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Connections between Lagrangian stochastic models and the closure theory of turbulence for stratified flows

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Abstract

An overview is given of some recently obtained results in the development of Lagrangian probability density function (PDF) methods for stratified turbulent flows. Turbulence is described in this approach as stochastic motion of particles and change of their properties in accord with usual budget equations of turbulence up to second order. This concept differs from the closure theory of turbulence in two ways. Firstly, reactions can be taken into account exactly. Secondly, this approach represents a new theory for turbulent mixing processes and it provides turbulence statistics for stratified flow. This is illustrated by considering the dispersion of buoyant particles, and by the calculation of third-order moments of the velocity–temperature PDF as well as the velocity PDF itself. The calculated buoyant plume rise is found to be in agreement with measurements in the atmosphere. The results for the turbulence statistics are shown to be in accord with water tank data and large-eddy simulation (LES) of a convective boundary layer. Finally, the advantages of applying such concepts to modelling transport, mixing and reaction of substances in stratified flows are pointed out.

Keywords: Stratified turbulent flow; Lagrangian stochastic models; Closure theory; Buoyant plume rise; Third-order correlations; Velocity-temperature; PDF

1. Introduction

Lagrangian stochastic models for the motion of fluid particles and change of particle properties appear to be a natural frame for the development of models for turbulent dispersion, scalar mixing and reaction in high-Reynolds number turbulent flows. One of the main advantages of Lagrangian methods over Reynolds-averaged Navier–Stokes (RANS) equations is that chemical reactions can be treated exactly (Pope, 1985). Just the required closure for non-linear reaction rates in RANS equation methods may cause errors by several orders of magnitude, if invalid approximations are applied (Pope, 1990; Fox, 1996). By considering the motion of all the fluid particles of the flow, these models define budgets for arbitrary moments of the velocity probability density function (PDF), so that the question arises as to the relationship of such Lagrangian models and usual Eulerian budget equations of turbulence. As observed by Pope (1994), such Lagrangian stochastic models can always be constructed in consistency with turbulence budget equations up to second order. These Lagrangian particle models then describe the one-point PDF of turbulent fluctuations, that depends only on a few assumptions on the pressure correlations and dissipation terms. Such relationships are instructive for both the Eulerian and the Lagrangian approaches. The Lagrangian models provide e.g. for the Eulerian approach criteria for the realizability of second-moment closures (Durbin and Speziale, 1994; Wouters et al., 1996). Inversely, the Eulerian budget equations may provide constraints for the design of Lagrangian models.

The extension of the Lagrangian PDF approach to stratified flow (for geophysical applications for instance) requires firstly an equation for the particle temperature, and secondly, the scaling of turbulence and buoyancy processes. A temperature equation for a particle can be derived e.g. by using relationships to the Eulerian budget theory (Heinz, 1997a). The closure of the pressure correlations and dissipation terms in the Eulerian equations leads to parametrizations for the time scales of the processes that are described in the Lagrangian framework, which means these scales are estimated in terms of the dissipation time scale and closure parameters, that appear as proportionality factors. The remaining problem is the estimation of the dissipation time scale. This is more challenging than for neutral flows, because the changes of this quantity may be remarkably larger due to buoyancy effects. This is found for instance for the buoyant plume rise (Heinz, 1998), that is considered in Section 4.

An overview of some recently obtained results and remaining questions in the development of Lagrangian PDF models

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for stratified turbulent reactive flow is given here. This is done by considering questions such as:

1. How is it possible to scale turbulence, buoyancy and mixing processes in particle methods for stratified flows?
2. What explanations for turbulent mixing processes and the turbulence statistics can be provided by Lagrangian PDF models that are consistent with turbulence budget equations?
3. What new chances are given for the solution of problems of practical relevance by the development of such models?

Lagrangian stochastic equations are described in Section 2 and solutions for the first question are pointed out in Section 3. These equations are then applied to the calculation of the buoyant plume rise (Section 4), the parametrization of third-order moments (Section 5) and the estimation of the vertical velocity PDF in convective turbulence (Section 6). The consequences of these results with respect to the last two questions are summarized finally.

2. Lagrangian stochastic equations

Let us consider linear stochastic Lagrangian equations, which are able to obey Eulerian budget equations up to second order (Heinz, 1997a). An equation for the change of the (potential) particle temperature $\Theta_L(t)$ (the subscript L refers to a Lagrangian quantity) in time t has to be considered in order to take buoyancy effects into account. It is advantageous to combine the particle velocity $\mathbf{U}_L(t)$ and temperature $\Theta_L(t)$ into the four dimensional particle state vector $\mathbf{Z}_L(t) = (\mathbf{U}_L(t), \Theta_L(t))$ in order to write these equations in a compact way. These equations for the particle position $\mathbf{x}_L$, velocity $\mathbf{U}_L$ and temperature Θ_L may be then written as (I runs from 1 to 3 only over velocity components in contrast to i, which runs from 1 to 4):

$$\frac{d}{dt} x^I_L(t) = Z^I_L, \tag{1a}$$

$$\frac{d}{dt} Z^i_L(t) = \langle a^i \rangle + G^{ij}\left(Z^j_L - \langle Z^j_E \rangle\right) + b^{ij} \frac{dW^j}{dt}, \tag{1b}$$

where dW^j/dt is a Gaussian process with vanishing mean values $\langle dW^j/dt \rangle = 0$ and uncorrelated values at different times, $\langle dW^i/dt(t) \cdot dW^j/dt'(t') \rangle = \delta_{ij}\delta(t-t')$. Here, δ_{ij} is the Kronecker delta, $\delta(t-t')$ is the delta function and $\langle \cdots \rangle$ denotes the ensemble average. Z^j_E is the j^{th} component of the vector $\mathbf{Z}_E = (\mathbf{U}_E, \Theta_E)$ that contains the Eulerian velocities $\mathbf{U}_E$ and the temperature Θ_E (the subscript E denotes an Eulerial quantity). Their position dependence is replaced in the Lagrangian equations by the actual particle position.

The Lagrangian equations (1a) and (1b) can be also written in terms of a Fokker–Planck equation (Gardiner, 1983; Risken, 1984) for the PDF of velocity and temperature fluctuations. Considering the motion of all the fluid particles of the flow, the solution of this equation then permits the calculation of the one-point turbulence statistics in time. Agreement with the budget equations for the mean quantities and all the variances of the velocity–temperature fields can be obtained by deriving the corresponding transport equations from the Lagrangian theory and comparing these equations with the Eulerian ones (Heinz, 1997a). The comparison of the equations of first-order for momentum and potential temperature determines then $\langle a^i \rangle$ as

$$\langle a^i \rangle = \nu \frac{\partial^2 \langle Z^i_E \rangle}{\partial x^K \partial x^K} + (\alpha - \nu) \frac{\partial^2 \langle Z^4_E \rangle}{\partial x^K \partial x^K} \delta_{i4} - \langle \rho \rangle^{-1} \frac{\partial \langle p \rangle}{\partial x^K} \delta_{Ki} - g\delta_{i3}, \tag{2}$$

where the Boussinesq approximation and the incompressibility constraint $\partial Z^K_E / \partial x^K = 0$ are applied. Here, p is the pressure, ρ the fluid density, ν the kinematic viscosity, α the coefficient of molecular heat transfer and g the acceleration due to gravity. The comparison of the Eulerian and Lagrangian equations of second-order for the variances permits the estimation of b^{ij} and G^{ij} in dependence on the pressure correlation and dissipation models. By adopting the Kolmogorov approximation (Kolmogorov, 1942), the matrix b is determined by

$$b^2 = \frac{1}{2\tau} \begin{pmatrix} C_0 q^2 & 0 & 0 & 0 \\ 0 & C_0 q^2 & 0 & 0 \\ 0 & 0 & C_0 q^2 & 0 \\ 0 & 0 & 0 & C_1 \langle \left(Z^4_E - \langle Z^4_E \rangle \right)^2 \rangle \end{pmatrix}, \tag{3}$$

where C_0 and C_1 are constants. The dissipation time scale τ is defined by $\tau = q^2/(2\langle \varepsilon \rangle)$, where $\langle \varepsilon \rangle$ denotes the mean dissipation rate of the turbulent kinetic energy (TKE) and q^2 is twice the TKE. The estimation of G is possible in accord with arbitrary models for pressure correlations, but the simple Rotta model (Rotta, 1951) is now applied in order to demonstrate the main features of the approach. Neglecting firstly rapid pressure terms related to a small parameter k_2 as justified for an unsheared boundary layer considered below, and secondly the influence of frequency fluctuations (Pope and Chen, 1990; Pope, 1991), G is given by

$$G = -\frac{1}{4\tau} \begin{pmatrix} k_1 & 0 & 0 & 0 \\ 0 & k_1 & 0 & 0 \\ 0 & 0 & k_1 & -4\beta g \tau \\ 0 & 0 & 0 & 2k_3 - k_1 \end{pmatrix} + \frac{1}{2} A V^{-1}. \tag{4}$$

The derivation of Eq. (4) provides simultaneously the relations $C_0 = (k_1 - 2)/3$ and $C_1 = 2k_3 - 2k_4 - k_1$ for the constants appearing in Eq. (3), where k_1, k_3 and k_4 are parameters that arise from the applied closure assumptions for the pressure correlation and dissipation terms. A is any four-dimensional antisymmetric matrix and V^{-1} the inverse matrix of second moments of the velocity–temperature fields with $V^{ij} = \langle z^i z^j \rangle$, where $z^i = Z^i_E - \langle Z^i_E \rangle$ are the Eulerian fluctuations.

We see, that the effect of the closure of the pressure correlation and dissipation terms in the Eulerian variance transport equations consists of the parametrizations of G and B in terms of the dissipation time scale τ and parameters k_1, k_3 and k_4, which describe the proportionality of all the involved time scales with τ. Thus, the estimation of this mean flow frequency $\omega = \tau^{-1}$ in dependence of shear and stratification is one of the key problems in this approach, because it scales the time scales of all the processes. The parameters k_1, k_3 and k_4 determine the quantitative features of the turbulence as e.g. the values of the anisotropy tensor, correlation coefficients or the power law of the buoyant plume rise.

The appearance of the unknown antisymmetric matrix A in Eq. (4) shows the non-uniqueness of Lagrangian equations that satisfy turbulence budget equations up to second order (Durbin and Speziale, 1994; Pope, 1994). This term causes additional couplings in the Lagrangian equations and consequently also additional correlations. For homogeneous and stationary turbulence one finds e.g. $\langle dZ^i_L(t)/dt \cdot Z^j_L(t) \rangle = 1/2 A^{ij}$, as can be derived from Eqs. (1a) and (1b) by calculating this correlation, separating $G\,V$ into a symmetric and an antisymmetric component and applying the transport equation for the variances to relate the symmetric part with B. Hence, in general also information about such correlations $\langle dZ^i_L(t)/dt \cdot Z^j_L(t) \rangle$ is required in order to estimate G completely, but these influences can be neglected in many cases. This is done also in the applications considered below.

3. Time scales estimation

The scaling of turbulence and buoyancy processes only within the Lagrangian framework is a non-trivial problem when complex conditions have to be considered, and just the above considered consistency constraints between the stochastic Lagrangian equations and the Eulerian budget equations indicate a way to solve it, because they provide a link between the Lagrangian frequencies G^{ij} and the mean Eulerian flow frequency $\omega = \tau^{-1}$.

The application of standard approaches (Wilcox, 1993) for the calculation of ω is complicated by two facts: stratification effects have to be included, and the consideration of spatial gradient terms of ω would increase remarkably the influence of errors in particle simulations. A feasible and robust frequency estimation can be derived (Heinz, 1998), if the particle frequency changes only under the influence of turbulence (as can be seen below from Eq. (5)) and is not directly influenced by spatial gradients of the frequency field. This condition is at least ensured for two benchmark turbulent flows with constant ratios of production to dissipation of TKE: homogeneous shear flow and the logarithmic layer of an equilibrium turbulent boundary layer (Speziale and Gatski, 1994). This approach opens a wide field of applications as e.g. the description of (atmospheric) boundary layer processes, where similar assumptions are often applied (Mellor and Yamada, 1982).

Let us consider a turbulent flow, where the joint velocity–temperature PDF depends only on the vertical coordinate, which is denoted now as $x^3 = z$ as usual. With respect to the applications considered below, a constant vertical gradient $\partial U/\partial z$ is assumed for the mean horizontal velocity $U(\text{along}\, x^1)$, and the influence of the mean vertical velocity and the gradients of triple correlations on the mean flow frequency are neglected. By taking stratification effects into account in standard methods for the estimation of this quantity, one finds

$$\frac{\mathrm{d}}{\mathrm{d}t'} T = C_{\varepsilon 2} - 1 - 2T(C_{\varepsilon 1} - 1) \cdot \left\{ -\frac{\hat{V}^{13}}{\hat{q}^2} + \frac{\hat{V}^{34}}{\hat{q}^2} \right\}, \tag{5}$$

where the dimensionless quantities $T = (\partial U/\partial z)/\omega$ and $t' = t \cdot (\partial U/\partial z)$ are introduced and $C_{\varepsilon 1} = 1.56$ and $C_{\varepsilon 2} = 1.9$ are constants. $\hat{V}^{13}, \hat{V}^{34}$ and $\hat{q}^2$ are dimensionless variances and twice the dimensionless TKE, respectively, that reflect the influence of the turbulence on T and satisfy the system of equations

$$\frac{\mathrm{d}}{\mathrm{d}t'} \begin{pmatrix} \hat{V}^{13} \\ \hat{V}^{14} \\ \hat{V}^{34} \\ \hat{V}^{33} \\ \hat{V}^{44} \\ \hat{q}^2 \end{pmatrix} = \frac{1}{T} \begin{pmatrix} -k_1/2 & T & 0 & -T & 0 & 0 \\ -\mathrm{Ri}T & -k_3/2 & -T & 0 & 0 & 0 \\ 0 & 0 & -k_3/2 & -\mathrm{Ri}T & T & 0 \\ 0 & 0 & 2T & -k_1/2 & 0 & (k_1-2)/6 \\ 0 & 0 & -2\mathrm{Ri}T & 0 & -k_4 & 0 \\ -2T & 0 & 2T & 0 & 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} \hat{V}^{13} \\ \hat{V}^{14} \\ \hat{V}^{34} \\ \hat{V}^{33} \\ \hat{V}^{44} \\ \hat{q}^2 \end{pmatrix}, \tag{6}$$

where $\mathrm{Ri} = (\beta g \partial\Theta/\partial z)/(\partial U/\partial z)^2$ is the gradient Richardson number, Θ the mean Eulerian potential temperature, and β the thermal expansion coefficient. The system (6) arises from the second-order moment equations which are used as budget equations for the derivation of the Lagrangian equations (1a)–(1b). The variances are normalized to twice the TKE at the initial time $q^2(t=0)$, and the variances related to temperature fluctuations (indicated by the superscript 4) appear multiplied with a factor $\beta g(\partial U/\partial z)^{-1}$.

The relation (5) is discussed in Section 4. This approach permits the description of the evolution of ω in accord with shear and stratification. The stationary predictions are rather similar to those of a frequency model, where T is calculated only from turbulence budget equations. The latter approach gives insight into the role of combinations of closure parameters k_1, k_3 and k_4 that can be interpreted as flow numbers (Heinz, 1998).

4. Buoyant plume rise

Let us consider now the application of the Eqs. (1a) and (1b) to the simulation of the buoyant plume rise. An accurate description of the turbulent mixing of the buoyant plume and surrounding flow (i.e. of the dependence of the mixing on initial plume and ambient flow properties) is in particular important for reactive plumes, because the mixing determines, whether chemical reactions between compounds that are distributed in the ambient air and the plume occur or not. Additionally, the mixing determines essentially the spatial patterns of the tracer distributions.

In the Eulerian approach, the buoyant plume rise is explained by entrainment and extrainment concepts. The idea of entrainment of air into plumes by plume-generated turbulence may provide the "two-thirds" power law for the buoyant plume rise (the mean plume height grows proportional to $t^{2/3}$), that is observed in a neutrally stratified and non-turbulent ambient flow (Briggs, 1975). For emissions into turbulent flows one observes that the plume follows at first the two-thirds power law and then levels off at later times, i.e. the mean plume height becomes constant. This effect is explained as extrainment, i.e. entrainment of plume material into the surrounding fluid due to the ambient turbulence. The description of these different mixing processes is related in the Eulerian approach to the introduction of parameters that cannot be derived directly from measurements and require different ad hoc assumptions for their estimation. Secondly, this approach does not provide the dispersion of plume particles.

Within the Lagrangian approach both the mean plume behaviour and the dispersion of plume material can be simulated (van Dop, 1992). The description of turbulent mixing processes has to be handled here by changes of time scales, and no theoretical basis seems to be available for their estimation within the Lagrangian framework for complex conditions. Thus, the characteristics of the plume behaviour had to be explained hitherto by different ad hoc assumptions on the time scale behaviour in the initial and final stage. This is related to questions as to the range of applicability of these assumptions and e.g. the influence of stratification effects.

Instead, the frequency estimations considered above can be applied, if the stochastic Lagrangian equations are chosen in accord with turbulence budget equations. The first term on the right-hand side of Eq. (5) provides a power law for the buoyant plume rise (due to T and growing proportionally to t') in accord with the entrainment idea. It is interesting to note that only this term appears in the original frequency equation of Kolmogorov (Wilcox, 1993). The second term on the right-hand side of Eq. (5) depends on the state of turbulence. It causes a decrease of T and consequently a levelling-off of the plume (see below). This is just the result of the extrainment idea.

In order to illustrate the advantage of the approach presented here let us consider the mean buoyant plume rise and the final rise that follow from Eqs. (1a) and (1b). The particles move only in the vertical direction $x^3 = z$ in the same flow field as considered in Section 3. By introducing the normalized particle height $Z = \langle x_{\mathrm{L}}^3 \rangle (\partial U/\partial z)^2 / B_0$ over the source, that means $\langle x_{\mathrm{L}}^3 \rangle (t=0) = 0$, the velocity $\mathrm{W} = \langle U_{\mathrm{L}}^3 \rangle (\partial U/\partial z)/B_0$ and the buoyancy $B = \beta g \langle \Theta_{\mathrm{L}} - \Theta \rangle / B_0$, where $B_0 = \beta g \langle \Theta_{\mathrm{L}} - \Theta \rangle$ $(t=0)$ is written for the initial buoyancy, the Lagrangian equations Eqs. (1a) and (1b) can be transformed for a neutral stratification into:

$$\frac{dZ}{dt'} = W, \tag{7a}$$

$$\frac{dW}{dt'} = -\frac{k_1}{4T}W + B, \tag{7b}$$

$$\frac{dB}{dt'} = -\frac{2k_3 - k_1}{4T}B, \tag{7c}$$

where t' is applied as above. The two-thirds power law can be obtained, if T is calculated only by the first term of the right-hand side of Eq. (5), which means, if the influence of the ambient turbulence is neglected. For large times one then obtains

$$Z = \frac{1}{m_1 m_2}\left(\frac{I}{C_{\varepsilon 2} - 1}\right)^{2-m_1} \cdot t'^{m_1}, \tag{8}$$

where $m_1 = 2 - (2k_3 - k_1)/(4[C_{\varepsilon 2} - 1])$ and $m_2 = 1 - (k_3 - k_1)/(2[C_{\varepsilon 2} - 1])$ are applied, and I is written for the initial value of T. For the derivation of Eq. (8), only the highest power of t' is taken into account and I is neglected with respect to t'. The change in time of the mean particle height over the source is independent of the shear, that drops out due to the definitions of Z, I and t'. Hence, the two-thirds power law is obtained, if $m_1 = 2/3$, i.e., if $k_3 = k_1/2 + 8[C_{\varepsilon 2} - 1]/3$.

The plume calculated by Eqs. (7a)–(7c) levels off, if the influence of the ambient turbulence is taken into account by considering also the second term on the right-hand side of Eq. (5). The final plume rise is numerically obtained to be

$$\langle x_L^3 \rangle = 1.838 \cdot I \cdot \lambda(I) \cdot \frac{B_0}{(\partial U/\partial z)^2}, \tag{9}$$

where λ is a factor between 0.4 and 1.0 in dependence on I. The levelling-off behaviour of the plume is explained within the Eulerian theory as a result of entrainment of plume material into the surrounding fluid due to the ambient turbulence (called extrainment by Netterville, 1990). The intensity of this process is characterized by a turbulence buffet frequency, that has to be estimated by different (debatable) ad hoc assumptions (Gangoiti et al., 1997). Instead, the relation (9) derived by the simulation of the turbulent mixing between plume and ambient air contains only measurable quantities, such that the turbulence buffet frequency is calculated here in terms of the shear $\partial U/\partial z$ and the parameters k_1 and $C_{\varepsilon 2}$ (Heinz, 1997b).

The curve, that follows only from the initial time scale (the second-term on the right-hand side of Eq. (5) is neglected), is shown in Fig. 1 together with the two-thirds power law curve (8) and the curve that follows from the solution of Eqs. (7a)–(7c) combined with Eqs. (5) and (6). The latter curve is indicated by HFM to point out to the use of the homogeneous (there are no spatial transport terms) frequency model (5) and (6). The equations Eqs. (7a)–(7c) are solved for the initial conditions $Z(t = 0) = 0, W(t = 0) = 0$ and $B(t = 0) = 1$, and Eq. (6) are solved by a Runge–Kutta procedure with initial conditions $\hat{V}^{ij} = 1/3\delta_{ij}$. The initial value $I = (\partial U/\partial z)/\omega(t = 0)$ is set to be 0.173 in accord with data of the Nanticoke plume rise measurements (Netterville, 1990), and $k_1 = 8.3$, $k_3 = 6.5$ (which guarantee the above condition for the power law) and $k_4 = 4.0$ are applied. These curves show the behaviour discussed above: the initial frequency provides asymptotically the two-thirds power law, and the influence of ambient turbulence leads to the levelling-off of the plume. By adopting $\lambda(0.173) = 0.77, B_0 = 0.764$ m s^{-2} and $\partial U/\partial z = 0.04$ s^{-1} according to the conditions of the Nanticoke measurements, one obtains $\langle x_L^3 \rangle = 116$ m. This agrees well with the measured results of $\langle x_L^3 \rangle = (119 \pm 40)$ m.

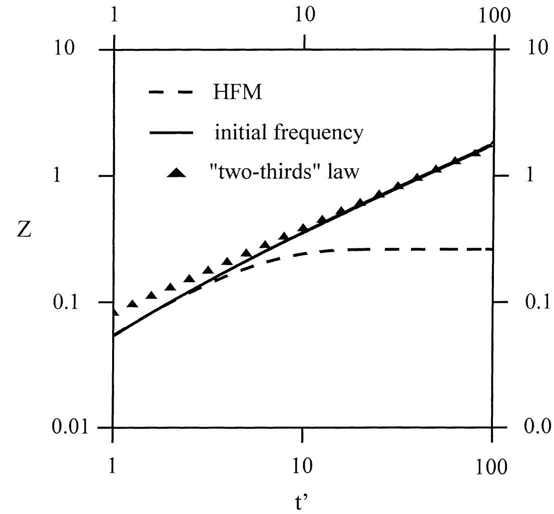

Fig. 1. The dashed line gives the normalized height Z as function of t' as obtained by Eqs. (7a)–(7c). The solid curve represents the initial rise, which follows from the initial particle frequency. The triangles represent the observed two-thirds power law.

5. Third-order moments

After this calculation of the turbulent mixing of buoyant particles with the ambient flow let us turn to the description of the turbulence statistics. The one-point (i.e. Eulerian) PDF of turbulent velocity and temperature fluctuations is determined by the Lagrangian stochastic equations Eqs. (1a) and (1b) or their Fokker–Planck equation. All the moments of this velocity–temperature PDF can be calculated through integrations over this PDF multiplied with the corresponding velocities and temperatures. The change of these moments is determined by their transport equations, that can be derived from the Fokker–Planck equation and represent parametrizations, because the moments of different order are related with each other. The expressions (2)–(4) for the coefficients of the Lagrangian equations (1a)–(1b) ensure that the first- and second-order moments of the velocity–temperature PDF change for arbitrary third- (and higher-) order moments according to usual budget equations derived in the closure theory of turbulence. Thus, all the moments that are higher than second-order can be obtained from Eqs. (1a) and (1b) as a consequence of these equations. This is considered next.

The vertical velocity PDF for convective turbulence, that is important for the design of dispersion models (see e.g. Wilson and Sawford, 1996), is investigated in Section 6. Second-order closure models require the knowledge of the third-order moments of the PDF. These are important ingredients of turbulence models for convective boundary layers, because the typical structures of these flows can only be explained by considering such turbulent transports. This relation between the third- and second-order moments is considered first and compared with corresponding parametrizations of the Eulerian closure theory.

In order to arrive at analytical solutions let us consider the transport equation for the third-order moments $T^{nlm} = \langle z^n z^l z^m \rangle$,

$$\frac{d}{dz}F^{klm3} = \frac{dV^{k3}}{dz}V^{lm} + \frac{dV^{l3}}{dz}V^{km} + \frac{dV^{m3}}{dz}V^{kl} + \Gamma^{kn}T^{nlm} + \Gamma^{ln}T^{nkm} + \Gamma^{mn}T^{nkl}, \tag{10}$$

which follows from Eqs. (1a) and (1b) by multiplying the corresponding Fokker–Planck equation with $z^k z^l z^m$ and integration over velocities and temperatures. Secondly, the often applied quasi-normality assumption is adopted for the fourth-order moments $F^{klmn} = \langle z^k z^l z^m z^n \rangle$. This means, that these terms are taken as products of second-order moments, $F^{klmn} = V^{kn}V^{lm} + V^{ln}V^{km} + V^{mn}V^{kl}$ (Millionshtchikov, 1941; Hanjalić, 1994). This approximation is the simplest of different possible assumptions (Heinz and Schaller, 1996). As above, the turbulence statistics is assumed to depend only on the vertical coordinate z, and $\Gamma^{ij} = G^{ij} - \mathrm{d}\langle Z_E^i \rangle / \mathrm{d}z \delta_{j3}$ is applied as an abbreviation. By inserting the approximation for F^{klmn} in Eq. (10) one obtains an algebraic equation system for the triple correlations. This can be solved (all the details can be found elsewhere (Heinz et al., 1997)), where some approximations are applied, which are justified for an unsheared convective boundary layer. For the triple correlations T^{333} and $T^{113} (= T^{223})$ of velocities one then obtains e.g.

$$T^{333} = -\frac{4\tau}{k_1}\left[\frac{\mathrm{d}V^{33}}{\mathrm{d}z} + 2\alpha_1\alpha_2(\beta g\tau)^2\frac{\mathrm{d}V^{44}}{\mathrm{d}z}\right]\{V^{33} - \alpha_1\beta g\tau V^{34}\} + \alpha_1\frac{8\tau}{k_1}\beta g\tau\frac{\mathrm{d}V^{34}}{\mathrm{d}z}\{V^{33} - 2\alpha_2\beta g\tau V^{34}\}, \quad (11)$$

$$T^{113} = -\frac{4\tau}{3k_1}\cdot\frac{\mathrm{d}V^{11}}{\mathrm{d}z}\{V^{33} - \alpha_1\beta g\tau V^{34}\}, \quad (12)$$

where $\alpha_1 = -4/(2k_3 - k_1)$ and $\alpha_2 = -4/(4k_3 - k_1)$ are introduced.

By adopting parametrizations for the vertical profiles of the variances according to the results of Canuto et al. (1994) for an unsheared convective boundary layer, one finds by means of Eqs. (11) and (12) for the vertical flux $T^{113} + \frac{1}{2}T^{333}$ of TKE the profile presented in Fig. 2. As can be seen, these data agree rather well with the results of LES, that are also presented. A similar behaviour is found for the triple correlation T^{333} of vertical velocities, that is given in Fig. 3. Similar deviations in the maxima of these curves are also found by applying different LES codes, that provide (normalized) values between 0.21 and 0.28. Small deviations in the behaviour of these curves near the surface appear also in the results of Canuto et al.

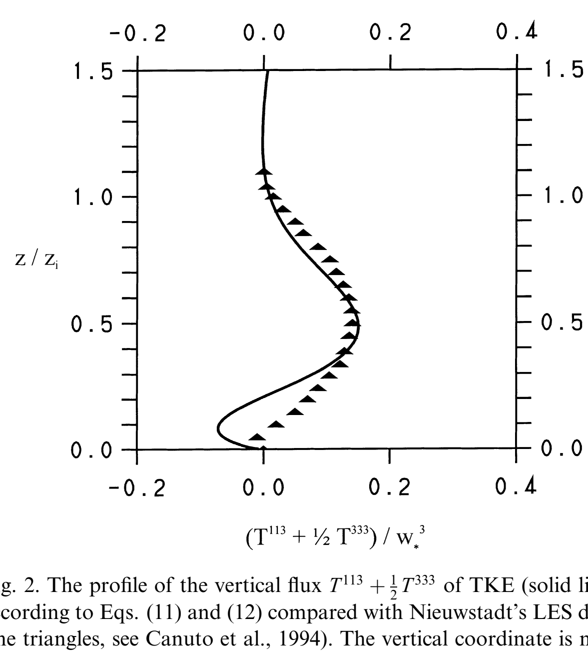

Fig. 2. The profile of the vertical flux $T^{113} + \frac{1}{2}T^{333}$ of TKE (solid line) according to Eqs. (11) and (12) compared with Nieuwstadt's LES data (the triangles, see Canuto et al., 1994). The vertical coordinate is normalized to the boundary layer height z_i, and the vertical flux of TKE is normalized to the cubic convective velocity scale $(w_*)^3$.

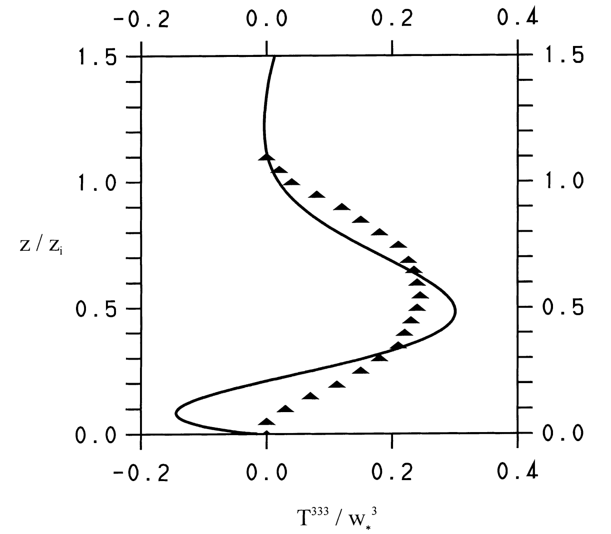

Fig. 3. The normalized vertical profile (solid line) of the third-order moments T^{333} of the velocity PDF according to Eq. (11) compared as in Fig. 2 with Nieuwstadt's LES data.

These derived third-order relations generalize the usual downgradient relation (Hanjalić, 1994) $T^{nlm} \sim \mathrm{d}V^{lm}/\mathrm{d}zV^{3n} + \mathrm{d}V^{nm}/\mathrm{d}zV^{3l} + \mathrm{d}V^{ml}/\mathrm{d}zV^{3m}$ by the incorporation of additional gradients of variances. It can be shown that the downgradient relation is recovered for a neutral flow, where interactions between the turbulent and the buoyant motion vanish (Heinz et al., 1997). The neglect of these additional terms would e.g. be related to the calculation of negative values of vertical flux of TKE in the lower half of the convective boundary layer, whereas it is found to be positive throughout the whole boundary layer in experiments.

Similar third-order relations can be derived by the closure of the Eulerian third-order transport equations (Canuto et al., 1994). However, this requires the introduction of additional closure parameters, which means essentially the setting of the quantitative contributions of all the gradients of the variances. It is obvious that this poses a non-trivial problem for complex flows. Instead, these contributions are obtained here in terms of the closure parameters k_1, k_3 and k_4 without any additional assumptions. Moreover, the Lagrangian approach ensures the realizability of the moments, such that no clipping procedures are required for the third-order terms in order to guarantee the realizability of the second-order moments.

6. Vertical velocity PDF

The usually applied concept of designing models for the turbulent dispersion of tracers is to ensure that the particles move in accord with given turbulence statistics. Thomson (1987) showed that such stochastic one-particle models require the knowledge of the one-point PDF of velocity fluctuations. However, this quantity is difficult to obtain for turbulent flows with structures, as e.g. the updrafts and downdrafts in the convective boundary layer.

Two methods had been applied hitherto to provide this velocity PDF for particle models. Firstly, the adjustment of assumed-shape PDF's to measurements (see e.g. Luhar et al., 1996), and secondly, the construction of the 'maximum missing information' (mmi) PDF proposed by Du et al. (1994a, b). The latter approach makes an optimal use of the available information on a turbulent flow, that means the velocity PDF is fitted to a given (even) number of low-order moments. A review of these developments was given recently by Wilson and Sawford (1996).

These applied concepts adjust the velocity PDF to given knowledge on the non-Gaussianity of the flow. A way to explain this non-Gaussianity and its dependence on mean-flow properties (as e.g. the mean temperature gradients) consists of the simulation of the turbulent flow by means of the stochastic equations presented in Section 2. Here, the non-Gaussianity is calculated in dependence of the mean velocity and temperature fields as well as the variances of these fields. Consequently, in contrast to the mmi approach no information on third- and fourth-order moments is required. Such a concept offers different advantages: (i) it may contribute to the assessment of different assumed-shape approaches, (ii) it may explain variations of the non-Gaussianity of the velocity PDF near the ground and top of the boundary layer, and (iii) it may provide this PDF under (strongly stable) conditions, where information about this quantity by measurements is very hard to obtain. Some first results of the application of this approach are described now.

The velocity–temperature PDF for convective turbulence is estimated by calculating the vertical motion of 500 000 particles and change of their temperatures according to the stochastic Lagrangian equations Eqs. (1a) and (1b), that are scaled as usually with the mixing layer height z_i, the convective velocity scale w_* and the temperature scale θ_*. The same vertical profiles are adopted for the mean values and variances (that enter into the equations by the drift term $\langle a^i \rangle = \partial V^{i3}/\partial z$, see Heinz, 1997a) of the velocity and temperature fields as in Section 5. At the initial time $t = 0$, the particles are distributed continuously between $0 \leqslant z/z_i \leqslant 1$. The initial values of the normalized particle velocities and temperatures are set to be $U_L^3/w_* = \Theta_L/\theta_* = (1 - z/z_i)R$, where R is a Gaussian distributed random variable with zero mean and unity variance. This assumption ensures a normalized vertical flux of heat $V^{34}/(\theta_* w_*) = 1 - z/z_i$ in accord with LES data (Canuto et al., 1994), that indicates the buoyancy in the lower part of the convective boundary layer. The particles are perfectly reflected at the boundaries (Physick, 1997), where their velocities and temperatures are set after the reflection to their negative values in order to ensure zero mean values of vertical velocity and temperature at the boundaries. The Lagrangian equations are solved with a time step of $w_*/z_i \mathrm{d}t = 0.03$ (Thomson, 1987). This calculation requires approximately 0.9 min CPU time per time step. The velocity PDF is calculated from the statistically stationary solution of these equations taking sample values in an interval of $\mathrm{d}z/z_i = 0.02$.

The results of these calculations are presented (without any smoothing procedure) for the heights $z/z_i = 0.69$, 0.44 and 0.19 in Figs. 4–6, respectively, and compared with the water tank measurements of Luhar et al. (1996). The calculated normalized PDF's $gw_*(w/w_*)$ (as usual, $U_E^3 - \langle U_E^3 \rangle = w$ is written) in the middle and upper boundary layer illustrate the ability of the presented approach to reflect the characteristic skewness of the velocity PDF in a convective boundary layer. The quantitative agreement between the calculations and tank data is good, apart from a small underestimate of the probability for the appearance of very small velocity values. This tendency is stronger expressed for the near-surface PDF. This fact is in accord with the deviations of the calculated third-order moments from the LES data as depicted in Fig. 3. A part of these deviations may be attributed to the expressions for the drift terms $\langle a^i \rangle = \partial V^{i3}/\partial z$, that are applied for the calculations presented here. These are chosen according to the conditions described by Canuto et al. in order to include the required

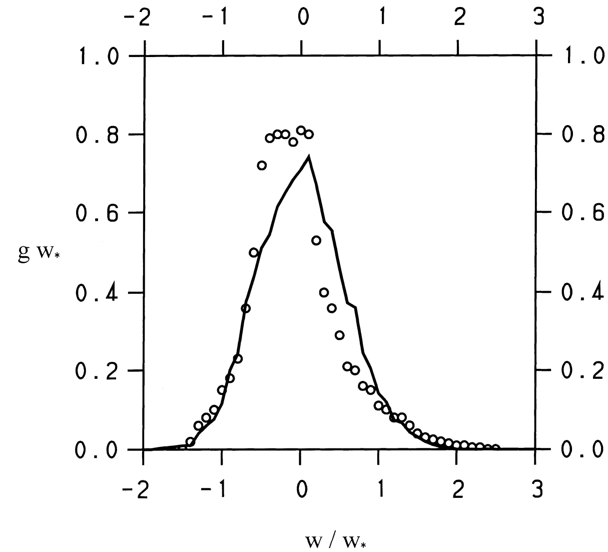

Fig. 4. The normalized PDF gw_* of vertical velocities w/w_* calculated by the Lagrangian particle model Eqs. (1a) and (1b) at $z/z_i = 0.69$ (solid line). The saline water tank data are given as circles, see Luhar et al. (1996).

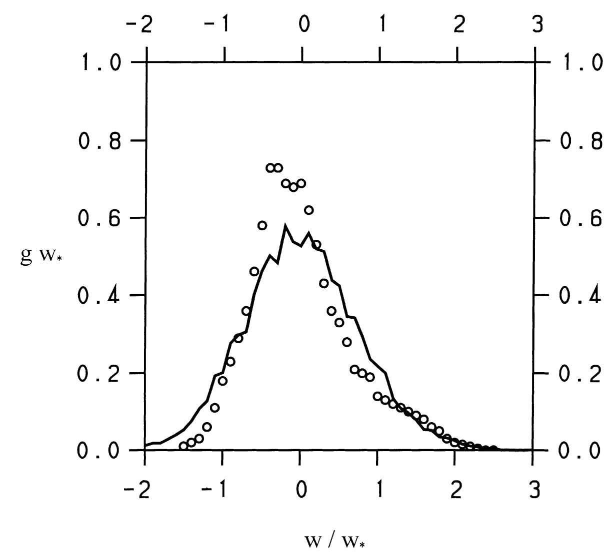

Fig. 5. The normalized PDF gw_* compared with water tank data as given in Fig. 4, but now at $z/z_i = 0.44$.

information on the temperature field, which was not measured in the water tank experiments. More extended comparisons then require simultaneous measurements of the statistics of the velocity and temperature fields in saline water tank studies or their calculation by LES. An improved agreement between the calculated near-surface PDF and measurements seems to be possible by adopting more complex closure models (see e.g. Craft et al., 1996).

7. Concluding remarks

It is demonstrated that the relationship between Lagrangian stochastic models and Eulerian Reynolds-averaged hydrodynamic equations for the moments up to second-order of the velocity and temperature fields may contribute remarkably to

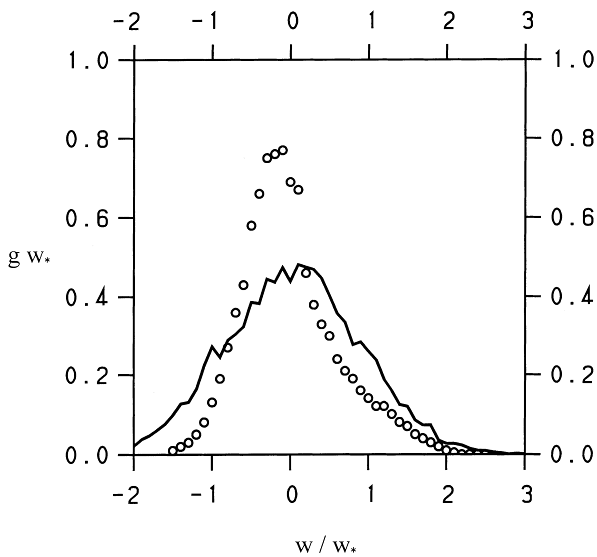

Fig. 6. The normalized PDF gw_* compared with water tank data as given in Fig. 4, but now at $z/z_i = 0.19$.

the development of theoretically well-founded methods for the simulation of stratified turbulent reactive flows. The Eulerian equations (with closed pressure correlation and dissipation terms) represent empirical budget equations for the turbulence, and the Lagrangian equations may provide with only a few assumptions a corresponding theory of the micro-processes as e.g. transport of momentum, heat, mass, their turbulent mixing and reactions between compounds. The Eulerian equations provide first of all for the Lagrangian equations parametrizations for the frequencies of all these processes by the applied pressure correlation and dissipation models (Section 2), whereas the Lagrangian equations provide criteria for the realizability of closures. For given parametrizations for the pressure correlations and the dissipation, the essential information to be required for both these methods is the time scale information, which means the calculation of the mean flow frequency for complex flows. This question is complicated by the needed incorporation of stratification effects, and a feasible calculation procedure is needed in order to limit the simulation effort in Lagrangian methods. It is explained in Section 3 how this problem can be solved, when the flow frequency is determined mainly by the local turbulence. This approach provides the dependence of the micro-processes on mean flow properties as shear and stratification, which means the variations of turbulent mixing processes are explained in this way.

The advantages of applying these Lagrangian PDF methods are illustrated here with respect to the simulation of the turbulent mixing between a buoyant plume and the surrounding fluid, as well as the calculation of the turbulence statistics for stratified flow. The buoyant plume rise theory solves two problems, because the mean plume rise as well as the dispersion are calculated simultaneously. The second difference to Eulerian approaches is given by the fact that the dynamics and intensity of turbulent mixing are simulated without ad hoc assumptions on entrainment and extrainment processes. These mixing processes and the two-thirds power law are explained as a consequence of the frequency model (5) and (6). The application of this approach to the parametrization of the third-order moments (see Section 5) solves two problems: Firstly, the contributions of variance gradient terms to these moments are calculated here as a consequence of the stochastic theory and not assumed as in Eulerian methods. Secondly, clipping procedures to ensure the realizability are avoided. Further improvements can be achieved by applying more complex parametrizations for the fourth-order terms (Heinz and Schaller, 1996), but this leads also to an enhanced computational effort. The calculation of one-point vertical velocity PDF for convective turbulence in Section 6 demonstrates in correspondence with the results of Section 5, that the typical features of this PDF can be explained in this way. This approach may provide a theory for the origin of non-Gaussianity and its variations in dependence on the gradients of the mean fields, but more investigations are needed here as discussed above.

What new changes are given for the solution of problems of practical relevance by the development of such stochastic particle models for stratified turbulence? An accurate description of the transport of reactive substances e.g. in the atmospheric boundary layer is essential in order to assess possible risks and to develop control strategies. The mixing processes determine the occurrence of chemical reactions, but their simulation is complicated by the considerable variation with the stratification. Invalid approximations for the description of these mixing processes and also the handling of non-linear reactions may cause errors by several orders of magnitude. In contrast to second-order closure methods, the considered Lagrangian particle models offer the possibility to treat arbitrary chemical reactions exactly and to simulate the turbulent mixing and its variations with shear and stratification, moreover they are still tractable computationally. Their computational requirements are much lower than those of LES, that is still restricted to flows within simplified geometries (at least with current capabilities) and that have the same closure problem for non-linear mean reaction rates as RANS equation methods. On the other hand, also LES may benefit from ongoing and future improvements of PDF methods (Givi, 1997), because the PDF methodology can be adopted for its subgrid-scale modelling as observed by Pope (1990). This approach avoids the closure problem for non-linear mean reaction rates, but it enhances the computational requirements. Further clarifications of the differences in the performances of these approaches (and their computational requirements) for the modelling of turbulent combustion in stratified flow remain as a challenge.

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