ANALYSIS AND MODELLING OF THE TURBULENT DIFFUSION OF TURBULENT HEAT FLUXES IN NATURAL CONVECTION

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ABSTRACT

Stably and unstably thermally stratified fluid layers are often encountered in practice ranging form environment to industry. There are examples of counter gradient heat fluxes occurring in such fluid layers containing a combination of both types of stratification. Simple standard heat flux models as employed e.g. in the *k*- ε - σ_i framework need to be improved for representing such behaviour of the turbulent heat fluxes. More complex algebraic models or even in some cases the full transport equations for the turbulent heat fluxes are therefore required. There, the triple correlation $\overline{u'_j u'_k T'}$ appears as an important closure term in the turbulent diffusion. Usually, this is modelled following the Daly and Harlow approximation, which has already been found to be not sufficiently accurate in buoyant flows.

In this paper, the transport equation for this triple correlation will be analyzed using Direct Numerical Simulation (DNS) data of two different flow types, for a internally heated fluid layer (IHL) and for Rayleigh-Bénard convection (RBC). Based on this study a Reynolds-Averaged Navier Stokes (RANS) model for the above closure term will be derived. Finally, this will be validated using the DNS data of both RBC and IHL which have different Rayleigh (Ra) and Prandtl (Pr) numbers.

INTRODUCTION

It is well known that $k - \varepsilon - \sigma_t$ type turbulence models need improvement for numerically investigating fluid flow involving both unstable and stable thermal stratification. One problem occurs in the turbulent heat flux model: The turbulent Prandtl number σ_t that is widely considered to be constant, depends on many parameters, e.g. here in stratified flows especially on the Richardson number (Venayagamoorthy et al. 2003). As often counter gradient heat fluxes are involved, more complex heat flux models need to be used. These are, e.g. algebraic approximations as in Launder (1988) or second order models basing on transport equations for the turbulent heat fluxes like summarized by Launder (1989) and for liquid metal flows in Carteciano and Grötzbach (2003). In the second order models, the triple correlation $\overline{u'_{j}u'_{k}T'}$ appears as an important closure term in the turbulent diffusion.

The other problem occurs in the turbulent shear stress model, because all models are basing on the k-equation which needs improvement for partially stably stratified flows: Following suggestions by Moeng and Wyngaard (1989) a way to improve the standard model by introducing buoyancy effects in the modelling of turbulent diffusion of khas been discussed in Chandra (2005). Considering the unusual dominance of the pressure term in the k-diffusion in RBC with or without imposed shear effects as shown by Domaradzki and Metcalfe (1988) and Wörner and Grötzbach (1998), a separate model for the pressurevelocity fluctuation correlation has been derived by Chandra and Grötzbach (2006). Using the transport equation for the velocity-fluctuation triple correlation its buoyancy-extended model is obtained by Chandra and Grötzbach (2007). There, the triple correlation $\overline{u'_i u'_k T'}$ also appears as closure term in the buoyancy contribution.

To deduce an improved model for this triple correlation, in the next section the flow features in IHL and RBC are discussed. These flows are used as vehicles for investigating this higher order correlation. The subsequent section will be presenting the derivation of the model for this triple correlation basing on a detailed study of its transport equation using DNS data. Finally, a validation of the derived model will be presented.

FLOW TYPES AND MODELLING REQUIREMENTS

DNS specifications

In this section some of the salient features of IHL and RBC analyzed from DNS data are presented. In RBC, the fluid layer between two infinite horizontal isothermal walls is heated uniformly from below and cooled from above. In

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IHL the fluid is internally heated by a uniform volumetric energy source and cooled by keeping both walls at a lower temperature than the fluid confined in-between; see the time-mean temperature profiles in figure 1.

The external Rayleigh number for RBC is $Ra_E = g\gamma\Delta T_w D^3/(v\kappa)$ and the internal Rayleigh number for IHL is $Ra_I = g\gamma q_v D^5/(v\kappa\lambda)$, where g is the gravity acceleration, γ is the volume expansion coefficient, ΔT_w is the wall temperature difference, D is the wall distance, q_v is the volumetric heat source, λ is the thermal conductivity, v and κ are the diffusivities for momentum and thermal energy, respectively. The Prandtl number of the fluid is $\Pr = v/\kappa$. Hereafter, external and internal Rayleigh numbers are referred to as Rayleigh number Ra.

The three-dimensional time-dependent TURBIT code, see Grötzbach (1987), which is based on a finite volume method has been employed for performing and analysing the DNS of RBC and IHL. Results obtained are already intensively used and validated for RBC in different fluids, e.g. in Grötzbach (1983), Wörner (1994), and Otić et al. (2005), and for IHL e.g. in Grötzbach (1987), Wörner et al. (1997), and Chandra (2005). A review on the details of the convective heat transfer in IHL is given by Kulacki and Richards (1985). The IHL may be considered as a representative of flow behaviour e.g. in chemically exothermal reactive flows, in nuclear reaction driven flows in stars, or even in the convective planetary boundary layer. Consequently, models that are developed for IHL may be adapted to numerical investigations e.g. of environmental and of certain chemical process flow problems.

For analysing the DNS results, homogeneity is assumed in the horizontal planes $X_1 - X_2$; thus, the statistical averaging is computed over these planes and over time. Such quantities are denoted by an over-bar (). In all figures this is represented by $\langle \rangle$. The fluctuation computed by using this average is indicated by ()".

Consequently, the heat transfer in each fluid layer reduces to a one-dimensional problem depending only on the vertical co-ordinate X₃. Also there is no horizontal mean flow, therefore the mean shear vanishes. For length scale the fluid layer height D, for temperature scale the wall temperature difference ΔT_w , for velocity scale $u_0 = (g\gamma\Delta T_w D)^{1/2}$, and for pressure scale (ρu_0^2) is used with ρ as the density. In IHL ΔT_w means its maximum value across the height of fluid layer. This is estimated apriori using the Damköhler number, see e.g. Grötzbach (1987). The present scaling results in $\operatorname{Re} = u_0 D / v = \sqrt{Gr} = \sqrt{Ra/Pr}$. In this study, the time averaged turbulent kinetic energy and its dissipation are denoted by $\overline{E'}$ and $\overline{\varepsilon'}$ instead of k and ε , respectively.

DNS analysis of IHL and RBC

Table 1 gives the specifications for the DNS that are the basis for numerically investigating the two different buoyant flows, IHL and RBC.



Figure 1: Vertical profiles of the mean temperature analyzed from DNS; IHL9(○), RBCA(♦).

Table 1: DNS specifications.

Flow type	Ra	Pr	Source
IHL	10^{7}	7	Wörner et al. (1997)
IHL	10^{9}	7	Chandra (2005)
RBC	6.3*10 ⁵	0.71	Wörner (1994)

The table reveals that the above DNS are performed for water (Pr = 7) and air (Pr = 0.71). Their validations are available in the respective sources. In the figures IHL with $Ra=10^7$, 10^9 and RBC with air are represented by IHL7, IHL9 and RBCA, respectively. All these DNS follow the spatial resolution requirements as proposed by Grötzbach (1983). Special attention has been given to avoid truncation of large scales by the periodic boundary conditions which are used in the horizontal directions.

The vertical statistical mean temperature profiles of IHL and RBC are shown in figure 1. In this and subsequent figures $X_3=1$ and $X_3=2$ indicate the positions of the lower and upper walls, respectively. This figure depicts the increase in temperature along the height in case of IHL that attains its maximum close to the upper wall. Therefore, most of the height of the fluid layer is stably stratified and only a small portion of the fluid layer close the upper wall is unstably stratified. The unstable stratification drives the vertical heat and momentum exchange, whereas the stable stratification attenuates this process. The standard $k - \varepsilon$ type RANS models are found to be not suitable for accounting such damping effect of stable stratification, see e.g. Davidson (1990). In RBC the decrease in temperature along the vertical direction reveals that the fluid layer is everywhere unstably stratified.

The vertical profile of the statistical turbulence kinetic energy in figure 2 demonstrates its strong in-homogeneity in IHL even at this high Ra. This is consistent with the strong damping effect in stable stratification. In RBC, this is almost homogeneous along the height of the fluid layer away from the near wall regions.



Figure 2: Vertical profiles of the mean turbulent kinetic energy analyzed from DNS; IHL9(○), RBCA(♦).

One of the important features of these flows can be explained based on their vertical profiles of the mean temperature in figure 1 and of the statistical turbulent heat fluxes as shown in figure 3. This reveals, indeed most of the height of the fluid layer in IHL is having a counter-gradient heat flux, which was already discussed in Grötzbach (1987) for a lower Ra. Whereas in RBC the statistical turbulent heat flux is almost homogenous, leaving the near wall regions. Nevertheless, the standard gradient diffusion heat flux model even fails to predict this homogeneous flux in RBC, see e.g. in Otić and Grötzbach (2007).

MATHEMATICAL MODELLING

Modelling concept

The most general models, which should reproduce counter gradient heat fluxes, are second order models like introduced e.g. by Donaldson (1973) or like it is used in a CFD code by Carteciano and Grötzbach (2003) in combining a first order low-Reynolds number $k - \varepsilon$ model with a full second order turbulent heat flux model. In the transport equations for the turbulent heat fluxes the turbulent diffusion appears as one of the closure terms. This consists of the partial derivatives of a triple correlation of velocity-temperature fluctuation $\overline{u'_{\mu}u'_{\mu}T'}$ and of a pressuretemperature fluctuation correlation p'T'. Usually they are modelled together by the Daly and Harlow (1970) approximation for the triple-correlation by almost neglecting the contribution from the pressure term as indicated in Launder (1989). It has already been shown by Chandra (2005) in modelling the analogous turbulent diffusion of kinetic energy that the involved pressure correlation term needs special attention in buoyant flows. Keeping this requirement and the statistical homogeneity of the considered fluid flows in view, the present paper

describes one way to improve the Daly and Harlow model for a separate modelling of $\overline{u_j'^2T'}$, along the vertical direction indicated by j=3.



Figure 3: Vertical profiles of the mean turbulent heat flux analyzed from DNS; IHL9(○), RBCA(♦).

Following simplifications are used for deriving the model for $\overline{u_2'^2T'}$:

A: The flow types are horizontally homogeneous and there is no horizontal mean flow so that these flows are shear free in the current averaging method.

B: The cross-correlations of the velocity fluctuations are smaller than their auto-correlations, i.e. $\overline{u'_i u'_j} \ll \overline{u'_j}^2$ for $i \neq j$, with i, j = 1, 2, 3.

Daly and Harlow model

The Daly and Harlow (hereafter referred to as DH) model for $\overline{u_3'^2T'}$ using simplifications A and B becomes:

$$\overline{u_3'^2 T'} \approx -C_{\theta} \frac{\overline{E'}}{\overline{\varepsilon'}} \left(2\overline{u_3'^2} \frac{\partial \overline{u_3' T'}}{\partial x_3} + \overline{u_3' T'} \frac{\partial \overline{u_3'^2}}{\partial x_3} \right).$$
(1)

Generally, C_{θ} is considered as constant coefficient with a value between 0.05 and 0.11. On the other hand Dol et al. (1997) had shown that this is not a constant and even can attend much higher values. A similar behaviour is observed by Wörner et al. (1997) in which they found that this coefficient needs to be increased by almost 100 times in IHL at $Ra = 10^8$. The analysis of our DNS data for RBC and IHL reveals that indeed the DH model needs both qualitative and quantitative improvement in these flow types, see figure 5. Further on, there are indications in literature that the involved coefficient may even depend on parameters like turbulent Reynolds number, $\operatorname{Re}_{t} = \overline{E'}^2 / (v \overline{\varepsilon'})$. Thus, there are possibilities to improve the existing DH model as given in equation 1.

Analysis of transport equation

As a first step in the derivation of the model for $u_3'^2T'$, its transport equation (2) as given in Dol (1998) has been analyzed using DNS data of IHL and RBC at different *Ra* and *Pr*. All the terms except the production due to Reynolds stresses and convection are closure terms. These two terms reduce to zero using the present statistical averaging.

$$\frac{\partial \overline{u_{3}^{2}T'}}{\partial t} = -\left(\overline{u_{k}} \frac{\partial \overline{u_{3}^{2}T'}}{\partial x_{k}}\right)$$
Convection
$$+\left(\overline{u_{3}^{2}} \frac{\partial \overline{u_{k}^{\prime}T'}}{\partial x_{k}} + 2\overline{u_{3}^{\prime}T'} \frac{\partial \overline{u_{3}^{\prime}u_{k}^{\prime}}}{\partial x_{k}}\right)$$
Prod. by Reynolds stress and turbulent heat fluxes (ProS)
$$-\left(\frac{\overline{u_{3}^{\prime}}^{2}u_{k}^{\prime}}{\partial x_{k}} + 2\overline{u_{3}^{\prime}u_{k}^{\prime}T'} \frac{\partial \overline{u_{3}}}{\partial x_{k}}\right) - \left(\frac{\partial \overline{u_{3}^{\prime}}^{2}u_{k}^{\prime}T'}{\partial x_{k}}\right)$$
Prod. due to mean Temp. and shear
$$+2\frac{Ra}{Re^{2}Pr}\left(\overline{u_{3}^{\prime}T'^{2}}\right)$$
Buoyaney(ProB)
$$+\frac{1}{Re}\left(\frac{\partial}{\partial x_{k}}\left\{2\overline{u_{3}^{\prime}T'} \frac{\partial u_{3}^{\prime}}{\partial x_{k}} + \frac{1}{Pr}\left\{\overline{u_{3}^{\prime}}^{2} \frac{\partial T'}{\partial x_{k}}\right\}\right)\right)$$
Molecular terms (M)
$$+2\left(\underbrace{\overline{p'}\left\{\frac{\partial u_{3}^{\prime}T'}{\partial x_{k}}\right\}}_{Press. transport} - \frac{\partial \overline{p'}u_{3}^{\prime}T'}{\partial x_{k}}\right)_{Press. transport}}_{(Dput)}\right)\delta_{k3}$$

$$-\frac{2}{Re}\left(\left(\left\{\frac{\partial u_{3}^{\prime}}{\partial x_{k}}\right\}^{2}T'\right) + \left(1 + \frac{1}{Pr}\right)\left\{\overline{u_{3}^{\prime}} \frac{\partial u_{3}^{\prime}}{\partial x_{k}} \frac{\partial T'}{\partial x_{k}}\right\}\right)$$
Dissipative terms (D)

Production due to the Reynolds stresses and turbulent heat fluxes (ProS), the turbulent transport (TurbT) and the dissipation (D) are generally used for deriving the DH model for heat fluxes as given in equation (1). Additionally, there are terms which can be significant in the different flow types. Therefore, all the terms in equation (2) that remain at the steady state are analyzed as shown in figure 4.

The figures also include the budget or out of balance of this equation which is calculated using all terms. This term is smaller than most other terms. This confirms that the flow is nearly fully developed, that equation (2) should be correct, and that the equation is also numerically correct realized in the analyzing software of the TURBIT code system.

The investigation of the other terms depicts the difficulty involved in classifying the terms in the transport equation, e.g. the production and dissipation show positive and negative contributions in certain regions. Thus, a separation of important terms by the formal classification may not be very useful for modelling. It can be inferred that, unlike the transport equations for second-order correlations, the equation for third-order correlations poses more challenges in modelling the involved closure terms. The only practical way of their approximation is to identify



Figure 4: Vertical profiles of all terms in equation (2) for IHL and RBC analyzed from DNS; ProS(•), -ProT(○),
-TurbT(x), ProB(+), Mol(◊), Pdut (◄), -Dput(-), -Diss(▼) and Budget(Δ).

those terms which may have higher importance based on their DNS analysis. This strategy has been employed in the present case.

The production due to Reynolds stresses and turbulent heat fluxes (ProS) and the turbulent transport (TurbT) have higher significance in RBC than in IHL. In accordance with the strong temperature gradient (see figure 1) the respective production term ProT is important close to the walls in both flows. The contributions of buoyancy (ProB) and dissipation (D) are comparable in IHL. The significance of pressure-transport (Dput) and strain (Pdut) near the walls in RBC can be justified to both the presence of a local region of high pressure fluctuations and of the turbulent heat flux. Special attention should be given to the molecular contribution (M) in the near wall region. The occurrence of 1/Pr in the molecular (M) and dissipative terms (D) shows that their contribution will be enhanced in liquid metals, see equation (2). Therefore, these observations reveal that in addition to the production due to Reynolds stresses (ProS), turbulent transport (TurbT) and dissipative terms (D), the production due to the temperature gradient (ProT), buoyancy contribution (ProB) and molecular terms (M) should be included in a model for $u_3^{\prime 2}T^{\prime}$.

Modelling of $\overline{u_3'^2 T'}$

In order to obtain the RANS model for $u_3'^2T'$ using its transport equation as given in equation (2), beside the

simplifications A and B following assumptions are employed:

- As the flow types are shear free, convection and production due to mean shear vanishes.

- Following a similar approach as in Hanjalić and Launder (1972) the pressure term (P) is modelled as in Rotta (1951) and the Dissipative terms (D) are modelled as a relaxation term as in Zeman and Lumley (1976),

$$P - D \approx -C \frac{\overline{u_3'^2 T'}}{\tau}$$
, with C as a coefficient.

Here, $\tau = \overline{E'}/\overline{\varepsilon'}$ is the typical turbulence time scale.

- The higher-order correlation in the turbulent transport TurbT is modelled as in Hanjalić and Launder (1972).

- As a first extension, the contribution of buoyancy ProB and production due to temperature gradient ProT will be introduced analogous to the turbulent diffusion of the temperature variance as in Dol et al. (1999).

- Considering high Re and moderate Pr the molecular terms (M) are not included.

- Assuming fully developed convection in the steady state, introducing the above simplifications in equation (2) and rearranging results in:

$$\overline{u_{3}^{\prime 2}T^{\prime}} \approx -C_{\theta 1}^{\prime} \frac{\overline{E^{\prime}}}{\overline{\varepsilon^{\prime}}} \left(2\overline{u_{3}^{\prime 2}} \frac{\partial \overline{u_{3}^{\prime}T^{\prime}}}{\partial x_{3}} + \overline{u_{3}^{\prime}T^{\prime}} \frac{\partial \overline{u_{3}^{\prime 2}}}{\partial x_{3}} + \overline{u_{3}^{\prime 3}} \frac{\partial \overline{T}}{\partial x_{3}} - 2\frac{Ra}{Re^{2}Pr} \overline{u_{3}^{\prime}T^{\prime 2}} \right)$$
(3)

In equation (3) $C'_{\theta 1} \sim 1/C$ is a coefficient. Considering the observations of Dol et al. (1997), Wörner et al. (1997) and Chandra (2005), $C'_{\theta 1} \approx C_{\theta 1} / \text{Re}_t^{\beta}$ with $\beta \approx 0.52$ and $C_{\theta 1} \approx 0.25$ is used here. This dependence is consistent with the directions by Daly and Harlow (1970) and by Launder (1989). This model (3) will be referred to as Daly and Harlow Extended (DHE) model. The DH model as in equation (1) contains only the first two terms on the rhs of the DHE model. The DHE model also includes the production due to the mean temperature gradient and the contribution of buoyancy. In this model the last two closure terms involve the higher-order correlations $\overline{u'_3}^3$ and $\overline{u'_3T'^2}$. The first one may be modelled according to Launder (1989). An improved model for the other closure term has been derived by Otić et al. (2005), which is validated with DNS data of RBC at different Pr.

VALIDATION

The DNS data at different Ra and Pr for the discussed flows are used for the validation of the extended DHE model for the triple-correlation in the turbulent diffusion of the turbulent heat flux. The DNS results for the triple correlation are given in Chandra and Grötzbach (2007). Here, the partial derivative of this term is used for evaluation as it appears in the heat flux diffusion term. The coefficient $C_a \approx 0.11$ is used in the DH model. For the



Figure 5: Profiles of the partial derivatives of triple correlation and its modelled values from equations (1) and (3) for IHL and RBC analyzed from DNS; DNS (\bullet), DH (\circ) and DHE (Δ).

DHE model the employed model coefficients are already discussed. The comparisons in figure 5 clearly indicate that considerable improvement is achieved in these flows with the extended model over the standard gradient approximation. The simple model produces not only quantitatively wrong diffusion data, but produces even a qualitatively wrong vertical distribution in IHL. In this flow type the extended model shows better qualitative and quantitative prediction except close to the lower wall. In RBC the DHE diffusion model reveals its better acceptability near the walls.

CONCLUSIONS

The simple gradient approximation for turbulent heat fluxes has limited application and accuracy for purely buoyant convection, especially while dealing with counter gradient heat fluxes. Consequently, attempts are still ongoing to derive more accurate models. In certain buoyancy driven flows, for example in the atmosphere, even the full transport equations for the heat fluxes may be preferred. This involves turbulent diffusion as one of the closure terms in which a triple correlation of the velocitytemperature fluctuation correlation appears. In this paper an extended version of the Daly and Harlow model for this closure term is derived. Subsequent validation reveals its better predictive capability compared to the simple gradient diffusion model. The developed extension requires an additional modelled transport equation for $\overline{u_3'}^2$, e.g. by Launder et al. (1975), and a closure for $\overline{u_3'}T'^2$, e.g. by Otić et al. (2005). Thus, even the modelled heat flux equations require special assumptions accounting for the large anisotropy which are inherent to buoyant flows.

The discussed DHE model for $\overline{u_3'^2T'}$ also occurs in the buoyancy extended diffusion model for the *k* equation, see Chandra and Grötzbach (2007). This means, the new DHE model not only allows for better treatment of the turbulent diffusion in all second order heat flux models, but also for a better modelling of the turbulent energy diffusion in all *k* - based turbulence models. Thus, this improved modelling is of major importance in buoyant flow calculations.

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