On a proper tensor-diffusivity model for large-eddy simulations of buoyancy driven flows

F.X. Trias, F. Dabbagh, A. Gorobets, and A. Oliva

1 Introduction

In this work, we plan to shed light on the following research question: *can we find a nonlinear 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 fails to provide a reasonable approximation for the SGS heat flux. This was shown in our work [1] where SGS features have been studied *a priori* for a Rayleigh-Bénard convection (RBC). We also concluded that nonlinear (or tensorial) models can give good approximations of the actual SGS heat flux. Briefly, the large-eddy simulation (LES) equations arise from applying a spatial commutative filter, with filter length δ, to the incompressible Navier-Stokes and thermal energy equations,

$$\partial_t \overline{u} + (\overline{u} \cdot \nabla)\overline{u} = (Pr/Ra)^{1/2} \;\; \nabla^2 \overline{u} - \nabla \overline{p} + \overline{f} - \nabla \cdot \tau, \tag{1}$$

$$\partial_t \overline{T} + (\overline{u} \cdot \nabla)\overline{T} = (Ra/Pr)^{-1/2} \nabla^2 \overline{T} \qquad\qquad - \nabla \cdot q, \tag{2}$$

where $\overline{u}$, $\overline{T}$ and $\overline{p}$ are respectively the filtered velocity, temperature and pressure, and the incompressibility constraint reads $\nabla \cdot \overline{u} = 0$. The SGS stress tensor, $\tau = \overline{u \otimes u} - \overline{u} \otimes \overline{u}$, and the SGS heat flux vector, $q = \overline{uT} - \overline{u}\overline{T}$, represent the effect of

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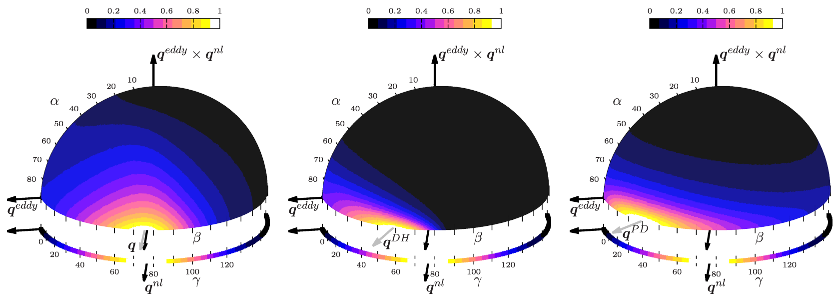

Fig. 1 Joint probability distribution functions (PDF) of the angles (α, β) plotted on a half unit sphere to show the orientation in the space of the mixed model. From left to right, alignment trends of the actual SGS heat flux, q, the Daly and Harlow [4] model (Eq. 6) and the Peng and Davidson [5] model (Eq. 5). For simplicity, the JPDF and the PDF magnitudes are normalized by its maximal. For details the reader is referred to [1].

the unresolved scales, and they need to be modeled in order to close the system. The most popular approach is the eddy-viscosity assumption, where the SGS stress tensor is assumed to be aligned with the local rate-of-strain tensor, $\mathsf{S} = 1/2(\nabla\overline{u} + \nabla\overline{u}^t)$, *i.e.* $\tau \approx -2\nu_e \mathsf{S}(\overline{u})$. By analogy, the SGS heat flux, q, is usually approximated using the gradient-diffusion hypothesis (linear modeling), given by

$$q \approx -\kappa_t \nabla\overline{T} \qquad (\equiv q^{eddy}). \tag{3}$$

Then, the Reynolds analogy assumption is applied to evaluate the eddy-diffusivity, κ_t, via a constant turbulent Prandtl number, Pr_t, *i.e.* $\kappa_t = \nu_e/Pr_t$. These assumptions have been shown to be erroneous to provide accurate predictions of the SGS heat flux [1]. Namely, *a priori* analysis showed that the eddy-diffusivity assumption, q^{eddy} (Eq. 3), is completely misaligned with the actual subgrid heat flux, q (see Figure 1, left). In contrast, the tensor diffusivity (nonlinear) Leonard model [2], which is obtained by taking the leading term of the Taylor series expansion of q,

$$q \approx \frac{\delta^2}{12}\mathsf{G}\nabla\overline{T} \qquad (\equiv q^{nl}), \tag{4}$$

provides a much more accurate *a priori* representation of q (see Figure 1, left). Here, $\mathsf{G} \equiv \nabla\overline{u}$ represents the gradient of the resolved velocity field. It can be argued that the rotational geometries are prevalent in the bulk region over the strain slots, *i.e.* $|\Omega| > |\mathsf{S}|$ (see Refs [1, 3]). Then, the dominant anti-symmetric tensor, $\Omega = 1/2(\mathsf{G} - \mathsf{G}^T)$, rotates the thermal gradient vector, $\nabla\overline{T}$, to be almost perpendicular to q^{nl} (see Eq.4). Therefore, the eddy-diffusivity paradigm is only supported in the not-so-frequent strain-dominated areas.

2 Nonlinear SGS heat flux models for large-eddy simulation

Since the eddy-diffusivity, q^{eddy}, cannot provide an accurate representation of the SGS heat flux, we turn our attention to nonlinear models. As mentioned above, the Leonard model [2] given in Eq.(4) can provide a very accurate *a priori* representation of the SGS heat flux (see Figure 1, left). However, the local dissipation (in the L2-norm sense) is proportional to $\nabla T \cdot \mathsf{G}\nabla T = \nabla T \cdot \mathsf{S}\nabla T + \nabla T \cdot \Omega \nabla T = \nabla T \cdot \mathsf{S}\nabla T$. Since the velocity field is divergence-free, $\lambda_1^{\mathsf{S}} + \lambda_2^{\mathsf{S}} + \lambda_3^{\mathsf{S}} = \nabla \cdot u = 0$, the eigenvalues of S can be ordered $\lambda_1^{\mathsf{S}} \geqslant \lambda_2^{\mathsf{S}} \geqslant \lambda_3^{\mathsf{S}}$ with $\lambda_1^{\mathsf{S}} \geqslant 0$ (extensive eigendirection) and $\lambda_3^{\mathsf{S}} \leqslant 0$ (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 can produce a finite-time blow-up. A similar problem is encountered with the nonlinear tensorial model q^{PD} proposed by Peng and Davidson [5],

$$q \approx C_t \delta^2 \mathsf{S}\nabla T \qquad (\equiv q^{PD}), \tag{5}$$

$$q \approx -\mathscr{T}_{SGS}\tau\nabla T = -\frac{1}{|\mathsf{S}|}\frac{\delta^2}{12}\mathsf{G}\mathsf{G}^T\nabla T \qquad (\equiv q^{DH}), \tag{6}$$

whereas the nonlinear model q^{DH} proposed by Daly and Harlow [4] relies on the positive semi-definite tensor $\mathsf{G}\mathsf{G}^T$. Here, $\mathscr{T}_{SGS} = 1/|\mathsf{S}|$ is the SGS timescale. Notice that the model proposed by Peng and Davidson, q^{PD}, can be viewed in the same framework if the SGS stress tensor is estimated by an eddy-viscosity model, *i.e.* $\tau \approx -2\nu_e \mathsf{S}$ and $\mathscr{T}_{SGS} \propto \delta^2/\nu_e$. These two models have shown a much better *a priori* alignment with the actual SGS heat flux, especially the DH model (see Figure 1, middle). Moreover, the DH is numerically stable since the tensor $\mathsf{G}\mathsf{G}^T$ is positive semi-definite. Hence, it seems appropriate to build models based on this tensor. However, the DH model does not have the proper near-wall behavior, *i.e.* $q \propto \langle v'T' \rangle = \mathscr{O}(y^3)$ where y is the distance to the wall. An analysis of the DH model leads to $\mathsf{G}\mathsf{G}^T\nabla\overline{T} \propto \mathscr{O}(y^1)$. Therefore, the near-wall cubic behavior is recovered if $\mathscr{T}_{SGS} \propto \mathscr{O}(y^2)$. This is not the case of the timescale used in the Daly and Harlow [4] model, *i.e.* $\mathscr{T}_{SGS} = 1/|\mathsf{S}| = \mathscr{O}(y^0)$.

At this point it is interesting to observe that new timescales, $\mathscr{T}_{SGS}$, 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 $\mathsf{G}\mathsf{G}^T$

$$q \approx -C_M \left(P^p_{\mathsf{G}\mathsf{G}^T} Q^q_{\mathsf{G}\mathsf{G}^T} R^r_{\mathsf{G}\mathsf{G}^T} \right) \frac{\delta^2}{12}\mathsf{G}\mathsf{G}^T\nabla T \qquad (\equiv q^{S2}) \tag{7}$$

where $P_{\mathsf{G}\mathsf{G}^T}$, $Q_{\mathsf{G}\mathsf{G}^T}$ and $R_{\mathsf{G}\mathsf{G}^T}$ are the first, second and third invariant of the $\mathsf{G}\mathsf{G}^T$ tensor. This tensor is proportional to the gradient model [6] given by the leading term of the Taylor series expansion of the subgrid stress tensor $\tau(\overline{u}) = (\delta^2/12)\mathsf{G}\mathsf{G}^T + \mathscr{O}(\delta^4)$. Then, the exponents p, q and r in Eq.(7), must satisfy the following equations

$$-6r - 4q - 2p = 1; \qquad 6r + 2q = s, \tag{8}$$

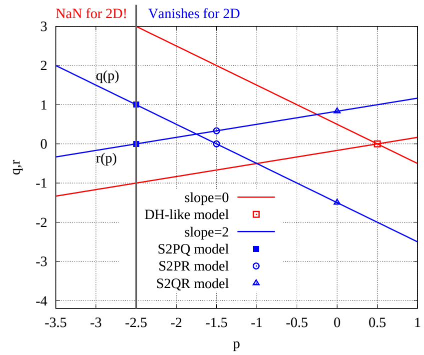

Fig. 2 Solutions of the linear system of Eq.(8) for $s = 0$ (red lines) and $s = 2$ (blue lines). Each (r, p, q) represents an tensor-diffusivity model with the form of Eq.(7).

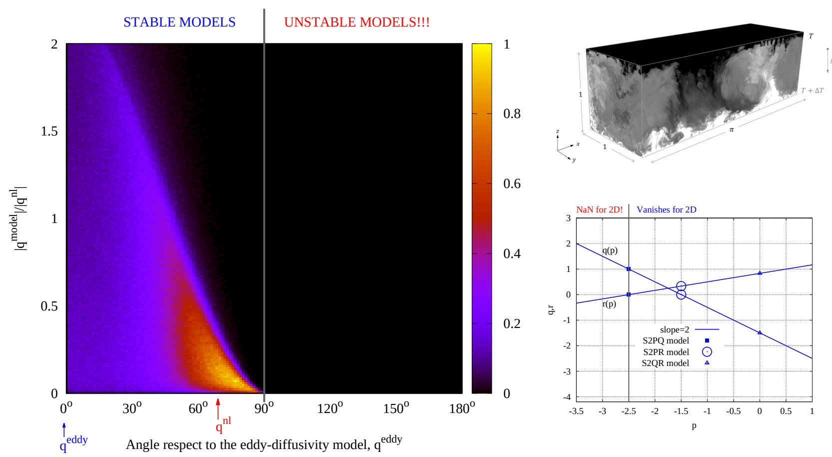

Fig. 3 Joint PDF for the S2PR model (Eq. 10) in the space $(|q^{PD}|/|q^{nl}|, \beta)$ where the angle β is defined in Figure 1. The analyzed data corresponds to the bulk region of the air-filled Rayleigh-Bénard configuration at $Ra = 10^{10}$ studied in Refs. [3, 1].

to guarantee that the differential operator has units of time, *i.e.* $[P^p_{\mathsf{GG}^T} Q^q_{\mathsf{GG}^T} R^r_{\mathsf{GG}^T}] = [T^1]$ 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 2. If we restrict ourselves to solutions with the proper near-wall scaling, *i.e.* $s = 2$ (blue lines in Figure 2), a family of p-dependent models follows. Restricting ourselves to solutions involving only two invariants of GG^T three models follow

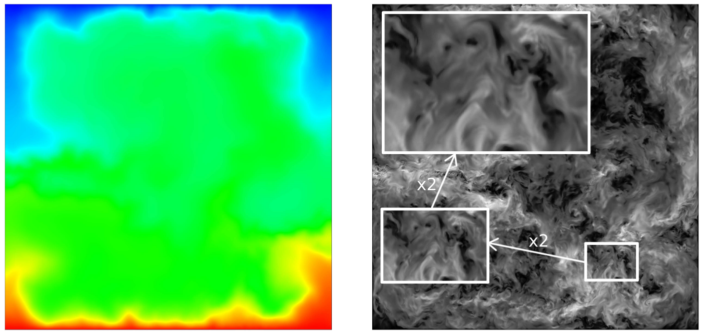

Fig. 4 An instantaneous picture of the temperature field (left) and velocity magnitude (right), $|u|$, of the DNS simulation of RBC at $Ra = 7.14 \times 10^7$ and $Pr = 0.005$ (liquid sodium) carried out using a mesh of $966 \times 966 \times 2048 \approx 1911M$ grid points.

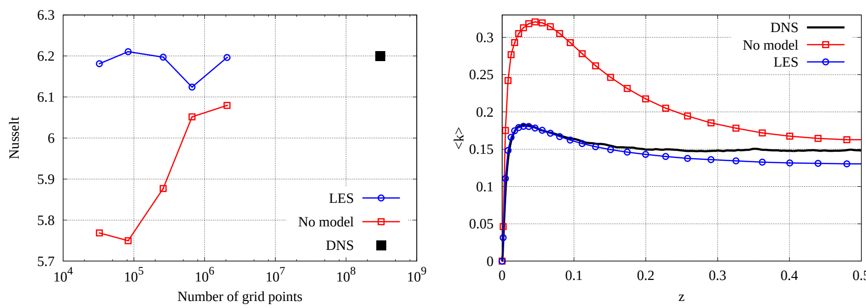

Fig. 5 Comparison of LES (and no-model) versus DNS results of RBC at $Ra = 7.14 \times 10^6$ and $Pr = 0.005$ (liquid sodium). LES results have been obtained using the eddy-viscosity model S3PQ proposed in Ref. [7]. Left: average Nusselt for different meshes. Right: turbulent kinetic energy at cavity mid-width for a $96 \times 52 \times 52$ mesh compared with the DNS results obtained with a mesh of $488 \times 488 \times 1280 \approx 305M$.

$$q^{S2PQ} = -C_{s2pq} P_{\mathsf{GG}^T}^{-5/2} Q_{\mathsf{GG}^T} \frac{\delta^2}{12} \mathsf{GG}^T \nabla \overline{T}, \tag{9}$$

$$q^{S2PR} = -C_{s2pr} P_{\mathsf{GG}^T}^{-3/2} R_{\mathsf{GG}^T}^{1/3} \frac{\delta^2}{12} \mathsf{GG}^T \nabla \overline{T}, \tag{10}$$

$$q^{S2QR} = -C_{s2qr} Q_{\mathsf{GG}^T}^{3/2} R_{\mathsf{GG}^T}^{5/6} \frac{\delta^2}{12} \mathsf{GG}^T \nabla \overline{T}, \tag{11}$$

for $p = -5/2$, $p = -1.5$ and $p = 0$, respectively. These three solutions are represented in Figure 2. Apart from being unconditionally stable, these models display very good *a priori* alignment trends in the bulk (see Figure 3) similar to the PD model (see Figure 1, middle) but also in the near-wall region. Hence, we consider that they are very good candidates for *a posteriori* LES simulations of buoyancy-driven flows.

3 Assessment of eddy-viscosity models at very low *Pr* numbers

At this stage, *a posteriori* results are necessary to assess the performance of the newly proposed SGS heat flux models. However, apart from the underlying numerics, such results will be strongly influenced by the SGS stress tensor model. Hence, we first aim to answer the following research question: *are eddy-viscosity models for momentum able to provide satisfactory results for turbulent Rayleigh-Bénard convection?* In order to shed light to this, a set of simulations at $Pr = 0.005$ (liquid sodium) have been carried out at $Ra = 7.14 \times 10^6$ and $Ra = 7.14 \times 10^7$. Figure 4 displays a snapshot of the temperature and velocity magnitude for the DNS simulation at the highest Ra. This clearly illustrates the separation between the smallest scales of temperature and velocity, *i.e.* the ratio between the Kolmogorov length scale and the Obukhov-Corrsin length scale is given by $Pr^{1/2}$ [8]. Therefore, for a $Pr = 0.005$ (liquid sodium) we have a separation of more than one decade. Hence, it is possible to combine a LES simulation for the velocity field with the numerical resolution of all the relevant scales of the thermal field. Regarding this, results shown in Figure 5 seem to confirm the adequacy of eddy-viscosity models for this kind of flows. Our future research plans include the extension of this analysis to higher Ra-numbers and testing *a posteriori* the new non-linear SGS heat flux models for air-filled RBC.

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