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On a physically-consistent nonlinear subgrid-scale heat flux model for LES of buoyancy driven flows

F.X. Trias*, F. Dabbagh*, A. Gorobets*,** and A.Oliva*
Corresponding author: xavi@cttc.upc.edu

* Heat and Mass Transfer Technological Center (CTTC),
Technical University of Catalonia, C/Colom 11, 08222 Terrassa (Barcelona)
** Keldysh Institute of Applied Mathematics, 4A, Miusskaya Sq., Moscow 125047, Russia

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 recent findings showing that the classical (linear) eddy-diffusivity assumption fails to provide a reasonable approximation for the SGS heat flux. This has been shown in our work [1] where SGS features have been studied *a priori* for a Rayleigh-Bénard convection. We have 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,

$$\partial_t \overline{\boldsymbol{u}} + (\overline{\boldsymbol{u}} \cdot \nabla)\overline{\boldsymbol{u}} = (Pr/Ra)^{1/2} \ \nabla^2 \overline{\boldsymbol{u}} - \nabla \overline{p} + \overline{\boldsymbol{f}} - \nabla \cdot \tau \, ; \qquad \nabla \cdot \overline{\boldsymbol{u}} = 0, \tag{1}$$

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

where $\overline{\boldsymbol{u}}$, $\overline{T}$ and $\overline{p}$ are respectively the filtered velocity, temperature and pressure. The SGS stress tensor, $\tau = \overline{\boldsymbol{u} \otimes \boldsymbol{u}} - \overline{\boldsymbol{u}} \otimes \overline{\boldsymbol{u}}$, and the SGS heat flux vector, $\boldsymbol{q} = \overline{\boldsymbol{u}T} - \overline{\boldsymbol{u}}\overline{T}$, represents the effect of 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, $\mathsf{S} = 1/2(\nabla\overline{\boldsymbol{u}} + \nabla\overline{\boldsymbol{u}}^t)$, *i.e.* $\tau \approx -2\nu_e \mathsf{S}(\overline{\boldsymbol{u}})$. By analogy, the SGS heat flux, $\boldsymbol{q}$, is usually approximated using the gradient-diffusion hypothesis (linear modeling), given by

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

Then, the Reynolds analogy assumption is applied to evaluate the eddy-diffusivity: κ_t is derived from the eddy-viscosity, ν_e, by a constant turbulent Prandtl number, Pr_t, independent of the instantaneous flow conditions, *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 in our recent work [1]. Namely, *a priori* analysis has shown that the eddy-diffusivity assumption, $\boldsymbol{q}^{eddy}$ (Eq. 3), is completely misaligned with the actual subgrid heat flux, $\boldsymbol{q}$ (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 $\boldsymbol{q}$,

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

provides a much more accurate *a priori* representation of $\boldsymbol{q}$ (see Figure 1, left). Here, $\mathsf{G} \equiv \nabla \overline{\boldsymbol{u}}$ 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 $\boldsymbol{q}^{nl}$ (see Eq.4). Therefore, the eddy-diffusivity paradigm is only applicable in the not-so-frequent strain-dominated areas.

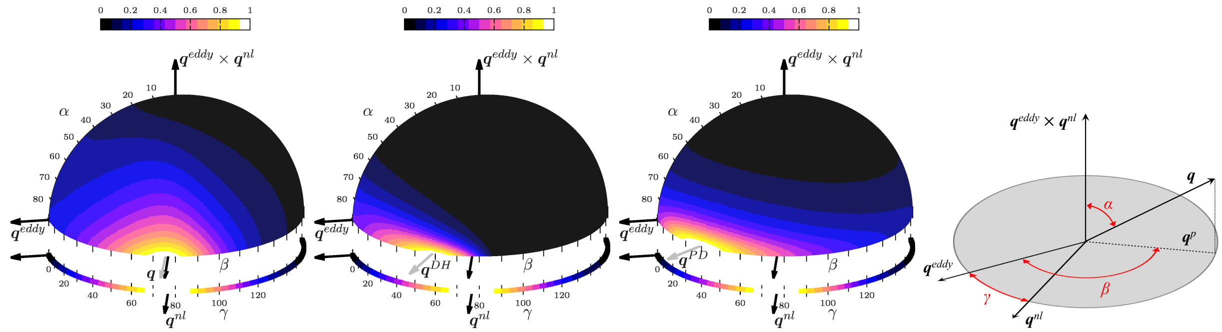

Figure 1: Joint probability distribution functions (PDF) of the angles (α, β) defined in the right figure and plotted on a half unit sphere to show the orientation trends in the space of the mixed model. The PDF of γ is shown along the bottom strip of each chart. Alignment trends of the actual SGS heat flux, $\boldsymbol{q}$ (left), the Daly and Harlow [4] model (see $\boldsymbol{q}^{DH}$ in Eq. 5) and the Peng and Davidson model [5] (see $\boldsymbol{q}^{PD}$ in Eq. 5) . For simplicity reasons, the JPDF and the PDF magnitudes are normalized by its maximal. For further details the reader is referred to our recent work [1].

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Since the eddy-diffusivity, $\boldsymbol{q}^{eddy}$, 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, top 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, $\lambda_1^{\mathsf{S}} + \lambda_2^{\mathsf{S}} + \lambda_3^{\mathsf{S}} = 0$, the eigensystem 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 produces a finite-time blow-up. A similar problem is encountered with the nonlinear tensorial model $\boldsymbol{q}^{PD}$ proposed by Peng and Davidson [5],

$$\boldsymbol{q} \approx C_t \delta^2 \mathsf{S} \nabla T \quad (\equiv \boldsymbol{q}^{PD}) \ ; \qquad \boldsymbol{q} \approx -\mathcal{T}_{SGS} \tau \nabla T = -\frac{1}{|\mathsf{S}|} \frac{\delta^2}{12} \mathsf{G}\mathsf{G}^T \nabla T \quad (\equiv \boldsymbol{q}^{DH}), \tag{5}$$

whereas the nonlinear model $\boldsymbol{q}^{DH}$ proposed by Daly and Harlow [4] relies on the positive semi-definite tensor $\mathsf{G}\mathsf{G}^T$. Here, $\mathcal{T}_{SGS} = 1/|\mathsf{S}|$ is an appropriate SGS timescale. Notice that the model proposed by Peng and Davidson, $\boldsymbol{q}^{PD}$, 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 $\mathcal{T}_{SGS} \propto \delta^2/\nu_e$. These two models have shown a much better *a priori* alignment with the actual SGS heat flux (see Figure 1). Furthermore, likewise the S3PQR eddy-viscosity models proposed in our work [6], we also want that the SGS heat flux model have the proper cubic near-wall behavior. This is not the case of any of the existing models. Corrections in this regard will be presented together with *a priori* and *a posteriori* studies of the nonlinear SGS heat flux models for RBC at $Ra = 10^{10}$ and $Ra = 10^{11}$. Results from LES simulations will be compared with the DNS results obtained in the on-going PRACE project *"Exploring new frontiers in Rayleigh-Bénard convection"*.

References

[1] F. Dabbagh, F. X. Trias, A. Gorobets, and A. Oliva. A priori study of subgrid-scale features in turbulent Rayleigh-Bénard convection. *Physics of Fluids*, 29:105103, 2017.

[2] A. Leonard. Large-eddy simulation of chaotic convection and beyond. *AIAA paper*, 97-0304, 1997.

[3] F. Dabbagh, F. X. Trias, A. Gorobets, and A. Oliva. On the evolution of flow topology in turbulent Rayleigh-Bénard convection. *Physics of Fluids*, 28:115105, 2016.

[4] B. J. Daly and F. H. Harlow. Transport equations in turbulence. *Physics of Fluids*, 13:2634, 1970.

[5] S. Peng and L. Davidson. On a subgrid-scale heat flux model for large eddy simulation of turbulent thermal flow. *International Journal of Heat and Mass Transfer*, 45:1393–1405, 2002.

[6] F. X. Trias, D. Folch, A. Gorobets, and A. Oliva. Building proper invariants for eddy-viscosity subgrid-scale models. *Physics of Fluids*, 27(6):065103, 2015.