Modeling of buoyancy and chemical reactions in a Lagrangian framework

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ABSTRACT

A conceptional approach was developed to describe turbulent diffusion in a high-Reynolds number flow in the Lagrangian framework by stochastic differential equations for particle motion. With respect to practical applications buoyancy effects and chemical reactions have to be considered additionally. It is described here, how this can be handled in the Lagrangian concept, where consistency between the Lagrangian and the Eulerian view is guaranteed for the means and variances of the quantities considered. This is achieved by calculating the coefficients appearing in the Lagrangian equations based on a turbulent timescale, which can be related to gradients of mean wind and temperature.

INTRODUCTION

It has been demonstrated e. g. by van Dop et al. [1], Thomson [2] and Sawford [3], that it is very convenient to describe particle motion in high Reynolds-number flows by stochastic differential equations. Accordingly, diffusion processes can be described in complex flows incorporating the effects of inhomogeneities, instationarities and non-Gaussianity in the turbulent velocity distribution and additionally close to sources. Only recently, the incorporation of buoyancy effects by a linear stochastic differential equation for the potential temperature is discussed by van Dop [4, 5] and a model for simulating chemical reactions in a turbulent flow was proposed e. g. by Pope [6]. However, it is in question in which way equations for fluid particle properties can be derived on a common basis, including the influences of both buoyancy and chemical reactions.

Starting from linear equations for particle position and velocity, potential temperature and stochastic equations for particle composition it was shown by Heinz and Schaller [7], that the coefficients appearing in these equations can be chosen exactly consistent with the transport equations for the corresponding Eulerian means and variances. Here a locally isotropic dissipation corresponding

to Kolmogorov [8] and a pressure redistribution resulting in a return-to isotropy according to Rotta's theory [9] are assumed. These Lagrangian coefficients are determined in terms of a turbulent timescale, which can be related to gradients in the mean velocity and temperature fields. Calculating these fields within the solution algorithm from Pope [6], the equations are given in a selfconsistent form. As a consequence, Lagrangian equations are derived so that consistency between the Lagrangian and Eulerian picture concerning the first two moments is guaranteed exactly. Because of the approximations of Kolmogorov and Rotta the equations for particle motion and potential temperature are linear. It is investigated in Heinz and Schaller [10, 11] in which way non-linearities and non-Gaussianity can be taken into account.

The topic of this paper is to show, how buoyancy effects and chemical reactions can be handled in the Lagrangian framework. In the next section the Lagrangian equations for particle motion, particle potential temperature and composition are represented. Due to the above mentioned approximations parameters appear, which characterize the ratios of timescales for the different processes considered. The estimation of these parameter values is shown in the following section. On this basis the influence of variations in the ratios of the timescales of the different processes can be studied.

LAGRANGIAN MODELS

Within the Lagrangian framework the flow is considered to consist of a certain number of fluid particles, each representing a constant mass (the sum of changing partial masses). The (time dependent) total mass is determined by the single particle mass multiplied by the (time dependent) total number of particles. Hence, equations for particle properties like position, potential temperature and mass fractions of chemical components have to be derived in correspondence with Eulerian budgets.

Thomson [2] gave a theoretical basis for the derivation of a nonlinear stochastic differential equation for particle motion. More recently, van Dop [4, 5] proposed a linear equation for particle potential temperature and discussed some problems in applying stochastic differential equations for scalar transport. Using this approach here, linear coupled stochastic differential equations for particle motion and particle potential temperature are proposed. Consequently, the equations for particle position $x_L(t)$ and velocity $U_L(t)$ at the time t read for the i-th component (i = 1, 2, 3, with summation over repeated subscripts),

$$\frac{d}{dt} x_L{}^i(t) = U_L{}^i(t), \tag{1a}$$

$$\frac{d}{dt} U_L{}^i(t) = \langle a^i \rangle + G^{ij}\left(U_L{}^j - U^j\right) + G^i(\Theta_L - \Theta) + b^{ij}\frac{dW^j}{dt}, \tag{1b}$$

where $<a^i>$, G^{ij}, G^i and b^{ij} are unknown coefficients and the subscript L refers to a Lagrangian quantity. The particle motion is coupled with the particle potential

temperature Θ_I, and U^i as well as Θ denote ensemble averages ($U^j = <U_E^{\;j}>$, $\Theta = <\Theta_E>$) of the corresponding Eulerian quantities (subscript E) depending on $x = x_I(t)$ and t. The first three terms give the systematic particle motion, whereas the last one describes the influence of a stochastic force characterized by the white noise dW^j/dt, which is a Gaussian process having a vanishing mean and uncorrelated values at different times,

$$\left\langle \frac{dW^i}{dt} \right\rangle = 0, \tag{2a}$$

$$\left\langle \frac{dW^i}{dt}(t) \frac{dW^j}{dt}(t') \right\rangle = \delta_{ij}\, \delta(t-t'). \tag{2b}$$

Here, δ_{ij} represents the Kronecker delta and $\delta(t-t')$ the delta function. In addition, the stochastic equation for the potential temperature of the particle reads

$$\frac{d}{dt}\Theta_I(t) = \langle a_\theta \rangle + S_\theta + G_\theta^{\;j}\left(U_I^{\;j} - U^j\right) + G_\theta\left(\Theta_I - \Theta\right) + b_\theta \frac{dW}{dt}, \tag{3}$$

where the coefficients $\langle a_\theta \rangle$, $G_\theta^{\;j}$, G_θ and b_θ have to be determined, S_θ being a source of loss or gain of potential temperature and dW/dt corresponds to one component of dW^i/dt. The fluid volume has a total mass $M(t)$, and the time depending number of particles $N = N(t)$ is calculated by

$$N(t) = \frac{M(t)}{\Delta m}, \tag{4}$$

where Δm is the constant mass associated with each particle.

The changing of composition is desribed by a mixing model proposed by Pope [6], avoiding problems related with the application of a stochastic differential equation for this process. According to that, with probability $1-N\,\Delta t/\tau_m$ in a time interval Δt the compositions of all stochastic particles $n=1$, N do not change, but with probability $N\,\Delta t/\tau_m$, the compositions of a pair of particles changes. Therefore, for two particles (selected at random and denoted by p and q) their values $M_L^{(p)}$ and $M_L^{(q)}$ are replaced by the common mean. This model can be written in the following way:

• with probabiliy $1-N\,\Delta t/\tau_m$,

$$M_L^{(n)}(t+dt) = M_L^{(n)}(t) + \left(\langle a_m \rangle + S_m\right)\Delta t, \quad n = 1, N, \tag{5a}$$

• with probability $N\,\Delta t/\tau_m$,

$$M_L^{(n)}(t+dt) = \frac{1}{2}\left(M_L^{(p)}(t) + M_L^{(q)}(t)\right) + \left(\langle a_m \rangle + S_m\right)\Delta t, \quad n = p, q \tag{5b}$$

$$M_L^{(n)}(t+dt) = M_L^{(n)}(t) + \left(\langle a_m \rangle + S_m\right)\Delta t, \quad n \neq p \text{ and } n \neq q, \tag{5c}$$

τ_m being the mass fraction timescale to be determined and $\mathbf{a}_m$ and $\mathbf{S}_m$ are vectors (with elements a_m^α, S_m^α, $\alpha = 1$, k) which have to be determined or given as source for loss and gain of substance analogous to S_0, respectively.

At fixed positions x the Lagrangian budgets have to be in accordance with Eulerian theory. To investigate these balances a mass density function

$$F(\hat{U}, \hat{M}, \hat{\Theta}, x, t)$$

notifying the probability to find values of the velocity, composition and potential temperature at the position x and to the time t between

$$\hat{U} + d\hat{U}, \hat{M} + d\hat{M}, \hat{\Theta} + d\hat{\Theta}$$

is introduced which is normalized to the mean fluid density $<\rho(x,t)>$,

$$\iiint F(\hat{U}, \hat{M}, \hat{\Theta}, x, t)\, d\hat{U}d\hat{M}d\hat{\Theta} = <\rho>. \tag{6}$$

For F a transport equation can be derived [7], which reads

$$\frac{\partial F}{\partial t} + \frac{\partial}{\partial x^i}\left\{\hat{U}^i F\right\} + \frac{\partial}{\partial \hat{M}_\alpha}\left\{S_\alpha F\right\} + \frac{\partial}{\partial \hat{\Theta}}\left\{S_0 F\right\} =$$

$$-\frac{\partial}{\partial \hat{U}^i}\left\{\left[\langle a^i\rangle + G^{ij}\left(\hat{U}^j - U^j\right) + G^i\left(\hat{\Theta} - \Theta\right)\right]F\right\} -$$

$$-\frac{\partial}{\partial \hat{\Theta}}\left\{\left[\langle a_\theta\rangle + G_\theta^i\left(\hat{U}^i - U^i\right) + G_0\left(\hat{\Theta} - \Theta\right)\right]F\right\} +$$

$$+\frac{\partial^2}{\partial \hat{U}^i \partial \hat{U}^j}\left\{B^{ij}F\right\} + \frac{1}{2}\frac{\partial^2}{\partial \hat{\Theta}^2}\left\{b_\theta^2 F\right\} - \frac{\partial}{\partial \hat{M}_\alpha}\left\{\langle a_\alpha\rangle F\right\} +$$

$$+2\tau_m^{-1}\left\{2^k \int d\hat{M}'\,\rho(\hat{M})\cdot\frac{F(\hat{M} + \hat{M}')}{\rho(\hat{M} + \hat{M}')}\cdot\frac{F(\hat{M} - \hat{M}')}{\rho(\hat{M} - \hat{M}')} - F\right\}, \tag{7}$$

where

$$B^{ij} = \frac{1}{2}b^{ik}b^{kj}. \tag{8}$$

Hence, a closed equation is obtained for the mass density function F. Solving it, all Eulerian moments and correlations of the quantities considered can be calculated by integration, for instance

$$U^i(x,t) = \rho^{-1}\iiint d\hat{U}d\hat{M}d\hat{\Theta}\ \hat{U}^i F(\hat{U}, \hat{M}, \hat{\Theta}, x, t),$$

or the elements V^{ij} of the variance matrix V,

$$V^{ij}(x,t) = \langle (U_E{}^i - U^i)(U_E{}^j - U^j) \rangle =$$

$$= \rho^{-1} \iiint d\hat{U} d\hat{M} d\hat{\Theta} \, (\hat{U}^i - U^i)(\hat{U}^j - U^j) F(\hat{U}, \hat{M}, \hat{\Theta}, x, t).$$

On the other hand, budget equations for the the first and second moments of the quantities considered can be calculated by multiplying (7) with the corresponding variables and integrating over the whole variable space.

CALCULATION OF LAGRANGIAN COEFFICIENTS

The coefficients appearing in the Lagrangian equations (1b), (3) and (5a-c) can be obtained by comparison of the transport equations for the means and variances calculated as described above from (7) with the corresponding averaged hydrodynamic equations, where the approximations of Kolmogorov [8] of locally isotropic dissipation and a pressure redistribution according to Rotta [9] are assumed. This leads to (without summation over α in (9b))

$$\langle a^i \rangle = \nu \Delta_x U^i - \rho^{-1} \frac{\partial \langle p \rangle}{\partial x^i} - g \delta_{i3}, \tag{9a}$$

$$\langle a_m{}^\alpha \rangle = -A_\alpha \Delta_x M_\alpha, \tag{9b}$$

$$\langle a_\theta \rangle = -A_\theta \Delta_x \Theta, \tag{9c}$$

for the coefficients $\langle a^i \rangle$, $\langle a_m{}^\alpha \rangle$, $\langle a_\theta \rangle$. Here, the Eulerian mean value $M_\alpha = \langle M_{E,\alpha} \rangle$ is introduced, $\langle p \rangle$ is the averaged pressure, g the acceleration due to gravity, ν being the kinematic viscosity and A_α, A_θ are molecular transport coefficients. From the equations for the second moments it follows that

$$G^{ij} = -\frac{q^2}{4\tau}\left(\frac{2}{3} + C_0\right) V^{-1 ij} - k_1 \frac{1}{4\tau}\left(V^{ik} - \frac{q^2}{3}\delta_{ik} \right) V^{-1 kj} +$$

$$+ k_2 \frac{q^2}{2}\left(\frac{\partial U^i}{\partial x^k} + \frac{\partial U^k}{\partial x^i} \right) V^{-1 kj}, \tag{10a}$$

$$G^i = \beta g \delta_{i3}, \tag{10b}$$

$$G_\theta = -\frac{2k_4 + C_1}{4\tau}, \tag{10c}$$

$$G_\theta{}^i = 0, \tag{10d}$$

with

$$C_0 = \frac{k_1 - 2}{3},$$ (11a)

$$C_1 = 2(k_3 - k_4) - k_1.$$ (11b)

Here, constant parameters k_1, k_2, k_3, k_4 appear caused by the approximations of Kolmogorov and Rotta. Providing that the transport of scalar correlations depends only on the turbulent properties of the medium leads to

$$\tau_m^{-1} = \frac{k_4^*}{\tau},$$ (12)

where the introduced k_4^* is equal to k_4 if $A_\theta = A_\alpha$, i. e. the coefficients for the transport of potential temperature and substance α must be equal.

Consequently, all coefficients are determined completely, using the introduced turbulent timescale τ. The latter can be calculated using second-order modelling, where the triple correlations in the second order moment equations are neglected and the flow is assumed to be in a steady state. In Heinz and Schaller [11] it is shown, that these assumptions are equivalent to a coarser rescaling of the equations considered. For simplicity, a vertical sheared horizontal wind is prescribed, so that

$$T^2 = \frac{1}{2A}\left(-B - \sqrt{B^2 - 4AC}\right)$$ (13)

follows for

$$T = \tau \sqrt{\left(\frac{\partial U^1}{\partial x^3}\right)^2 + \left(\frac{\partial U^2}{\partial x^3}\right)^2}.$$ (14)

Here,

$$A = \frac{16}{3}(4k_4 + 3k_1 + k_1 k_4)Ri(Ri - Ri_c),$$

$$B = \frac{4}{3}k_1 k_3\left[(7k_4 + 3k_1 + k_1 k_4)Ri - k_3 k_4 \frac{k_1 - 2}{k_1}\right],$$

$$C = k_1^2 k_3^2 k_4,$$

and Ri is the gradient Richardson number defined by

$$Ri = \frac{\beta g \frac{\partial \Theta}{\partial x^3}}{\left(\frac{\partial U^1}{\partial x^3}\right)^2 + \left(\frac{\partial U^2}{\partial x^3}\right)^2}.$$

Furthermore, the critical Richardson number Ri_c is given by

$$Ri_c = \frac{(k_1 - 2)(k_3 - k_4)}{4k_4 + 3k_1 + k_1 k_4},$$

limiting the applicability of (13) to $Ri \leq Ri_c$.

ESTIMATION OF PARAMETERS

The estimation of the constants k_1 - k_4 is considered in detail by Wichmann and Schaller [12]. The values of Mellor and Yamada [13] for k_1, k_2, k_3, k_4,

$$k_1 = 6.0,$$

$$k_2 = 0.08,$$

$$k_3 = 7.5,$$

$$k_4 = 1.66,$$

seem to represent the most general constants [12]. One obtains the universal constants C_0, C_1 of Kolmogorov theory as

$$C_0 = 1.3,$$

$$C_1 = 5.7.$$

Comparisons with values obtained by other authors can be found in Heinz and Schaller [7,10]. In particular, for the ratios of timescales of transport of potential temperature to that of kinetic energy $\tau_\theta / \tau = - G_\theta^{-1} / \tau$ follows

$$\frac{\tau_\theta}{\tau} = \frac{4}{2k_3 - k_1} = 0.44,$$

whereas (13) with $A_\theta = A_\alpha$ leads to

$$\frac{\tau_m}{\tau} = \frac{1}{k_4} = 0.60.$$

CONCLUSIONS

Starting from linear coupled stochastic differential equations for particle motion and potential temperature as well as a stochastic mixing model for changes of compositions it is shown that the coefficients appearing in the Lagrangian equations can be chosen in accordance with the Eulerian transport equations up to the second order. Here, a timescale τ appears wich can be related with gradients of the wind- and potential temperature fields. Values for the remaining unknown parameters k_1, k_2, k_3, k_4, are given above. This consistent approach to

incorporate buoyancy effects and chemical reactions into Lagrangian modelling of turbulent diffusion provides a suitable basis to study the influence of ratios of the timescales for turbulent transport, transport of potential temperature and substances.

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