowest Ra -number is analyzed because the integration period of the DNS at $Ra = 7.14 \times 10^7$ is too short to have well-converged statistics. Moreover, among the four eddy-viscosity models studied, only those ones (S3QR and WALE) that have the proper near-wall behavior are shown here. Again, the eddy-viscosity models introduce great improvement with respect to the no-model solution. It is noteworthy that the results obtained without SGS model seem to be far away from the asymptotic behavior: namely, the solution with the finer grid is significantly worse compared with the solution obtained with the coarser one. This is not the case for the LES simulations. Actually, results obtained with the finer grid are in good agreement with the DNS solution. All these results seem to confirm the suitability of the eddy-viscosity assumption for buoyancy-driven flows.

4 Building a proper SGS heat flux model

4.1 Exploring nonlinear SGS heat flux models

In this work, we focus on finding a nonlinear tensorial SGS heat flux model with good physical and mathematical properties, that provides an accurate approximation of the actual SGS heat flux for buoyancy-driven turbulence. As mentioned before, (linear) eddy-diffusivity (see Eq. 7) assumption cannot provide an accurate representation of the SGS heat flux, $\mathbf{q}$; hence, we turn our attention to (nonlinear) tensorial models. The least to be expected from an SGS model is to keep the stability of the numerical solution. This is not the

Fig. 6 Joint PDF for the Peng and Davidson model (Eq. 10) in the space $(|q^{PD}|/|q^{nl}|, \beta)$ where the angle β is defined in Figure 2. The analyzed data corresponds to the bulk region of the air-filled Rayleigh-Bénard configuration at $Ra = 10^{11}$.

case of the Leonard (Eq. 9) and the Peng and Davidson models (Eq. 10). Both of them have directions of negative diffusivity that make the model numerically unstable. This is clearly observed in Figure 6 where the joint PDF (JPDF) for the Peng and Davidson model (Eq. 10) in the space $(|q^{PD}|/|q^{nl}|, \beta)$ is displayed. This *a priori* analysis has been carried out using a set of instantaneous fields corresponding to a new air-filled DNS computed using 8192 CPUs of the MareNostrum 4 supercomputer [49] on a mesh of 5.7 billion grid points ($2048 \times 1662 \times 1662$). Likewise our previous DNS [3], a fourth-order symmetry-preserving spatial discretization [40] has been used together with a self-adaptive second-order explicit time-integration scheme [41]. For details about the mesh refinement criteria, the reader is referred to our previous work [3]. It is worth noticing that both models collapse to the same formula for $\beta = 0$, *i.e.* $q^{PD} = q^{nl} \propto q^{eddy}$, since they corresponds to flow topologies with null rate-of-rotation, $\Omega = 0$. This can be also observed in Figure 6. On the other hand, the model proposed by Daly and Harlow [25] (see Eq. 12) does not suffer these numerical instabilities since the tensor $\mathbf{GG}^T$ is positive semi-definite. Furthermore, this model shows a rather good *a priori* alignment with the actual SGS heat flux (see Figure 2, bottom left). Hence, hereafter we will consider nonlinear models based on the symmetric second-order tensor, $\mathbf{GG}^T$. Notice that this tensor is proportional to the gradient model [26] given by the leading term of the Taylor series expansion of the SGS stress tensor, $\tau = (\delta^2/12)\mathbf{GG}^T + \mathcal{O}(\delta^4)$, assuming an isotropic filter length, δ ; therefore, it provides an accurate representation of the SGS stress tensor activity.

Fig. 7 Near-wall scaling of $\langle v'T' \rangle$ for the air-filled RBC configurations at $Ra = 10^8$ and $Ra = 10^{10}$ studied in Refs. [3, 13].

4.2 Imposing the right near-wall scaling

It can be shown that due to the no-slip condition and the incompressibility constraint, the production of turbulent kinetic energy follows a cubic behavior near the wall [39]. This leads to the well-known near-wall cubic behavior condition for the eddy-viscosity, *i.e.* $\nu_e = \mathcal{O}(y^3)$. The WALE model [16], the σ -model [17], the model proposed by Ryu and Iaccarino [50], the S3PQR models [18] and the vortex-stretching-based eddy-viscosity model [38] are examples thereof. A similar analysis can be performed for the SGS heat flux, $\mathbf{q}$. Namely, due to the no-slip condition and the incompressibility constraint, $\nabla \cdot \mathbf{u} = 0$, the stream-wise, wall-normal and span-wise velocity components and the temperature have the following scalings

$$u = ay + \mathcal{O}(y^2); \quad v = by^2 + \mathcal{O}(y^3); \quad w = cy + \mathcal{O}(y^2); \quad T = dy + \mathcal{O}(y^2), \quad (17)$$

where y is the distance to the wall and $a(x, z), b(x, z), c(x, z), d(x, z)$ are smooth functions that do not depend on y . Hence, the actual SGS heat flux, $\mathbf{q}$, also follows a cubic behavior near the wall, *i.e.*

$$\mathbf{q} \propto \langle v'T' \rangle = \mathcal{O}(y^3). \quad (18)$$

The results displayed in Figure 7 confirms that this cubic scaling is valid for $y^+ \lesssim 8$. Let us consider now the near-wall scaling of the Daly and Harlow model given in Eq.(12),

$$\mathbf{G} \propto \begin{pmatrix} y & 1 & y \\ y^2 & y & y^2 \\ y & 1 & y \end{pmatrix}; \quad \nabla T \propto \begin{pmatrix} y \\ 1 \\ y \end{pmatrix} \implies \mathbf{G}\mathbf{G}^T \nabla \bar{T} \propto \begin{pmatrix} y \\ y^2 \\ y \end{pmatrix} = \mathcal{O}(y^1). \quad (19)$$

	P_{GG^T}	Q_{GG^T}	R_{GG^T}
Formula	$2(Q_\Omega - Q_S)$	$V_G^2 + Q_G^2$	R_G^2
Wall-behavior	$\mathcal{O}(y^0)$	$\mathcal{O}(y^2)$	$\mathcal{O}(y^6)$
Units	$[T^{-2}]$	$[T^{-4}]$	$[T^{-6}]$

Table 1 Properties of the first, second and third invariants of the GG^T tensor where $Q_\Omega = -1/2tr(\Omega^2)$, $Q_S = -1/2tr(S^2)$, $Q_G = -1/2tr(G^2)$ are the second invariants of Ω , S and G , respectively, and $R_G = \det(G)$ is the third invariant of G . Finally, the invariant V_G^2 is equal to the L^2 -norm of the vortex-stretching term, *i.e.* $V_G^2 = |\mathbf{S}\boldsymbol{\omega}|^2$, where $\boldsymbol{\omega} = \nabla \times \mathbf{u}$ is the vorticity. For further details the reader is referred to Ref. [18].

Therefore, the near-wall cubic behavior is recovered if the SGS timescale, $\mathcal{T}_{SGS}$, would scale quadratically. This is not the case of the timescale used in the Daly and Harlow [25] model, *i.e.* $\mathcal{T}_{SGS} = 1/|S| = \mathcal{O}(y^0)$, therefore, $\mathbf{q}^{DH} = \mathcal{O}(y^1)$.

At this point, it is interesting to observe that new timescales, $\mathcal{T}_{SGS}$, can be derived by imposing restrictions on the differential operators they are based on. For instance, let us consider models that are based on the invariants of the tensor GG^T

$$\mathbf{q} \approx -C_M (P_{GG^T}^p Q_{GG^T}^q R_{GG^T}^r) \frac{\delta^2}{12} GG^T \nabla \bar{T} \quad (\equiv \mathbf{q}^{PQR}) \quad (20)$$

where P_{GG^T} , Q_{GG^T} and R_{GG^T} are the first, second and third invariant of the GG^T tensor. This tensor is proportional to the gradient model [26] given by the leading term of the Taylor series expansion of the subgrid stress tensor $\tau(\bar{\mathbf{u}}) = (\delta^2/12)GG^T + \mathcal{O}(\delta^4)$. Formulae of these invariants, their wall behavior and their units are given in Table 1. Then, the exponents p , q and r in Eq.(20), must satisfy the following linear equations

$$-6r - 4q - 2p = 1; \quad 6r + 2q = s, \quad (21)$$

to guarantee that the differential operator has units of time, *i.e.* $[P_{GG^T}^p Q_{GG^T}^q R_{GG^T}^r] = [T]$ and a slope s for the asymptotic near-wall behavior, *i.e.* $\mathcal{O}(y^s)$. Solutions for $q(p, s) = -(1+s)/2 - p$ and $r(p, s) = (2s+1)/6 + p/3$ are displayed in Figure 8. If we restrict ourselves to solutions with the proper near-wall scaling, *i.e.* $s = 2$ (solid lines in Figure 8), a family of p -dependent models follow

$$\mathbf{q} \approx -C_{s2pq} \left(P_{GG^T}^p Q_{GG^T}^{-(p+3/2)} R_{GG^T}^{(2p+5)/6} \right) \frac{\delta^2}{12} GG^T \nabla \bar{T} \quad (\equiv \mathbf{q}^{S2PQR}). \quad (22)$$

Hereafter, this family of models is referred as S2PQR-model. Restricting ourselves to solutions involving only two invariants of GG^T three models are found,

$$\mathbf{q}^{S2PQ} = -C_{s2pq} P_{GG^T}^{-5/2} Q_{GG^T} \frac{\delta^2}{12} GG^T \nabla \bar{T}, \quad (23)$$

$$\mathbf{q}^{S2PR} = -C_{s2pr} P_{GG^T}^{-3/2} R_{GG^T}^{1/3} \frac{\delta^2}{12} GG^T \nabla \bar{T}, \quad (24)$$

$$\mathbf{q}^{S2QR} = -C_{s2qr} Q_{GG^T}^{3/2} R_{GG^T}^{5/6} \frac{\delta^2}{12} GG^T \nabla \bar{T}, \quad (25)$$

Fig. 8 Solutions for the linear system of Eq.(21) for $s = 0$ (dashed line) and for the correct slope $s = 2$ (solid line). Each (p, q, r) solution represents a SGS heat flux model of the form given in Eq.(20).

for $p = -5/2$, $p = -1.5$ and $p = 0$, respectively. These three solutions are also represented in Figure 8.

4.3 *A priori* analysis in the bulk region

The alignment trends of the new family of SGS heat flux models given in Eq.(22) have also been studied *a priori* in the bulk region for the RBC at $Ra = 10^{11}$ [49]. Results for different values of p are displayed in Figure 9. In this case, the value of the model constants, C_{s2pqr} , is computed imposing that the average magnitude of the model, $\mathbf{q}^{S2PQR}$, is equal to the average magnitude of the actual SGS heat flux, $\mathbf{q}$. The values of the constants as a function of p are shown in Figure 10 together with the values obtained for the two lower Ra -numbers [3]. It is worth noticing that the differences between the two highest Ra -numbers are minimal; this may indicate that an asymptotic regime has been reached at $Ra = 10^{11}$. Even more important, the relatively small differences observed between the lowest ($Ra = 10^8$) and the highest ($Ra = 10^{11}$) Rayleigh number indicates that a constant value of C_{s2pqr} can be assumed independently of the turbulent regime. Moreover, the ratios between the computed constant at different Ra -numbers are almost independent of the value of the p -exponent. Therefore, our choice among all the potential S2PQR models can be based on their alignment trends (see Figure 9). Models corresponding to values of $p < -5/2$ are not considered because divisions by zero may occur (see Eq. 22) since the invariant $R_{GG^T} = \det(GG^T) = \det(G)\det(G^T) = \det^2(G)$ vanishes for 2D flows. Moreover, most-frequent events should have locations

Fig. 9 Same as Figure 6. In this case, the S2PQR model (Eq. 22) is analyzed for different values of the p -exponent. Horizontal and vertical axis labels are the same as in Figure 6.

with similar angles to those displayed for the Leonard model, $\mathbf{q}^{nl}$, *i.e.* $\beta \approx 68^\circ$ in the horizontal axis and $|\mathbf{q}^{S2PQR}|/|\mathbf{q}^{nl}| \sim 1$ in the vertical axis. In this regard, models with $p \gtrsim -1.4$ tend to have not-so-frequent events with very large values of $|\mathbf{q}^{S2PQR}|/|\mathbf{q}^{nl}|$. To compensate this, most-frequent events tend to be represented in the region with very low values of $|\mathbf{q}^{S2PQR}|/|\mathbf{q}^{nl}|$. This could be compensated by changing the model constant; however, this would exaggerate even more those not-so-frequent events with very large values of $|\mathbf{q}^{S2PQR}|/|\mathbf{q}^{nl}|$. Within the range $-5/2 \leq p \lesssim 1.4$, the S2PR model ($p = -1.5$) given by Eq.(24) seems to be an excellent candidate: it combines numerical stability with good alignment trends (see Figure 11, for details) with the actual SGS heat flux, $\mathbf{q}$, and switches off for 2D flows. Furthermore, since it based on only two invariants, it is computationally cheaper.

4.4 *A priori* analysis in the near-wall region

Among all the potential S2PQR models given in Eq.(22) we have chosen the S2PR model ($p = -1.5$) given in Eq.(24) because of their good alignment trends with the actual SGS heat flux, $\mathbf{q}$. This analysis has been carried out

Fig. 10 Values of the model constants, C_{s2pqr} , for the family of the p -dependent SGS heat flux models given in Eq.(22). They are computed imposing that the average magnitude of the model, q^{S2PQR} , in the bulk region is equal to average magnitude of the actual SGS heat flux, q . The data used correspond to our previous DNS [3] at $Ra = 10^8$ and $Ra = 10^{10}$, and the new DNS simulation at $Ra = 10^{11}$ [49,51].

Fig. 11 Same as Figure 6. In this case, the S2PR model (Eq. 24) is analyzed.

using the DNS data corresponding to an air-filled RBC at $Ra = 10^{11}$ [49]. The same analysis has been carried out for the two lowest Ra -numbers, *i.e.* $Ra = \{10^8, 10^{10}\}$, showing very similar trends; therefore, these results are not shown here for the sake of brevity. Apart from having a good representation of q in the bulk region, a SGS heat flux model should have a proper behavior in the near-wall region. This actually motivated the above-explained construction of this family of models (see Section 4.2), *i.e.* the SGS heat flux should vanish in the near-wall region following the right cubic scaling given in Eq.(18). Here, we analyze *a priori* the new S2PR model in the near-wall region of the air-filled

Fig. 12 Same as Figure 6. In this case, the Peng and Davidson model (left) given in Eq.(10) and the new S2PR model (right) given in Eq.(24) are analyzed in the near-wall region.

RBC at $Ra = 10^{11}$ [49]. Results are displayed in Figure 12 together with the same analysis for the Peng and Davidson model (Eq. 10). The first remarkable observation is that most-frequent events are almost perpendicular to the eddy-diffusivity model, *i.e.* $\beta \approx 90^\circ$. This can be easily explained by analyzing the near-wall behavior of the angle β ,

$$\cos \beta^m = \frac{\mathbf{q}^{eddy} \cdot \mathbf{q}^m}{|\mathbf{q}^{eddy}| |\mathbf{q}^m|}, \quad (26)$$

for different nonlinear models. Here, $\mathbf{q}^m$ represents a modeled SGS heat flux. Namely,

$$\cos \beta^{S2} = \cos \beta^{DH} = \frac{\nabla \bar{T} \cdot \mathbf{G} \mathbf{G}^T \nabla \bar{T}}{|\nabla \bar{T}| |\mathbf{G} \mathbf{G}^T \nabla \bar{T}|} = \frac{|\mathbf{G}^T \nabla \bar{T}|^2}{|\nabla \bar{T}| |\mathbf{G} \mathbf{G}^T \nabla \bar{T}|} = \mathcal{O}(y^1), \quad (27)$$

$$\cos \beta^{PD} = \frac{\nabla \bar{T} \cdot \mathbf{S} \nabla \bar{T}}{|\nabla \bar{T}| |\mathbf{S} \nabla \bar{T}|} = \mathcal{O}(y^1), \quad (28)$$

$$\cos \beta^{nl} = \frac{\nabla \bar{T} \cdot \mathbf{G} \nabla \bar{T}}{|\nabla \bar{T}| |\mathbf{G} \nabla \bar{T}|} = \mathcal{O}(y^1). \quad (29)$$

These scalings follow straightforwardly from the near-wall scalings given in Eqs.(19): $\mathbf{G}^T \nabla \bar{T} = \mathcal{O}(y^1)$, $\nabla \bar{T} = \mathcal{O}(y^0)$, $\mathbf{G} \mathbf{G}^T \nabla \bar{T} = \mathcal{O}(y^1)$, $\nabla \bar{T} \cdot \mathbf{S} \nabla \bar{T} = \mathcal{O}(y^1)$, $\mathbf{S} \nabla \bar{T} = \mathcal{O}(y^0)$, $\nabla \bar{T} \cdot \mathbf{G} \nabla \bar{T} = \mathcal{O}(y^1)$ and $\mathbf{G} \nabla \bar{T} = \mathcal{O}(y^0)$. This explains why all these models tend to $\beta \approx 90^\circ$ in the near-wall region. Apart from this, we can also explain why the S2PR model (see Figure 12, right) also tends to zero in the vertical axis; namely, $|\mathbf{q}^{S2PR}|/|\mathbf{q}^{nl}| = \mathcal{O}(y^3)$. Conversely, the Peng and Davidson model (see Figure 12, left) does not tend to zero since both $\mathbf{G} \nabla \bar{T} = \mathcal{O}(y^0)$ and $\mathbf{S} \nabla \bar{T} = \mathcal{O}(y^0)$ do not vanish in the near-wall region. However, a more detailed analysis reveals why the ratio $|\mathbf{q}^{PD}|/|\mathbf{q}^{nl}|$ tends to 1/2. Namely, recalling the definition of the rate-of-strain tensor given in Eq.(8) and the scalings $\mathbf{G} \nabla \bar{T} = \mathcal{O}(y^0)$ and $\mathbf{G}^T \nabla \bar{T} = \mathcal{O}(y^1)$, the ratio between

$|\mathbf{q}^{PD}|/|\mathbf{q}^{nl}|$ follows

$$\lim_{y \rightarrow 0^+} \frac{\mathbf{q}^{PD}}{\mathbf{q}^{nl}} = \lim_{y \rightarrow 0^+} \frac{|\mathbf{S}\nabla\bar{T}|}{|\mathbf{G}\nabla\bar{T}|} = \lim_{y \rightarrow 0^+} \frac{1}{2} \frac{|\mathbf{G}\nabla\bar{T} + \mathbf{G}^T\nabla\bar{T}|}{|\mathbf{G}\nabla\bar{T}|} = \frac{1}{2}. \quad (30)$$

Apart from this, a very important proportion of the events are in the unstable side showing again that the Peng and Davidson model cannot be used as standalone SGS heat flux model since it produces a finite-time blow-up.

5 Concluding remarks and future research

A *a priori* analysis using DNS data of RBC at high Ra -numbers clearly shows that classical (linear) eddy-diffusivity assumption, $\mathbf{q}^{eddy} \propto \nabla\bar{T}$, is completely misaligned with the actual SGS heat flux, $\mathbf{q} = \overline{\mathbf{u}T} - \overline{\mathbf{u}}\bar{T}$. In the quest for more accurate models, we have first studied and confirmed the suitability of the eddy-viscosity assumption for buoyancy-driven turbulent flows. To do so, we have carried out *a posteriori* tests for different LES models at very low Prandtl numbers (liquid sodium, $Pr = 0.005$): since the ratio between the Kolmogorov length scale and the Obukhov-Corrsin length scale is given by $Pr^{3/4}$, in this case, it is possible to combine an LES simulation for the velocity field, $\overline{\mathbf{u}}$, with the numerical resolution of all the relevant scales of the thermal field, T . Then, different nonlinear SGS heat flux models have been studied *a priori* using DNS results of an air-filled ($Pr = 0.7$) RBC at Rayleigh number up to 10^{11} . Existing models such as the nonlinear Leonard model, $\mathbf{q}^{nl} \propto \mathbf{G}\nabla\bar{T}$, or the Peng and Davidson model, $\mathbf{q}^{PD} \propto \mathbf{S}\nabla\bar{T}$ can exhibit good alignment trends in the bulk region; however, they are unstable and, therefore, they cannot be used as standalone SGS heat flux model. Conversely, the model proposed by Daly and Harlow, $\mathbf{q}^{DH} \propto \mathbf{G}\mathbf{G}^T\nabla\bar{T}$ does not suffer these numerical problems since the tensor $\mathbf{G}\mathbf{G}^T$ is positive semi-definite. Moreover, this model shows a rather good *a priori* alignment with the actual SGS heat flux in the bulk region; however, it fails to provide a good approximation in the near-wall region, a crucial aspect for any SGS model. In this regard, we have proposed a new family of SGS heat flux models given in Eq.(22) that incorporates the correct cubic scaling in the near-wall region, *i.e.* $\mathbf{q} \propto \mathcal{O}(y^3)$. Among all the possible candidates, we have chosen the so-called *S2PR* model

$$\mathbf{q}^{S2PR} = -C_{s2pr} P_{\mathbf{G}\mathbf{G}^T}^{-3/2} R_{\mathbf{G}\mathbf{G}^T}^{1/3} \frac{\delta^2}{12} \mathbf{G}\mathbf{G}^T \nabla\bar{T}, \quad (31)$$

with $C_{s2pr} \approx 12.02$: it shows a very good representation of the SGS heat flux both in direction and magnitude. Moreover, apart from fulfilling a set of desirable properties (locality, Galilean invariance, numerical stability, proper near-wall behavior, and automatically switch-off for laminar and 2D flows), the proposed model is well-conditioned, and has a low computational cost and no intrinsic limitations for statistically in-homogeneous flows. Hence, it seems to be well suited for engineering applications [52]. In this regard, the proper calculation of the subgrid characteristic length on unstructured grids [53] or

the (dynamic?) determination of model constant are relevant issues that may affect the performance. Another point of interest for future studies could be the adaptation of the model for the SGS transport of chemical species for LES simulation of combustion processes [54, 55]. Apart from this, our future research plans also include the extension of this analysis to higher Ra -numbers and testing *a posteriori* the new non-linear SGS heat flux model for air-filled RBC problems.

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Compliance with Ethical Standards

Conflict of Interest: The authors declare that they have no conflict of interest.

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