Available online at www.sciencedirect.com
ScienceDirect
International Journal of Heat and Fluid Flow 29 (2008) 743–751
International Journal of HEAT AND FLUID FLOW
www.elsevier.com/locate/ijhff

Analysis and modelling of the turbulent diffusion of turbulent heat fluxes in natural convection

Laltu Chandra [1], Günther Grötzbach *

Forschungszentrum Karlsruhe, Institut für Kern- und Energietechnik, Postfach 3640, 76021 Karlsruhe, Germany

Received 31 October 2007; received in revised form 23 January 2008; accepted 24 January 2008
Available online 19 March 2008

Abstract

In stably and unstably stratified fluid layers there are often highly anisotropic and counter gradient heat fluxes occurring. Standard heat flux models as the isotropic k–ε–σ_t model need to be improved for representing such behaviour. More complex algebraic models or even in some cases the full transport equations for the turbulent heat fluxes are therefore required. There, a triple correlation appears as an important closure term in the turbulent diffusion. Usually, this is modelled following Daly and Harlow, which has already been found to be not sufficiently accurate in buoyant flows. In this paper, some of the salient features of an internally heated fluid layer (IHL) and of Rayleigh–Bénard convection (RBC) are discussed basing on direct numerical simulation (DNS) data. In IHL a counter gradient heat flux occurs over a wide region. The transport equation for the triple correlation is analyzed using the DNS data. Based on this study a Reynolds-Averaged Navier Stokes (RANS) model for this closure term is derived which covers the influence of the fluid Prandtl number (Pr) and of buoyancy. The model is validated using the DNS data of both RBC and IHL for different Rayleigh and Prandtl numbers.

Keywords: Turbulent heat flux diffusion; Thermal stratification; Anisotropy; Counter gradient heat flux; DNS; RANS

1. Introduction

It is well known that the commonly used k–ε–σ_t type turbulence models need improvement for numerically investigating fluid flow involving buoyancy influences with unstable and stable thermal stratification. Such models are basing on gradient diffusion, assume isotropic turbulent diffusivities for momentum and heat, and apply the Reynolds analogy to approximate the turbulent diffusivity for heat by means of a turbulent Prandtl number σ_t. One problem occurs in the turbulent heat flux model: The turbulent Prandtl number is widely considered to be constant; instead it depends on many parameters, see e.g. Kays (1994). Here in stratified flows it depends especially on the Richardson number (Venayagamoorthy et al., 2003). As often counter gradient and strongly anisotropic heat fluxes are involved, more complex models need to be used as discussed in Launder (1988), Hanjalić (2002) and Grötzbach (2007). These are, e.g. algebraic approximations as in Launder (1988), Otić and Grötzbach (2007), or second order models basing on the transport equations for the turbulent heat fluxes as deduced e.g. in Donaldson (1973). In the turbulent heat flux equations 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 practically relevant models are basing on the k-equation for the turbulent kinetic energy 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 k has been discussed in Chandra (2005). Considering the unusual dominance of the pressure term in the k-diffusion in Rayleigh–Bénard convection with or without imposed shear

* Corresponding author. Tel.: +49 7247 82 4477; fax: +49 7247 82 4837.
E-mail address: groetzbach@iket.fzk.de (G. Grötzbach).
[1] Presently with the Equipe-MoST, LEGI, B.P. 53, 38041, Grenoble, Cedex 09, France.

0142-727X/$ - see front matter © 2008 Elsevier Inc. All rights reserved.
doi:10.1016/j.ijheatfluidflow.2008.01.009

effects as shown by Domaradzki and Metcalfe (1988) and Wörner and Grötzbach (1998), a separate model for the pressure-velocity fluctuation correlation has been derived by Chandra and Grötzbach (2007a). Using the transport equation for the velocity-fluctuation triple correlation its buoyancy-extended model is obtained by Chandra and Grötzbach (2007b). There, the triple correlation $\overline{u_j'u_k'T'}$ also appears as closure term in the buoyancy contribution.

The current status of modelling of this triple correlation especially for the turbulent heat flux diffusion can be found e.g. in Launder (1989), Dol et al. (1999) and Hanjalić (2002), to name a few. They have given a broader review on the modelling for turbulent stresses and heat fluxes for complex or buoyancy influenced flows. Daly and Harlow (1970) proposed a model which is widely used. A model for meteorological applications is deduced in Donaldson (1973).

Lai and So (1990) compared some of the models going back to the Launder-school in practical channel flow applications and concluded that the modelling would not be critical. In contrast, for liquid metal flows modelling extensions are required, see e.g. in Carteciano and Grötzbach (2003). And for buoyancy dominated flows at Prandtl numbers different from one the DNS analyses by Wörner and Grötzbach (1995) and Wörner et al. (1997) also show that the current modelling is insufficient so that a model adaptation to low Prandtl number flows is proposed.

To deduce an improved model for $\overline{u_j'u_k'T'}$ for convection in horizontal fluid layers, which accounts for the high anisotropy in buoyant flows, the next section explains some of the flow features of an internally heated fluid layer (IHL) and of Rayleigh–Bénard convection (RBC). 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 correlation basing on a detailed study of its transport equation using DNS data. Finally, a validation of the derived model will be presented.

2. Flow types and modelling requirement

2.1. Flow type specifications

The analysis and modelling in this work is based on DNS data for two buoyant horizontal fluid layers, the standard RBC and the less common IHL. In this section both are shortly introduced and some of the salient features are analyzed. In RBC, the fluid layer between two infinite horizontal isothermal walls is heated uniformly from below and cooled from above. In 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 vertical time-mean temperature profiles in Fig. 1. 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.

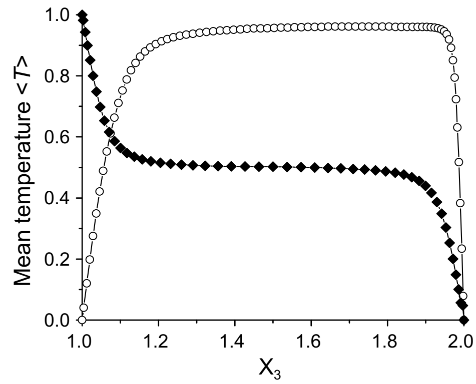

Fig. 1. Vertical profiles of the mean temperature analyzed from DNS; IHL9 (○), RBCA (♦).

The flows are characterized by the external Rayleigh number $Ra_E = g\gamma\Delta T_w D^3/(\nu\kappa)$ for RBC and by the internal Rayleigh number $Ra_I = g\gamma\, q_v D^5/(\nu\kappa\lambda)$ for IHL, 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, ν and κ are the diffusivities for momentum and thermal energy, respectively. The Prandtl number of the fluid is $Pr = \nu/\kappa$. Hereafter, external and internal Rayleigh numbers are referred to as Rayleigh number Ra .

For analysing the DNS results, following the standard approach 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 and their fluctuations are denoted by standard over-bar $\overline{()}$ and $()'$, respectively. In all figures these are shown by $\langle\ \rangle$ and $()''$. Consequently, the heat transfer in each fluid layer reduces to a one-dimensional problem depending only on the vertical co-ordinate X_3. Also there is no horizontal mean flow, therefore the mean shear vanishes.

The results are made dimensionless by using the following scales: For length scale the fluid layer height D is used, 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 the fluid layer. This value is problem dependent; it is estimated a priori using the Damköhler number $Da = q_v D^2/(\lambda\Delta T_w)$. For fully developed convection one gets $Da = Nu_b + Nu_t$ which is computed from available correlations for the Nusselt number Nu_b at the bottom wall and Nu_t at the top wall, see e.g. Kulacki and Richards (1985), Grötzbach (1987), and Schmidt et al. (1997). The present scaling results in $Re = u_0 D/\nu = \sqrt{Gr} = \sqrt{Ra/Pr}$. 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.

2.2. DNS analysis of IHL and RBC

The three-dimensional time-dependent TURBIT code has been employed for performing and analysing the DNS of RBC and IHL, see Grötzbach (1987). It is based on a finite volume method of second order. An Euler–Leapfrog Crank Nicolson scheme is applied for integration in time, see e.g. Wörner (1994) for more details. Results obtained are already validated and intensively used 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), (1989), Wörner et al. (1997), and Chandra (2005).

Table 1 gives the specifications for the DNS that are the basis for numerically investigating the two different buoyant flows, IHL and RBC. 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 $Ra = 5 \times 10^6$, 10^7, 10^8, 10^9 and RBC with air are represented by IHL6, IHL7, IHL8, IHL9 and RBCA, respectively. All these DNS use finer grids than follow from 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 both horizontal directions, because both flow types react very sensitive on large scale truncation. This is inferred by analyzing the two point correlation coefficients in the horizontal direction for the velocity fluctuations. In all these simulations these coefficients remain close to zero for a distance of half the length of the horizontal extension L_1 of the computational domain, see e.g. Grötzbach (1989) and Chandra (2005).

The vertical statistical mean temperature profiles of IHL and RBC are shown in Fig. 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. From there cold plumes plunge downward into the hot core of the fluid layer; see e.g. Kulacki and Richards (1985), Wörner et al. (1997, 1998). The unstable stratification drives this vertical heat and momentum exchange, whereas the stable stratification attenuates this process. The standard k–ε type RANS models are found to be not suitable for accounting such damping effect of stable stratification, see e.g. Davidson (1990), Hattori and Nagano (2007). In RBC the decrease in temperature along the vertical direction reveals that the fluid layer at this Ra is everywhere unstably stratified.

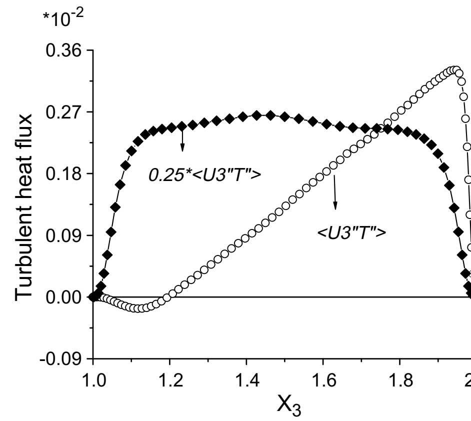

Fig. 2. Vertical profiles of the mean turbulent heat flux analyzed from DNS; IHL9 (○), RBCA (♦).

One of the important features of these flows can be explained based on their vertical profiles of the statistical mean temperature in Fig. 1 and of the turbulent heat fluxes as shown in Fig. 2. This reveals, indeed most of the height of the fluid layer in IHL is having a positive heat flux, which means an upward directed heat transport towards the temperature maximum; thus, a counter-gradient heat flux occurs as was already discussed in Grötzbach (1987) for a lower Ra. As a consequence, any gradient type heat flux model, and so also the turbulent Prandtl number concept, will fail to predict the heat flux in this flow type. In RBC the statistical turbulent heat flux is almost homogenous, leaving the near wall regions. Nevertheless, the standard gradient diffusion heat flux model also fails to predict this homogeneous flux in RBC, see e.g. in Otić and Grötzbach (2007). Also from Hattori and Nagano (2007) the need of improvements in the standard k–ε type RANS models for the turbulent momentum transfer can be inferred to achieve a more accurate description of the stably stratified boundary layer.

The vertical profile of the statistical turbulence kinetic energy in Fig. 3 demonstrates its strong vertical in-homogeneity in IHL even at this high Ra. This is consistent with

Table 1
DNS specifications

Flow type	Ra	Pr	Domain size $L_1 \times L_2 \times D$	Grid	Source
IHL	5×10^6	7	$5 \times 5 \times 1$	$100 \times 100 \times 35$	Schmidt et al. (1997), Wörner et al. (1997)
IHL	10^7	7	$5 \times 5 \times 1$	$128 \times 128 \times 39$	”
IHL	10^8	7	$4 \times 4 \times 1$	$160 \times 160 \times 55$	”
IHL	10^9	7	$4 \times 4 \times 1$	$320 \times 320 \times 77$	Chandra (2005)
RBC	6.3×10^5	0.71	$7.92 \times 7.92 \times 1$	$200 \times 200 \times 39$	Wörner (1994)

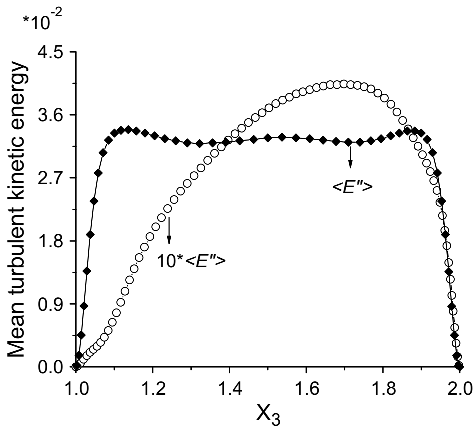

Fig. 3. Vertical profiles of the mean turbulent kinetic energy analyzed from DNS; IHL9 (○), RBCA (♦).

the strong damping effect in the stably stratified region. In RBC, the distribution is almost homogeneous along the height of the fluid layer away from the near wall regions.

2.3. Modelling requirement

The most general models, which should be capable of reproducing 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–ε 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 $\overline{u'_j u'_k T'}$ and of a pressure-temperature fluctuation correlation $\overline{p'T'}$. 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 horizontal homogeneity of the considered flows in view, the present paper describes one way to improve the Daly and Harlow model for a separate modelling of $\overline{u'^2_j T'}$ along the vertical direction indicated by $j = 3$.

Following simplification is used for analysing models and for deriving the extended model for $\overline{u'^2_3 T'}$:

A: The flow types are horizontally homogeneous (x_1 and x_2 derivatives are statistically zero) and there is no horizontal mean flow so that these flows are shear free in the current averaging method.

The widely used Daly and Harlow model (hereafter referred to as DH) for $\overline{u'^2_3 T'}$ using simplification A becomes:

$$\overline{u'^2_3 T'} \approx -C_\theta \frac{\overline{E'}}{\overline{\varepsilon'}} \left(2\overline{u'^2_3} \frac{\partial \overline{u'_3 T'}}{\partial x_3} + \overline{u'_3 T'} \frac{\partial \overline{u'^2_3}}{\partial x_3} \right) \qquad (1)$$

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 the DNS data in Fig. 4 reveals that this model may only be partially accepted in predicting the vertical positions of minima near the walls for RBC, but it is certainly inadequate for IHL. Here $C_\theta = 0.11$ is used. It can be inferred from this comparison that the DH model needs both qualitative and quantitative improvement in these flow types. Moreover, special attention should be given for modelling stably stratified fluid layers as in IHL. Further on, there are indications in literature that the involved coefficient may even depend on parameters like turbulence Reynolds number, $Re_\tau = \overline{E'}^2/(\nu\overline{\varepsilon'})$. Thus, there are possibilities and needs to improve the existing DH model as given in Eq. (1).

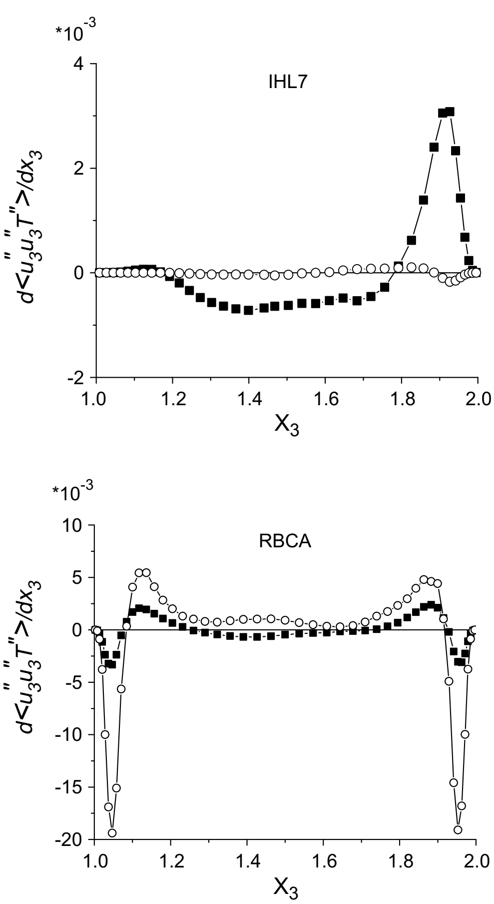

Fig. 4. Profiles of the partial derivatives of triple correlation and its modelled values from Eq. (1) for IHL7 & RBCA analyzed from DNS; DNS (■), DH (○).

3. Mathematical modelling

In this section one way is described to improve the model for the triple correlation.

3.1. Analysis of transport equation

As a first step in the derivation of the model for $\overline{u_3'^2T'}$, its transport Eq. (2) as given in Dol (1998) has been analyzed using DNS data of IHL and RBC at different Ra and Pr. Using the present scaling, $Ra/(Re^2Pr)=1$. All the terms except the production due to Reynolds stresses and convection are closure terms. In the considered horizontal fluid layers, these two terms reduce to zero using the present statistical averaging.

$$
\begin{aligned}
\frac{\partial \overline{u_3'^2T'}}{\partial t} = & -\underbrace{\left(\overline{u}_k \frac{\partial \overline{u_3'^2T'}}{\partial x_k}\right)}_{\text{Convection}} \\
& +\underbrace{\left(\overline{u_3'^2}\,\frac{\partial \overline{u_k'T'}}{\partial x_k}+2\overline{u_3'T'}\,\frac{\partial \overline{u_3'u_k'}}{\partial x_k}\right)}_{\text{Prod. by Reynolds stress and turbulent heat fluxes (ProS)}} \\
& -\underbrace{\left(\underbrace{\overline{u_3'^2u_k'}\,\frac{\partial \overline{T}}{\partial x_k}}_{\text{ProT}}+2\overline{u_3'u_k'T'}\,\frac{\partial \overline{u}_3}{\partial x_k}\right)}_{\text{Prod. due to mean Temp. and shear}}-\underbrace{\left(\frac{\partial \overline{u_3'^2u_k'T'}}{\partial x_k}\right)}_{\text{Tur. transport (TurbT)}} \\
& +\underbrace{2\frac{Ra}{\mathrm{Re}^2\,\mathrm{Pr}}\left(\overline{u_3'T'^2}\right)}_{\text{Buoyancy (ProB)}} \\
& +\underbrace{\frac{1}{\mathrm{Re}}\left(\frac{\partial}{\partial x_k}\left\{2\,\overline{u_3'T'\frac{\partial u_3'}{\partial x_k}}+\frac{1}{\mathrm{Pr}}\left\{\overline{u_3'^2\,\frac{\partial T'}{\partial x_k}}\right\}\right\}\right)}_{\text{Molecular terms (M)}} \\
& +\underbrace{2\left(\underbrace{\overline{p'\left\{\frac{\partial u_3'T'}{\partial x_k}\right\}}}_{\substack{\text{Press. strain}\\ (Pdut)}}-\underbrace{\frac{\partial \overline{p'u_3'T'}}{\partial x_k}}_{\substack{\text{Press. transport}\\ (Dput)}}\right)\delta_{k3}}_{\text{Pressure terms (P)}} \\
& -\underbrace{\frac{2}{\mathrm{Re}}\left(\left(\overline{\left\{\frac{\partial u_3'}{\partial x_k}\right\}^2 T'}\right)+\left(1+\frac{1}{\mathrm{Pr}}\right)\left\{\overline{u_3'\,\frac{\partial u_3'}{\partial x_k}\,\frac{\partial T'}{\partial x_k}}\right\}\right)}_{\text{Dissipative terms (D)}}.
\end{aligned}
\tag{2}
$$

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 Eq. (1). Additionally, there are terms which can be significant in the different flow types. Therefore, all the terms in Eq. (2) that remain at the steady state are analyzed as shown in Fig. 5. The DNS analyzed data for the triple correlation $\overline{u_3'^2T'}$ are shown in Fig. 6.

The data in Fig. 5 include the budget or out of balance of the transport Eq. (2) which is calculated using all terms. This term is smaller than most other terms. This confirms that the flow is nearly fully developed, that Eq. (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 all other terms depicts the difficulty involved in classifying the terms in the transport equation, e.g. the production due to stresses and heat fluxes and dissipation show positive and negative contributions in certain regions. These regions are not always consistent with those, in which positive or negative values for $\overline{u_3'^2T'}$ occur, see Fig. 6. Thus, a separation of important terms by the formal classification may not be very useful for modelling, because it has to be concluded that other terms obviously also give considerable contributions. 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 developing a model is to identify those terms in Fig. 5 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 Fig. 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. Also it can be inferred that a part of the production of the triple correlation is due to ProB in both flow types. 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 Eq. (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 $\overline{u_3'^2T'}$.

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

In order to obtain the RANS model for $\overline{u_3'^2T'}$ using its transport equation as given in Eq. (2), beside the simplification A following assumptions are employed:

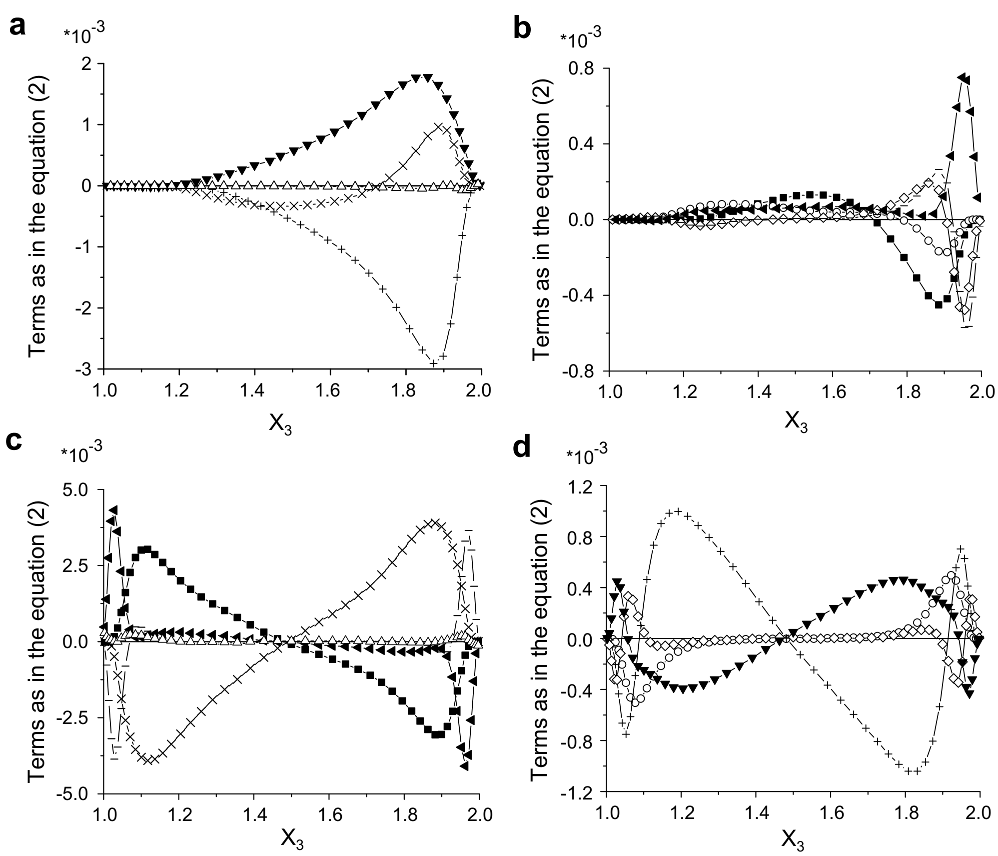

Fig. 5. Vertical profiles of all terms in Eq. (2) for IHL7 in (a, b) and RBCA in (c, d) analyzed from DNS; ProS (■), -ProT (○), -TurbT (×), ProB (+), Mol (◇), Pdut (◀), -Dput (-), -D (▼) and Budget (△), see also Chandra and Grötzbach (2007b).

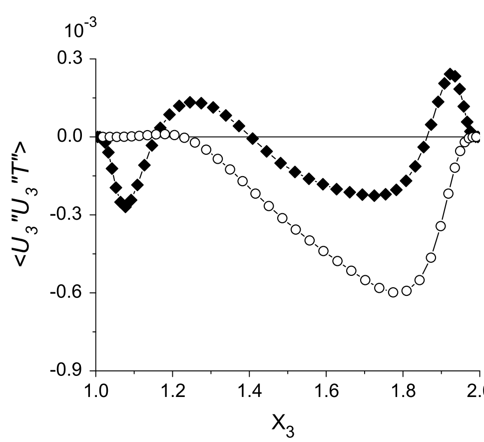

Fig. 6. Vertical profiles of triple correlation analyzed from DNS; IHL7 (○) and RBCA (⧫).

– 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),

$$P - D \approx -C\frac{\overline{u_3'^2T'}}{\tau},$$

with C as a coefficient. Here, typically the turbulent time scale of the velocity fluctuations $\tau = \overline{E'}/\overline{\varepsilon'}$ is used.
– The higher-order correlation in the turbulent transport TurbT is modelled as in Hanjalić and Launder (1972),

$$\overline{u_3'^2\, u_k'T'} \approx (\overline{u_3'^2}\;\overline{u_k'T'}) + 2(\overline{u_3'u_k'}\;\overline{u_3'T'}).$$

– Using simplification A gives:

$$\mathrm{ProS} - \mathrm{TurbT} = -\left(2\overline{u_3'^2}\frac{\partial\overline{u_3'T'}}{\partial x_3} + \overline{u_3'T'}\frac{\partial\overline{u_3'^2}}{\partial x_3}\right).$$

– 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 Eq. (2) and rearranging results in:

$$\overline{u_3'^2T'} \approx -C'_{\theta 1}\frac{\overline{E'}}{\overline{\varepsilon'}}\left(\begin{array}{c}2\overline{u_3'^2}\frac{\partial\overline{u_3'T'}}{\partial x_3} + \overline{u_3'T'}\frac{\partial\overline{u_3'^2}}{\partial x_3}\\ +\overline{u_3'^3}\frac{\partial\overline{T}}{\partial x_3} - 2\frac{Ra}{Re^2Pr}\overline{u_3'T'^2}\end{array}\right). \quad (3)$$

If the mean velocity gradients are not negligible then their contributions to the production and convection as shown in Eq. (2) have to be included in the model which needs additional investigations. In Eq. (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), $C'_{\theta 1} \approx C_{\theta 1}/Re_\tau^\beta$ with $\beta \approx 0.52$ and $C_{\theta 1} \approx 0.25$ is used here. This dependence on the turbulence Reynolds number is consistent with the directions by Daly and Harlow (1970) and by Launder (1989). As an example, this behaviour has been shown in Fig. 7b for IHL at a certain height point. Same values of parameters are used for RBC in which the statistical turbulent heat flux is mostly homogeneous along the height of the fluid layer. It may be expected that a functional description of β on height could be even more accurate.

Moreover, Fig. 7a reveals that the DNS analyzed values of the turbulence Reynolds number Re_τ are having different order of magnitudes in IHL and RBC. This is consistent with the damping and driving influence of stable and unstable thermal stratification on the turbulence mixing, respectively.

The new model as in Eq. (3) will be referred to as Daly and Harlow Extended model (DHE). The DH model as in Eq. (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 $\overline{u_3'T'^2}$. The first one may be modelled according to Launder (1989) as it is

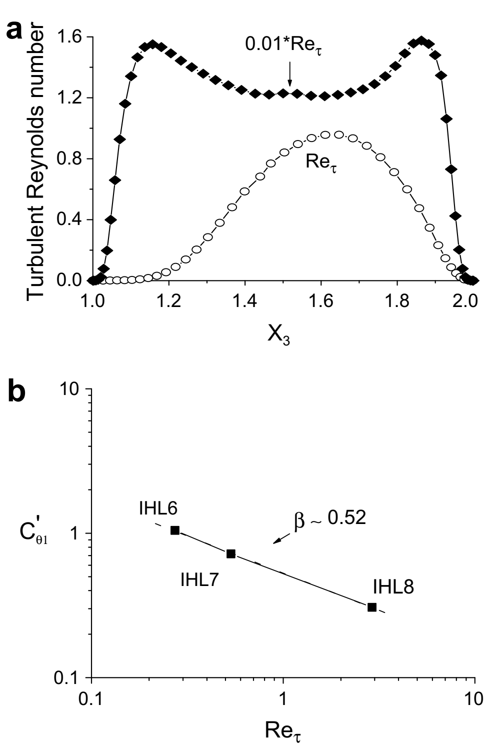

Fig. 7. (a) Turbulence Reynolds number analyzed from DNS; IHL7 (○), RBCA (♦); (b) coefficient $C'_{\theta 1}$ in Eq. (3) analyzed from DNS data for IHL at $X_3 \approx 1.4$; DNS (■), Linear fit (–).

indicated by 'Mod' in Eq. (4). Combining his model with Eq. (3) results in:

$$\overline{u_3'^2T'} \approx -C'_{\theta 1}\frac{\overline{E'}}{\overline{\varepsilon'}}\left(\begin{array}{c} 2\overline{u_3'^2}\frac{\partial \overline{u_3'T'}}{\partial x_3} + \overline{u_3'T'}\frac{\partial \overline{u_3'^2}}{\partial x_3} \\ \underbrace{-C_\mu \overline{u_3'^2}\frac{\overline{E'}}{\overline{\varepsilon'}}\left(\frac{\partial \overline{u_3'^2}}{\partial x_3}\right)\frac{\partial \overline{T}}{\partial x_3}}_{\text{Mod}} \\ -2\frac{Ra}{Re^2 Pr}\overline{u_3'T'^2}\end{array}\right) \quad (4)$$

C_μ is the well known coefficient of the k–ε model. An improved model for the other closure term, i.e. for the triple correlation $\overline{u_3'T'^2}$, has been derived by Otić et al. (2005). It is validated with DNS data of RBC at different Pr. The triple correlation follows as the solution of the following equation:

$$\overline{u_3'T'^2} \approx -C_{\theta 2}\left[\frac{2}{Re\sqrt{Pr}}\tau \Delta_x \overline{u_3'T'^2} + \frac{\overline{E'}^2}{\overline{\varepsilon'}}\frac{\partial \overline{T'^2}}{\partial x_3}\right]$$

Here $C_{\theta 2}$ is an empirical coefficient and Δ_x is a Laplacian operator. For $C_{\theta 2}$ a value of 0.11 has been preferred by Otić et al. (2005). To account for the influence of the molecular Prandtl number of the fluid a mixed time scale for the velocity and temperature fluctuations is chosen:

$$\tau = \sqrt{\frac{\overline{E'}}{\overline{\varepsilon'}}\frac{\overline{T'^2}}{\overline{\varepsilon'_T}}}$$

Thus, the above model has to be complemented by the additional transport equations for the temperature variance, as it is anyway needed for the production term due to buoyancy in the heat flux equation, and its dissipation $\overline{\varepsilon'_T}$. The velocity-fluctuation auto-correlations $\overline{u_3'^2}$ follow automatically when the second order heat flux model involving the closures (3) or (4) for the turbulent heat flux diffusion is used in the framework of a second-order shear stress model or when it is combined at least with a buoyancy extended algebraic shear stress model.

4. 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 results for the triple correlation are given in Chandra and Grötzbach (2007b). Here, the partial derivative of this term is used for evaluation as it appears in the turbulent heat flux diffusion term. The coefficient $C_\theta = 0.11$ is used in the DH model. For the DHE model as given in Eq. (3) the employed model coefficients are already discussed. The comparisons in Fig. 8 clearly indicate that considerable improvement is achieved in these flows with the extended model over the standard DH 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

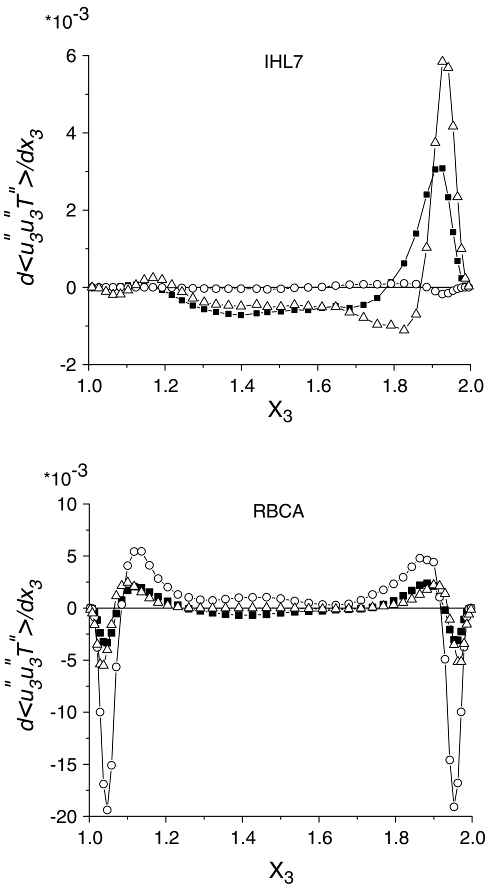

Fig. 8. Profiles of the partial derivatives of triple correlation and its modelled values from Eqs. (1) and (3) for IHL7 & RBCA analyzed from DNS; DNS (■), DH (○) and DHE (Δ).

better qualitative and quantitative predictions except close to the lower wall. In RBC the DHE diffusion model reveals its better acceptability near the walls.

5. 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 velocity-temperature fluctuation correlation appears. In this paper an extended version of the Daly and Harlow model for this turbulent heat flux diffusion is derived, Eq. (3). This also includes formal contributions of buoyancy and production due to temperature gradient to the triple correlation. The influence of the molecular Prandtl number of the fluid is also included. Subsequent validation reveals its better predictive capability compared to the simple gradient diffusion model. The developed extension requires an additional model for $\overline{u_3'^2}$, which will anyway be available when the second order heat flux model is combined with a second order shear stress model or with an algebraic shear stress model as e.g. in Launder et al. (1975). In addition a closure for $\overline{u_3' T'^2}$ is needed, as 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 $\overline{u_3'^2 T'}$ also occurs in the buoyancy extended diffusion model for the k equation, see Chandra and Grötzbach (2007b). 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 kinetic energy diffusion in all k-based turbulence models for momentum transfer. Thus, this improved modelling is of major importance in calculations of buoyant flows.

Acknowledgements

The authors wish to convey sincere thanks to the Institut für Kern- und Energietechnik, Forschungszentrum Karlsruhe GmbH, Germany and to the team MoST, LEGI, National Polytechnic Institute Grenoble, France for supporting the presentation of the precursor paper at the 5th International Symposium on Turbulence and Shear Flow Phenomena, Munich, Germany.

References

Carteciano, L.N., Grötzbach, G., 2003. Validation of Turbulence Models in the Computer Code FLUTAN for a Free Hot Sodium Jet in Different Buoyancy Flow Regimes. FZKA 6600.

Chandra, L., 2005. A Model for The Turbulent Diffusion of Turbulent Kinetic Energy in Natural Convection. PhD Thesis, Univ. Karlsruhe, Germany, FZKA 7158.

Chandra, L., Grötzbach, G., 2007a. A RANS Model for The Velocity Pressure Fluctuation Correlation. In: Progress in Turbulence II, Springer Proceedings in Physics 109, Oberlack, M. et al. (Eds.), ISBN: 3-540-32602-2, pp. 185–188.

Chandra, L., Grötzbach, G., 2007b. Analysis and modeling of the turbulent diffusion of turbulent kinetic energy in natural convection. Flow, Turb. Comb. 79, 133–154.

Daly, B.J., Harlow, F.H., 1970. Transport equations in turbulence. Phys. Fluids 18, 2634–2649.

Davidson, L., 1990. Second-order corrections of the k–ε model to account for non-isotropic effects due to buoyancy. Int. J. Heat Mass Transfer 33, 2599–2608.

Dol, H.S., Hanjalić, K., Kenjereš, S., 1997. A comparative assessment of the second-moment differential and algebraic models in turbulent natural convection. Int. J. Heat Fluid Flow 18, 4–14.

Dol, H. S., 1998. Turbulence Models for Natural Convection in Side-Heated Enclosures. PhD Thesis, Technische Universiteit Delft, Nederlands.

Dol, H.S., Hanjalić, K., Versteegh, T.A.M., 1999. A DNS-based thermal second-moment closure for buoyant convection at vertical walls. J. Fluid Mech. 391, 211–247.

Domaradzki, J.A., Metcalfe, W., 1988. Direct numerical simulations of the effect of shear on turbulent Rayleigh–Bénard convection. J. Fluid Mech. 193, 499–531.

Donaldson, C. duP., 1973. Construction of a dynamic model of the production of atmospheric turbulence and the dispersal of atmospheric pollutants. In: Haugen, D.A. (Ed.), Workshop on Micrometeorology, Amer. Met. Society, pp. 313–392.

Grötzbach, G., 1983. Spatial resolution requirements for direct numerical simulation of the Rayleigh–Bénard convection. J. Comput. Phys. 49, 241–264.

Grötzbach, G., 1987. Direct numerical and large Eddy simulation of turbulent channel flows. In: Cheremisinoff, N.P. (Ed.), Encyclopaedia of Fluid Mechanics, Complex Flow Phenomena and Modeling, vol. 6. Gulf Publishing Company, Houston, pp. 1337–1391.

Grötzbach, G., 1989. Turbulent heat transfer in an internally heated fluid layer. In: Iwasa, Y. et al. (Eds.), Refined Flow Modelling and Turbulence Measurements. Un. Ac. Press, Tokyo, pp. 267–275.

Grötzbach, G., 2007. Anisotropy and Buoyancy in Nuclear Turbulent Heat Transfer – Critical Assessment and Needs for Modelling. FZKA 7363.

Hanjalić, K., Launder, B.E., 1972. A Reynolds stress model of turbulence and its application to thin shear flows. J. Fluid Mech. 52, 609–638.

Hanjalić, K., 2002. One point closure models for buoyancy-driven turbulent flows. Annual Rev. Fluid Mech. 34, 321–347.

Hattori, H., Nagano, Y., 2007. Numerical study of turbulent thermal boundary layer under various stable stratifications. In: Friedrich, R. et al., (Eds.), Proceedings of the Fifth International Symposium on Turbulence and Shear Flow Phenomena, vol. 2, Munich, pp. 481–486.

Kays, W.M., 1994. Turbulent Prandtl number – where are we? J. Heat Transfer 116, 284–295.

Kulacki, F.A., Richards, D.E., 1985. Natural convection in plane layers and cavities with volumetric energy sources. In: Kakać, S., Aung, W., Viskanta, R. (Eds.), Natural Convection – Fundamentals and Applications, Hemisphere, pp. 179–255.

Lai, Y.G., So, R.M.C., 1990. Near-wall modeling of turbulent heat fluxes. Int. J. Heat Mass Transfer 33, 1429–1440.

Launder, B.E., Reece, G.J., Rodi, W., 1975. Progress in the development of a Reynolds-stress turbulence closure. J. Fluid Mech. 68, 537–566.

Launder, B.E., 1988. On the computation of convective heat transfer in complex turbulent flows. ASMEC J. Heat Transfer 110, 1112–1128.

Launder, B.E., 1989. Second-moment closure: present... and future? Int. J. Heat Fluid Flow 10, 282–300.

Moeng, C.–H., Wyngaard, J.C., 1989. Evaluation of turbulent transport and dissipation closures in second-order modeling. J. Atmos. Sci. 46, 2311–2330.

Otić, I., Grötzbach, G., Wörner, M., 2005. Analysis and modelling of the temperature variance equation in turbulent natural convection for low-Prandtl-number fluids. J. Fluid Mech. 525, 237–261.

Otić, I., Grötzbach, G., 2007. Turbulent heat flux and temperature variance dissipation rate in natural convection in Lead-Bismuth. Nucl. Sci. Eng. 155, 489–496.

Rotta, J., 1951. Statistische Theorie nichthomogener Turbulenz, 1. Mitteilung. Zeitschrift für Physik 129, 547–572.

Schmidt, M., Wörner, M., Grötzbach, G., 1997. Direkte numerische Simulation der Konvektion in einer Fluidschicht mit interner Wärmequelle. FZKA 5916.

Venayagamoorthy, S.K., Koseff, J.R., Ferziger, J.H., Shih, L.H., 2003. Testing of RANS turbulence models for stratified flows based on DNS data. Annual Research Briefs, Center for Turbulence Research, 127–138.

Wörner, M., 1994. Direkte Simulation turbulenter Rayleigh–Bénard-Konvektion in flüssigem Natrium. PhD Thesis, Univ. Karlsruhe, Germany, KfK 5228.

Wörner, M., Grötzbach, G., 1995. Modelling the molecular terms in the turbulent heat flux equation for natural convection. In: Proceedings of the 10th Symposium on Turbulent Shear Flows, Pennsylvania State Univ., State College, Pennsylvania, USA, 2, pp. P2-73–P2-78.

Wörner, M., Schmidt, M., Grötzbach, G., 1997. Direct numerical simulation of turbulence in an internally heated convective fluid layer and implications for statistical modelling. J. Hydraulic Res. 35, 773–797.

Wörner, M., Grötzbach, G., 1998. Pressure transport in direct numerical simulations of turbulent natural convection in horizontal fluid layers. Int. J. Heat Fluid Flow 19, 150–158.

Zeman, O., Lumley, J.L., 1976. Modeling buoyancy driven mixed layers. J. Atmos. Sci. 33, 1974–1988.