Turbulence, Heat and Mass Transfer 5
K. Hanjalić, Y. Nagano and S. Jakirlic (Editors)

A New Irreducible Dynamic Nonlinear Tensor-Diffusivity SGS Heat-Flux Model for LES of Convective Flows

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Abstract — In this paper, a new irreducible dynamic nonlinear tensor diffusivity model based on Noll's formulation is proposed for representing the subgrid-scale (SGS) heat flux. In contrast to the conventional eddy diffusivity type models, the proposed model does not require the alignment between the SGS heat flux and the resolved scalar gradient, and therefore allows for a more realistic geometrical representation of the SGS heat flux. Due to the inclusion of nonlinearity, the new SGS heat flux model improves the numerical stability of the simulations and can be applied locally in the flow without resorting to plane averaging for stable computation of the model coefficients.

1. Introduction

During the past five years, dynamic SGS heat flux (HF) models for large-eddy simulation (LES) of thermal convective flows have advanced from models based on a scalar eddy diffusivity to those based on a tensor diffusivity. Peng and Davidson [1] proposed a *dynamic linear tensor diffusivity heat flux model* (DLTDM-HF) for studying a buoyancy driven turbulent flow. Porté-Agel *et al.* [2] introduced a *dynamic two-parameter mixed heat flux model* (DTPMM-HF) for an investigation of the SGS HF in the atmospheric boundary layer. The concept of dynamic modelling for the SGS HF vector began with the work of Moin *et al.* [3] in 1991, soon after the proposal of the dynamic SGS stress modelling approach by Germano *et al.* [4]. In their work, Moin *et al.* [3] proposed the *dynamic eddy diffusivity heat flux model* (DEDM-HF), which assumes that the SGS HF vector is instantaneously proportional to and aligned with the resolved temperature gradient. The DEDM-HF uses a linear constitutive relation, analogous to Fourier's law for describing molecular heat conduction. For modelling of turbulent heat fluxes, this linear constitutive relation is not in general consistent with the physics of turbulent convection. The above mentioned models of Peng and Davidson [1] and Porté-Agel *et al.* [2] abandon the linear eddy-diffusivity assumption and allow for non-alignment between the SGS heat flux vector and the resolved temperature gradient, thereby improving the physical representation of the SGS scalar transport processes.

In continuum physics, the theory of tensor invariants and functions is essential for modelling the nonlinear constitutive relations required for describing crystal classes, viscoelastic phenomenon and non-Newtonian fluids. The modern development of the rigorous formulation of nonlinear constitutive laws using tensor functions derives largely from the pioneering efforts of Reiner [5] and Rivlin [6] in the late 1940's. Since these seminal works, the mathematical theory of tensor invariants and functions, and its application to the formulation of nonlinear constitutive relations in the area of continuum mechanics have been extensively developed [7]. The objective this research is to use the theory of tensor functions to formulate a new dynamic nonlinear tensor diffusivity model for representing the SGS heat flux.

2. SGS Heat Flux Models

In the LES approach, a filtered scalar transport equation needs to be solved for determining the filtered scalar field in an incompressible flow, viz.

$$\frac{\partial \bar{\theta}}{\partial t} + \frac{\partial (\bar{u}_j \bar{\theta})}{\partial x_j} = \alpha \frac{\partial^2 \bar{\theta}}{\partial x_j \partial x_j} - \frac{\partial h_j}{\partial x_j}, \tag{1}$$

where $\bar{\theta}$ represents the filtered scalar (temperature), α is the molecular thermal diffusivity, and $h_j \stackrel{\text{def}}{=} \overline{u_j\theta} - \bar{u}_j\bar{\theta}$ is the SGS scalar- (heat-) flux which needs to be modelled to close this governing equation. In this paper, we consider three SGS heat flux models which we summarize as follows:

(1) Dynamic Linear Eddy-Diffusivity Model [3]

The dynamic SGS heat flux model of Moin *et al.* [3], referred to as the DEDM-HF, expresses the SGS heat flux as

$$h_j = -C_{\theta E}\bar{\Delta}^2|\bar{S}|\frac{\partial\bar{\theta}}{\partial x_j}, \tag{2}$$

where $|\bar{S}| \stackrel{\text{def}}{=} (2\bar{S}_{ij}\bar{S}_{ij})^{1/2}$ and $\bar{\Delta}$ is the grid-level filter size. The model coefficient can be obtained by minimizing the residual of the vector identity ($L_j = H_j - \tilde{h}_j$) using the least squares method, viz.

$$C_{\theta E} = -\frac{L_jP_j}{P_jP_j}, \tag{3}$$

where $L_j \stackrel{\text{def}}{=} \widetilde{\bar{u}_j\bar{\theta}} - \tilde{\bar{u}}_j\tilde{\bar{\theta}}$, $H_j \stackrel{\text{def}}{=} \widetilde{\overline{u_j\theta}} - \tilde{\bar{u}}_j\tilde{\bar{\theta}}$ is the test-grid-level SGS heat flux, $P_j \stackrel{\text{def}}{=} a_j^E - \tilde{b}_j^E$ is the differential vector, and $b_j^E \stackrel{\text{def}}{=} \bar{\Delta}^2|\bar{S}|\frac{\partial\bar{\theta}}{\partial x_j}$ and $a_j^E \stackrel{\text{def}}{=} \tilde{\bar{\Delta}}^2|\tilde{\bar{S}}|\frac{\partial\tilde{\bar{\theta}}}{\partial x_j}$ are the grid-level and test-grid-level base vector functions, respectively.

(2) Dynamic Linear Tensor Diffusivity Model of Peng and Davidson [1]

Peng and Davidson [1] proposed a dynamic linear tensor diffusivity heat flux model (DLTDM-HF), which avoids the unphysical linear scalar eddy diffusivity assumption embodied in the DEDM-HF. This model has the form

$$h_j = -D_{jk}^L\frac{\partial\bar{\theta}}{\partial x_k} = C_{\theta S}\bar{\Delta}^2\bar{S}_{jk}\frac{\partial\bar{\theta}}{\partial x_k}, \tag{4}$$

where the tensor diffusivity is a linear tensor function of $\bar{S}_{ij}$, viz. $D_{jk}^L = -C_{\theta S}\bar{\Delta}^2\bar{S}_{jk}$. The dynamic model coefficient can be similarly obtained using the least squares method as $C_{\theta S} = -L_jQ_j/Q_jQ_j$, where $Q_j \stackrel{\text{def}}{=} a_j^S - \tilde{b}_j^S$ is the differential vector, and $b_j^S \stackrel{\text{def}}{=} -\bar{\Delta}^2\bar{S}_{jk}\frac{\partial\bar{\theta}}{\partial x_k}$ and $a_j^S \stackrel{\text{def}}{=} -\tilde{\bar{\Delta}}^2\tilde{\bar{S}}_{jk}\frac{\partial\tilde{\bar{\theta}}}{\partial x_k}$.

(3) A New Irreducible Dynamic Nonlinear Tensor Diffusivity SGS Heat Flux Model

According to the theory of tensor invariants and functions, a vector-valued function of a second-order symmetric tensor M and a vector **v** can be represented by Noll's formula [7] as follows:

$$\mathbf{h} = \phi_0\mathbf{v} + \phi_1\mathbf{M}\mathbf{v} + \phi_2\mathbf{M}^2\mathbf{v}, \tag{5}$$

where ϕ_i ($i = 0, 1, 2$) is of the form of $\phi_i = \phi_i(I_M, II_M, III_M, I_v, I_{Mv}, II_{Mv})$. Here, $I_M = \text{tr}\mathbf{M}$, $II_M = \text{tr}\mathbf{M}^2$ and $III_M = \text{tr}\mathbf{M}^3$ are the three independent irreducible invariants of M, $I_v = \mathbf{v}\cdot\mathbf{v}$ is the invariant of **v**, and $I_{Mv} = \mathbf{v}\cdot\mathbf{M}\mathbf{v}$ and $II_{Mv} = \mathbf{v}\cdot\mathbf{M}^2\mathbf{v}$ are the two irreducible invariants for M and **v**. Noll's formula provides the irreducible and complete tensor function of M and **v**, which forms the basis for our proposed *dynamic irreducible nonlinear tensor diffusivity model for the SGS heat flux* (DNTDM-HF), viz.

$$h_j = -D_{jk}^N\frac{\partial\bar{\theta}}{\partial x_k} = -C_{\theta E}\bar{\Delta}^2|\bar{S}|\frac{\partial\bar{\theta}}{\partial x_j} + C_{\theta S}\bar{\Delta}^2\bar{S}_{jk}\frac{\partial\bar{\theta}}{\partial x_k} + C_{\theta N}\bar{\Delta}^2\frac{\bar{S}_{ji}\bar{S}_{ik}}{|\bar{S}|}\frac{\partial\bar{\theta}}{\partial x_k}, \tag{6}$$

where the tensor diffusivity is a nonlinear irreducible tensor function of $\bar{S}_{ij}$, viz.

$$D_{jk}^N = C_{\theta E}\bar{\Delta}^2|\bar{S}|\delta_{jk} - C_{\theta S}\bar{\Delta}^2\bar{S}_{jk} - C_{\theta N}\bar{\Delta}^2\bar{S}_{ji}\bar{S}_{ik}/|\bar{S}|. \tag{7}$$

Introducing the base vector functions: $b_j^N = -\bar{\Delta}^2\frac{\bar{S}_{ji}\bar{S}_{ik}}{|\bar{S}|}\frac{\partial\bar{\theta}}{\partial x_k}$ and $a_j^N = -\tilde{\bar{\Delta}}^2\frac{\tilde{\bar{S}}_{ji}\tilde{\bar{S}}_{ik}}{|\tilde{\bar{S}}|}\frac{\partial\tilde{\bar{\theta}}}{\partial x_k}$, the SGS heat flux at the grid-level [Eq. (6)] can be simplified as

$$h_j = -C_{\theta E}b_j^E - C_{\theta S}b_j^S - C_{\theta N}b_j^N, \tag{8}$$

and similarly, the constitutive relation for the SGS heat flux at the test-grid-level can be expressed as

$$H_j = -C_{\theta E}a_j^E - C_{\theta S}a_j^S - C_{\theta N}a_j^N. \tag{9}$$

By substituting Eqs. (8) and (9) into the vector identity ($L_j = H_j - \tilde{h}_j$), a 3×3 matrix system for computing the model coefficients is obtained, viz.

$$[P_j, Q_j, R_j]\cdot[C_{\theta E}, C_{\theta S}, C_{\theta N}]^T = -L_j, \tag{10}$$

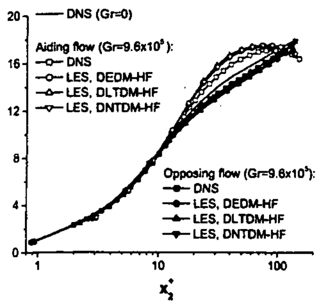

Figure 1: Mean streamwise velocity profile.

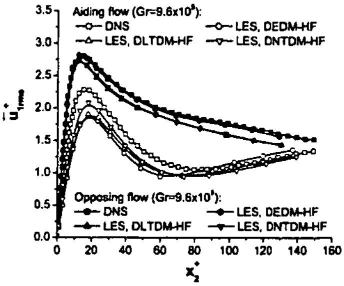

Figure 2: RMS of streamwise velocity fluctuations.

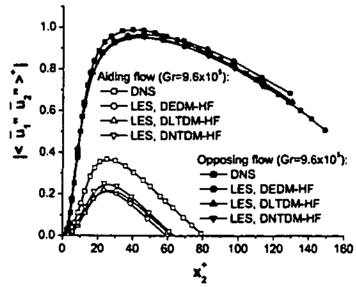

Figure 3: Resolved Reynolds stress.

for $j = 1$, 2 and 3. Here, $R_j \stackrel{\text{def}}{=} a_j^N - \tilde{b}_j^N$ is the differential vector associated with $\frac{\bar{S}_{ji}\bar{S}_{ik}}{|\bar{S}|}\frac{\partial\bar{\theta}}{\partial x_k}$. Unlike the conventional method which relies on the least squares method for obtaining the model coefficients, Eq. (10) is directly based on the vector identity. In addition, because δ_{jk}, $\bar{S}_{jk}$ and $\bar{S}_{ji}\bar{S}_{ik}$ are linearly independent, P_j, Q_j and R_j are linearly independent. Therefore, the solution to Eq. (10) for the three model coefficients of the proposed DNTDM-HF exists locally for an instantaneous flow field.

3. Preliminary Numerical Results

In order to validate the proposed approach, numerical simulations have been performed based on a combined forced and natural convective vertical channel flow following the test case of Kasagi and Nishimura [9], who investigated the flow and temperature fields using direct numerical simulation (DNS). The Grashof and Reynolds numbers (based on half channel width δ and wall friction velocity u_τ) for the test case are $Gr = 9.6 \times 10^5$ and $Re_\tau = 150$, respectively. The computational domain is $5\pi\delta \times 2\delta \times 2\pi\delta$ and a nonuniform coarse grid of $48 \times 32 \times 48$ is used for discretizing the streamwise (x_1), wall-normal (x_2) and spanwise (x_3) dimensions, respectively. Three different SGS HF models, namely, the conventional DEDM-HF [3] and DLTDM-HF [1], and the proposed DNTDM-HF are used for closure of Eq. (1). To close the filtered momentum equation, the dynamic nonlinear SGS stress model (DNM) [8] was adopted in all the test cases. In presenting the results, quantities nondimensionalized using the wall friction velocity u_τ and wall friction temperature T_τ are denoted using a superscript "+".

Figure 1 shows the predicted mean velocity profile using wall coordinates. In comparison with the purely forced convection case ($Gr = 0$, Kuroda *et al.* [10]), the velocity profile for the aiding flow deforms and a logarithmic region no longer exists near the hot wall; while near the cold wall, the velocity profile for the opposing flow shifts downwards. From the figure, it is observed that the performance of the three tested SGS HF models is similar. This is due to the fact that for all the test cases, the same DNM is used for modelling the SGS stress and the influence of the buoyancy on the fluid dynamics is limited in this mixed convection. Figure 2 shows the root-mean-square (RMS) of the resolved streamwise velocity fluctuations. Since the effect of buoyancy on the flow field is to make the opposing flow more turbulent, the values of $\bar{u}^+_{1rms}$ are enhanced near the cold wall and suppressed near the hot wall. From the figure, it is observed that the prediction of $\bar{u}^+_{1rms}$ by the DEDM-HF is closer to the DNS results on the opposing side; however, the predictions of both the DLTDM-HF and DNTDM-HF agree more with the DNS results on the aiding side, especially in the buffer layer. Figure 3 shows the resolved Reynolds stresses $\left|\langle\bar{u}_1''\bar{u}_2''\rangle^+\right|$, which indicates that the prediction of the proposed DNTDM-HF is slightly closer to the DNS results on the aiding side in comparison with the other two SGS HF models.

From Figs. 4–6, it is evident that the buoyancy force creates a striking difference between the aiding and opposing flows. Figure 4 compares the mean temperature profiles predicted by the different models. Due to the existence of buoyancy, the temperature profile for both the aiding and opposing flows deviates

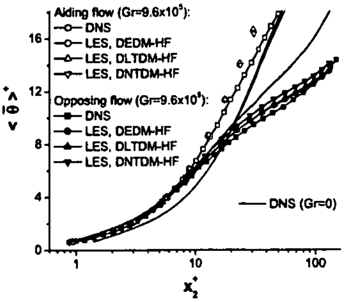

Figure 4: Mean temperature profile.

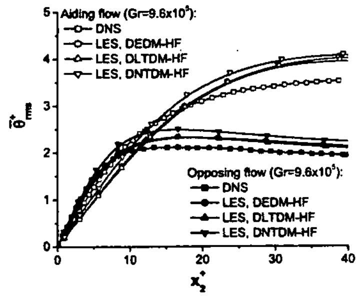

Figure 5: RMS of temperature fluctuations.

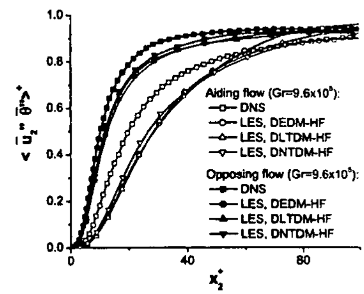

Figure 6: Resolved wall-normal turbulent heat flux.

from that of a passive scalar ($Gr = 0$). From the figure, it is observed that the DNTDM-HF yields a result that is slightly closer to the DNS data on the aiding side, however, it overpredicts the temperature on the opposing side. Figures 5 and 6 show the predicted resolved temperature fluctuation $\bar{\theta}^+_{rms}$ and wall-normal turbulent heat flux $\langle \bar{u}''_2 \bar{\theta}'' \rangle^+$, respectively. The temperature fluctuation $\bar{\theta}^+_{rms}$ is slightly overpredicted by the DNTDM-HF for both the aiding and opposing flows. However, as shown in Fig. 6, the prediction of $\langle \bar{u}''_2 \bar{\theta}'' \rangle^+$ by the DNTDM-HF agrees better with the DNS data in comparison with the other two models.

In conclusion, although the performance of the DNTDM-HF is, in general, similar to those of the DEDM-HF and DLTDM-HF in terms of the prediction of resolved quantities demonstrated in the paper, the DNTDM-HF is advantageous in term of tensor theory and geometrical properties. The constitutive relation of the DNTDM-HF based on $\bar{S}_{ij}$ is complete and irreducible, includes the conventional models (i.e., DEDM-HF of Moin *et al.* [3] and DLTDM-HF of Peng and Davidson [1]) as special cases, and allows for a non-alignment between h_j and $\partial\bar{\theta}/\partial x_j$. A more extensive comparative numerical study is being conducted to obtain a more comprehensive understanding of the proposed SGS HF model.

References

1. S.-H. Peng and L. Davidson. On a subgrid-scale heat flux model for large-eddy simulation of turbulent thermal flow. *Int. J. Heat Mass Trans.*, 45:1393-1405, 2002.
2. E. Porté-Agel, M. Parlange, C. Meneveau and W. Eichinger. A priori field study of the subgrid-scale heat fluxes and dissipation in the atmospheric surface layer. *J. Atmos. Sci.*, 58:2673-2698, 2001.
3. P. Moin, K. Squires, W. Cabot and S. Lee. A dynamic subgrid-scale model for compressible turbulence and scalar transport. *Phys. Fluids A*, 3:2746-2757, 1991.
4. M. Germano, U. Piomelli, P. Moin and W. H. Cabot. A dynamic subgrid-scale eddy viscosity model. *Phys. Fluids A*, 3:1760-1765, 1991.
5. M. Reiner. A mathematical theory of dilatancy. *Amer. J. Math.*, 67:350-362, 1945.
6. R. S. Rivlin. Large elastic deformations of isotropic materials. iv. further developments of the general theory. *Philos. Trans. R. Soc. Lond. A*, 241:379-397, 1948.
7. Q.-S. Zheng. Theory of representations for tensor functions–a unified invariant approach to constitutive equations. *Appl. Mech. Rev.*, 47:545-587, 1994.
8. B.-C. Wang and D. J. Bergstrom. A dynamic nonlinear subgrid-scale stress model. *Phys. Fluids*, 17(035109):1-15, 2005.
9. N. Kasagi and M. Nishimura. Direct numerical simulation of combined forced and natural turbulent convection in a vertical plane channel. *Int. J. Heat Fluid Flow*, 18:88-99, 1997.
10. A. Kuroda, N. Kasagi and M. Hirata. Direct numerical simulation of turbulent plane Couette-Poiseuille flows: effect of mean shear rate on the near-wall turbulence structures. in *Proc. Turbul. Shear Flows 9 (Edited by F. Durst et al.)*, pp. 241–257, Springer-Verlag, 1995.