Stochastic Lagrangian Models for Turbulent Dispersion in Atmospheric Boundary Layer

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Abstract — A one-particle 3D stochastic Lagrangian model in for transport of particles in horizontally-homogeneous atmospheric surface laeyr with arbitrary one-point probability density function of Eulerian velocity fluctuations is suggested. A uniquely defined Lagrangian stochastic model in the class of well-mixed models is constructed from physically plausible assumptions: (i) in the neutrally stratified horizontally homogeneous surface layer, the vertical motion is mainly controlled by eddies whose size is of order of the current height; and (ii), the streamwise drift term is independent of the crosswind velocity. Numerical simulations for neutral stratification have shown a good agreement of our model with the well known Thomson's model, with Flesch & Wilson's model, and with experimental measurements as well. However there is a discrepancy of these results with the results obtained by Reynolds' model.

Keywords: Horizontally homogeneous turbulence, Lagrangian stochastic models, well-mixed condition, consistency principle, uniqueness problem, neutrally stratified surface layer.

1 Introduction

This paper deals with one-particle stochastic Lagrangian models (LS) for 2D and 3D turbulent transport. Here we treat the flow in the Atmospheric Boundary Layer (ABL) as a fully developed turbulence (i.e., a flow with very high Reynolds number) and consider it as a random velocity field (u, v, w) which is assumed to be incompressible. Therefore, the trajectories of particles in such flows are stochastic processes. To simulate these stochastic processes, two different approaches are known in the literature. The first one is based on the numerical solution of the system of random equations

$$\frac{\partial X}{\partial t} = u(X, Y, Z, t), \quad \frac{\partial Y}{\partial t} = v(X, Y, Z, t), \quad \frac{\partial Z}{\partial t} = w(X, Y, Z, t). \tag{1.1}$$

Here $X(t), Y(t), Z(t)$ are the coordinates of the Lagrangian trajectory at the time t. The random fields u, v, w are simulated by Monte Carlo methods (e.g., see Drummond et.al., 1984; Fung et.al., 1992; Kraichnan, 1970; Sabelfeld, 1991; Sabelfeld and Kurbanmuradov, 1990; Turfus and Hunt, 1987), and the random trajectories are then obtained by numerical solution of (1.1) with the relevant initial data.

In the second approach the true trajectory $X(t), Y(t), Z(t)$ is assumed to be approximated by a model trajectory $\hat{X}(t), \hat{Y}(t), \hat{Z}(t)$, a solution to a stochastic differential equation of Ito type (e.g., see Sawford, 1985; Thomson, 1987; Wilson and Sawford, 1996, and the list of references in these papers):

$$\begin{aligned} d\hat{X} &= \hat{U} dt, \quad d\hat{Y} = \hat{V} dt, \quad d\hat{Z} = \hat{W} dt, \\ d\hat{U} &= a_u\, dt + b_u\, dB_u(t), \quad d\hat{V} = a_v\, dt + b_v\, dB_v(t), \\ d\hat{W} &= a_w\, dt + b_w\, dB_w(t). \end{aligned} \tag{1.2}$$

Here we denote by $\hat{U}, \hat{V}, \hat{W}$ the components of the model Lagrangian velocity, $B_u(t), B_v(t)$ and $B_w(t)$ are three standard independent Wiener processes; a_u, a_v, a_w and b_u, b_v, b_w are generally functions of $(t, \hat{X}, \hat{Y}, \hat{Z}, \hat{U}, \hat{V}, \hat{W})$.

Ideally, one would have an approximation such that the true and the model Lagrangian velocities coincide:

$$\begin{aligned} \hat{U}(t) &= u(\hat{X}(t), \hat{Y}(t), \hat{Z}(t), t), \\ \hat{V}(t) &= v(\hat{X}(t), \hat{Y}(t), \hat{Z}(t), t), \quad \hat{W}(t) = w(\hat{X}(t), \hat{Y}(t), \hat{Z}(t), t) \end{aligned} \tag{1.3}$$

which would assure that the true and model trajectories are the same. However it is unrealistic to satisfy (1.3), therefore one uses different consistency principles. Namely, the general *consistency principle* says that the statistics of the model process $\hat{X}(t), \hat{Y}(t), \hat{Z}(t)$, $\hat{U}(t), \hat{V}(t), \hat{W}(t)$ satisfies the same relations satisfied by the true process $X(t)$, $Y(t)$, $Z(t)$, $U(t), V(t), W(t)$, where

$$\begin{aligned} U(t) &= u(X(t), Y(t), Z(t), t), \quad V(t) = v(X(t), Y(t), Z(t), t), \\ W(t) &= w(X(t), Y(t), Z(t), t) \end{aligned}$$

are the components of the true Lagrangian velocity.

Two consistency principles used in the literature are:

(A) Consistency with the Kolmogorov similarity theory,

(B) Consistency with Thomson's well-mixed condition.

Here (A) reads

$$\langle (dU)^2 \rangle = \langle (dV)^2 \rangle = \langle (dW)^2 \rangle = C_0 \varepsilon dt,$$

and

$$\langle dU\, dV \rangle = \langle dU\, dW \rangle = \langle dW\, dV \rangle = 0,$$

where dU, dV, dW are the components of the increments of the Lagrangian velocity, ε is the mean rate of the dissipation of turbulence energy, C_0 is the universal constant (e.g., Monin and Yaglom, 1975; Sawford, 1985; Thomson, 1987); here and in what follows, the angle brackets stand for the ensemble average.

Note that (A) implies (e.g., see Thomson, 1987) that in (1.2), all the terms b_u, b_v, b_w are equal to $\sqrt{C_0\varepsilon}$:

$$b_u = b_v = b_w = \sqrt{C_0 \varepsilon}. \qquad (1.4)$$

Thomson's well-mixed condition can be rigorously derived from Novikov's integral relation (Novikov, 1969)

$$p_E(u, v, w; x, y, z, t) = \int_{R^3} p_L(x, y, z, u, v, w; x_0, y_0, z_0, t) dx_0 dy_0 dz_0. \qquad (1.5)$$

Here p_E is the probability density function (pdf) of the Eulerian velocity u, v, w, in the fixed point x, y, z, at the time t, and p_L is the joint pdf of the true Lagrangian phase point X, Y, Z, U, V, W defined by the trajectory started at x_0, y_0, z_0.

It is natural to require that the pdf of the model phase point governed by (1.2), say $\hat{p}_L$, satisfies

$$p_E(u, v, w; x, y, z, t) = \int_{R^3} \hat{p}_L(x, y, z, u, v, w; x_0, y_0, z_0, t) dx_0 dy_0 dz_0. \qquad (1.6)$$

Note that (1.6), the Focker-Planck-Kolmogorov equation for $\hat{p}_L$ and (1.4) lead to the well-mixed condition due to Thomson (1987):

$$\begin{aligned} &\frac{\partial p_E}{\partial t} + u\frac{\partial p_E}{\partial x} + v\frac{\partial p_E}{\partial y} + w\frac{\partial p_E}{\partial z} + \frac{\partial}{\partial u}(a_u p_E) + \frac{\partial}{\partial v}(a_v p_E) + \frac{\partial}{\partial w}(a_w p_E) \\ &\quad = \frac{C_0 \varepsilon}{2} \left\{ \frac{\partial^2 p_E}{\partial u^2} + \frac{\partial^2 p_E}{\partial v^2} + \frac{\partial^2 p_E}{\partial w^2} \right\}. \end{aligned} \qquad (1.7)$$

It is convenient to rewrite this equation in the form given by Thomson (1987):

$$\frac{\partial p_E}{\partial t} + u\frac{\partial p_E}{\partial x} + v\frac{\partial p_E}{\partial y} + w\frac{\partial p_E}{\partial z} + \frac{\partial}{\partial u}(\phi_u) + \frac{\partial}{\partial v}(\phi_v) + \frac{\partial}{\partial w}(\phi_w) = 0, \tag{1.8}$$

where

$$\phi_u = a_u p_E - \frac{C_0\varepsilon}{2}\frac{\partial p_E}{\partial u},\ \phi_v = a_v p_E - \frac{C_0\varepsilon}{2}\frac{\partial p_E}{\partial v},\ \phi_w = a_w p_E - \frac{C_0\varepsilon}{2}\frac{\partial p_E}{\partial w}.$$

The vector function $\phi = (\phi_u, \phi_v, \phi_w)$ is not uniquely defined from (1.8). Indeed, a series of solutions can be obtained by adding to ϕ an arbitrary vector-function whose divergence in velocity space is zero.

It should be noted that in one-dimensional case, the well-mixed condition uniquely defines the LS model even for non-Gaussian p_E (Thomson, 1987). In multi-dimensional case, the *uniqueness problem* can be formulated as follows: give physically plausible assumptions which define uniquely the function ϕ in (1.8).

The first 3D LS model satisfying (1.8) was suggested by Thomson (1987). The pdf p_E in his model has a Gaussian form, and the drift terms a_u, a_v, a_w have a quadratic dependence on the velocity. Another example of a model (suggested by Borgas; see, e.g., Wilson and Flesch, 1997) with quadratic drift term and Gaussian p_E was studied in Sawford and Guest (1988). They have found that the Borgas model gives slightly different results compared to Thomson's model. Reynolds (1997) has constructed a two-parametric class of well-mixed models, also quadratic and with Gaussian p_E, which includes Thomson's and Borgas' models. He demonstrated that two different models from his class produce essentially different predictions of the turbulent dispersion.

Non-Gaussian form of p_E in 2D case was treated by Flesch and Wilson (1992). To extract a unique model in the class of well-mixed models, they suggested the following assumption: the term $(\phi_u/p_E, \phi_w/p_E)$ accelerates particles directly towards (or away from) the origin of (u, w) space. A 3D generalization of this model is given by Monti and Leuzzi (1996). Further generalization of the approach of Flesch and Wilson (1992) was given in Wilson and Flesch (1997): the vector $(\phi_u/p_E, \phi_w/p_E)$ is chosen so that there is no preferred direction of rotation of the velocity fluctuation vector ("zero-spin" models). However as shown by Reynolds (1998), this approach does not solve the uniqueness problem.

It should be emphasized that all the above mentioned LS models deal with quite general inhomogeneous turbulents flows. It is therefore difficult to formulate physically motivated assumptions which, together with the well-mixed condition uniquely define the LS model. Therefere it is reasonable to consider special classes of turbulent flows (e.g., horizontally homogeneous) whose specific features can be used to construct uniquely the LS models under assumptions with credible physical basis.

In the present paper we treat a 3D horizontally homogeneous surface layer with a general form of p_E, and formulate a physically plausible assumption about the structure of the drift terms a_u, a_v, a_w. This assumption uniquelly defines our model in the class of well-mixed models. The model proposed is essentially different from all the models cited above, in particular, for Gaussian p_E, our model, being in this case also quadratic in velocities, is generally not in the class of models given by Reynolds (1997); we mention only the case of ideally neutral stratification (i.e., the Obukhov-Monin length scale is infinite: $L = \infty$): in this case our model belongs to Reynolds' class if the parameter C_1 is chosen as $C_1 = C_0 u_*^4/2\sigma_w^4$, and $C_2 = 0$ (see Appendix B).

In Section 2 we formulate the Assumption which ensures the unique definition of our model for the horizontally homogeneous neutrally stratified surface layer. Comparison with other stochastic Lagrangian models and experimental measurements is given in Section 3. Convective case is treated in Section 4. The behaviour of trajectories of our model near the boundary is analysed in Section 5. In Appendix A the drift terms are derived in the Gaussian case. In Appendix B we analyse how our model relates to Reynolds' and "zero-spin" classes of models.

2 Neutrally stratified boundary layer

2.1 General case of Eulerian pdf

We consider a horizontally homogeneous incompressible ABL in the half-space $R^3_+ = \{(x, y, z) : z \geq 0\}$, where x, y are the horizontal coordinates, and z is the vertical coordinate. Thus it is assumed that the mean velocity has no vertical component. It is supposed in this section that the mean velocity vector is not changing his direction with height, it is directed along the X-axis, and the crosswind velocity fluctuations are symmetric with respect to the plane XZ. Thus the mean velocity vector is $(\bar{u}(z, t), 0, 0)$, while p_E does not depend on x, y.

We will write the pdf p_E in the form

$$p_E(u, v, w; z, t) = p'_E(u', v', w'; z, t)$$

where $u' = u - \bar{u}(z, t)$, $v' = v$ and $w' = w$.

By (1.4), the equation (1.2) in these variables has the form:

$$\begin{aligned} dX &= (U' + \bar{u}(Z, t))dt,\ dY = V'dt,\ dZ = W'dt, \\ dU' &= a'_u(t, Z, U', V', W')dt + \sqrt{C_0\varepsilon}\, dB_u(t), \\ dV' &= a'_v(t, Z, U', V', W')dt + \sqrt{C_0\varepsilon}\, dB_v(t), \\ dW' &= a'_w(t, Z, U', V', W')dt + \sqrt{C_0\varepsilon}\, dB_w(t). \end{aligned} \tag{2.1}$$

To simplify the notation, here and in what follows we omit the hat sign introduced in Section 1 to denote the model trajectory.

The well-mixed condition in new variables is

$$\begin{aligned} &\frac{\partial p'_E}{\partial t} + w'\frac{\partial p'_E}{\partial z} + \frac{\partial}{\partial u'}(a'_u p'_E) + \frac{\partial}{\partial v'}(a'_v p'_E) + \frac{\partial}{\partial w'}(a'_w p'_E) \\ &\quad = \frac{C_0\varepsilon}{2}\left\{\frac{\partial^2 p'_E}{\partial (u')^2} + \frac{\partial^2 p'_E}{\partial (v')^2} + \frac{\partial^2 p'_E}{\partial (w')^2}\right\}. \end{aligned} \tag{2.2}$$

Now we give our main assumption about the structure of the Lagrangian model (2.1).

Assumption. *We assume in addition to the well-mixed condition that:*
(i) the vertical drift term does not depend on the horizontal velocity components: $a'_w = a'_w(t, z, w')$;
(ii) the streamwise term a'_u *does not depend on the crosswind velocity* v': $a'_u = a'_u(t, z, u', w')$.

This assumption meets the conditions of a surface layer with neutral (or close to) stratification. Indeed, all the contributions to the vertical motions can be divided into two parts: the first comes from the vortices whose sizes are smaller or close to the current height z, and the second is due to the large horizonatally streched vortices. The second part of the contribution is much smaller than the first one since the vertical velocities in such horizontal streched vortices are much smaller than that of the small vortices whose sizes are of the order of the current height. The first part comes mainly from isotropic vortices of the inertial subrange. But in the isotropic case, the well-mixed condition leads to the dependence $a'_w = a'_w(t,z,w')$ (e.g., see Wilson and Sawford, 1996) which gives us the motivation of the point (i) in our assumption. As to the point (ii), we note that the coordinate system is chosen so that $\langle u'v'\rangle = 0$, $\langle v'w'\rangle = 0$, but $\langle u'w'\rangle \neq 0$, which suggests the approximation $a'_u = a'_u(t,z,u',w')$.

The approximation formulated in the point (ii) is reasonable if the mean velocity is dominating over the fluctuated part. Otherwise, for instance in convective case, this approximation fails, and the velocity components u' and v' must enter the drift terms symmetrically. In Section 3 we will treat this case separately.

Note that the dependence $a'_u = a'_u(t,z,u',w')$ holds also both for Thomson's and Reynolds' model, see Appendix B.

Thus the model (2.1), in view of the Assumption reads

$$\begin{aligned} dX &= (U' + \bar{u}(Z,t))dt,\ dY = V'dt,\ dZ = W'dt, \\ dU' &= a'_u(t,Z,U',W')dt + \sqrt{C_0\varepsilon}\, dB_u(t), \\ dV' &= a'_v(t,Z,U',V',W')dt + \sqrt{C_0\varepsilon}\, dB_v(t), \\ dW' &= a'_w(t,Z,W')dt + \sqrt{C_0\varepsilon}\, dB_w(t). \end{aligned} \tag{2.3}$$

Integrating (2.2) over u' and v' yields

$$\frac{\partial p'_{1E}}{\partial t} + w'\frac{\partial p'_{1E}}{\partial z} + \frac{\partial}{\partial w'}(a'_w(t,z,w')p'_{1E}) = \frac{C_0\varepsilon}{2}\frac{\partial^2 p'_{1E}}{\partial (w')^2}\,, \tag{2.4}$$

where

$$p'_{1E} = p'_{1E}(w';z,t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} p'_E(u',v',w';z,t)\,du'dv'. \tag{2.5}$$

Here we have assumed that

$$a'_u p'_E,\ a'_v p'_E,\ \frac{\partial p'_E}{\partial u'},\ \frac{\partial p'_E}{\partial v'} \quad \text{all tend to zero as} \quad (u')^2 + (v')^2 \to \infty.$$

Similarly, the integration of (2.2) over v' leads to

$$\begin{aligned} &\frac{\partial p'_{2E}}{\partial t} + w'\frac{\partial p'_{2E}}{\partial z} + \frac{\partial}{\partial u'}(a'_u(t,z,u',w')p'_{2E}) + \frac{\partial}{\partial w'}(a'_w(t,z,w')p'_{2E}) \\ &\quad = \frac{C_0\varepsilon}{2}\left(\frac{\partial^2 p'_{2E}}{\partial (u')^2} + \frac{\partial^2 p'_{2E}}{\partial (w')^2}\right), \end{aligned} \tag{2.6}$$

where

$$p'_{2E} = p'_{2E}(u', w'; z, t) = \int_{-\infty}^{\infty} p'_E(u', v', w'; z, t)\, dv'. \tag{2.7}$$

Now, under the assumption about the behaviour in the infinity, it is possible to define uniquely the coefficients a'_u, a'_v and a'_w. Indeed, from (2.4) one gets a'_w, then from (2.6) one finds a'_u, and from (2.2) one obtains a'_v. This yields

$$a'_w(t, z, w) = \frac{1}{p'_{1E}(w; z, t)} \left\{ \frac{C_0\varepsilon}{2} \frac{\partial p'_{1E}}{\partial w} - \left(\frac{\partial f_{1E}}{\partial t} + \frac{\partial F_{1E}}{\partial z} \right) \right\}, \tag{2.8}$$

where

$$f_{1E}(w; z, t) = \int_{-\infty}^{w} p'_{1E}(w'; z, t)\, dw',$$

$$F_{1E}(w; z, t) = \int_{-\infty}^{w} w' p'_{1E}(w'; z, t)\, dw',$$

and

$$a'_u(t, z, u, w)$$

$$= \frac{1}{p'_{2E}} \left\{ \frac{C_0\varepsilon}{2} \left(\frac{\partial p'_{2E}}{\partial u} + \frac{\partial^2 f_{2E}}{\partial w^2} \right) - \left(\frac{\partial f_{2E}}{\partial t} + w \frac{\partial f_{2E}}{\partial z} \right) - \frac{\partial}{\partial w} \left(a'_w f_{2E} \right) \right\}, \tag{2.9}$$

where

$$f_{2E}(u, w; z, t) = \int_{-\infty}^{u} p'_{2E}(u', w; z, t)\, du'.$$

Finally,

$$a'_v(t, z, u, w) = \frac{1}{p'_E} \left\{ \frac{C_0\varepsilon}{2} \left(\frac{\partial^2 f_E}{\partial u^2} + \frac{\partial p'_E}{\partial v} + \frac{\partial^2 f_E}{\partial w^2} \right) - \left(\frac{\partial f_E}{\partial t} + w \frac{\partial f_E}{\partial z} \right) \right.$$

$$\left. - \frac{\partial}{\partial u} (a'_u f_E) - \frac{\partial}{\partial w} \left(a'_w f_E \right) \right\}, \tag{2.10}$$

where

$$f_E(u, v, w; z, t) = \int_{-\infty}^{v} p'_E(u, v', w; z, t)\, dv'.$$

Thus the coefficients (2.8)-(2.10) define a unique stochastic model (2.3) through p'_E.

In the case when the crosswind velocity fluctuations are independent of the streamwise and vertical fluctuations, i.e., if

$$p'_E(u, v, w; z, t) = p'_{2E}(u, w; z, t) p_{vE}(v; z, t) \tag{2.11}$$

then the expression (2.10) for the crosswind drift term can be simplified:

$$a'_v(t, z, u, v, w) = \frac{C_0\varepsilon}{2p_{vE}} \frac{\partial p_{vE}}{\partial v} - \frac{1}{p_{vE}} \frac{\partial f_{vE}}{\partial t} - \frac{w}{p_{vE}} \frac{\partial f_{vE}}{\partial z}, \tag{2.12}$$

where

$$f_{vE}(v) = \int_{-\infty}^{v} p_{vE}(v')\, dv'.$$

2.2 Gaussian pdf

We present here expressions for the coefficients to (2.3) for Gaussian pdf p_E. Recall that we deal here with horizontally homogeneous turbulence, and use a coordinate system where the direction of the mean velocity coincides with the X-axes, and the crosswind velocity fluctuations are symmetric relative to the plane XZ. Therefore, the Gaussian pdf p_E has the form

$$
\begin{aligned}
p'_E(u,v,w;z,t) \;=\; & \frac{1}{2\pi\sigma_{u/w}\sigma_w}\exp\left\{-\frac{1}{2\sigma^2_{u/w}}(u-\rho w)^2-\frac{w^2}{2\sigma^2_w}\right\} \\
& \times\;\frac{1}{\sqrt{2\pi}\sigma_v}\exp\left\{-\frac{v^2}{2\sigma^2_v}\right\},
\end{aligned}
\tag{2.13}
$$

where

$$
\sigma_{u/w}=\frac{\Delta^{1/2}}{\sigma_w},\qquad \rho=\frac{\overline{uw}}{\sigma^2_w},\qquad \Delta=\sigma^2_u\sigma^2_w-(\overline{uw})^2,
$$

and σ^2_u, σ^2_v, σ^2_w are the variances of the x-, y- and z- velocity components, respectively.

Using the result given in Section 2.1 we obtain (see Appendix A) the following expressions:

$$
a'_w(t,z,w)=-\left(\frac{C_0\varepsilon}{2\sigma^2_w}-\frac{1}{\sigma_w}\frac{\partial\sigma_w}{\partial t}\right)w+\frac{1}{2}\frac{\partial\sigma^2_w}{\partial z}\left(\frac{w^2}{\sigma^2_w}+1\right), \tag{2.14}
$$

$$
\begin{aligned}
a'_u(t,z,u,w) = & -\frac{C_0\varepsilon(1+\rho^2)}{2\sigma^2_{u/w}}(u-\rho w)+\frac{\rho}{2\sigma^2_w}\left(C_0\varepsilon+\frac{\partial\sigma^2_w}{\partial t}\right)w \\
& +\frac{\rho}{2}\frac{\partial\sigma^2_w}{\partial z}\left(\frac{w^2}{\sigma^2_w}+1\right)-\left(\frac{\partial\rho}{\partial t}+w\frac{\partial\rho}{\partial z}\right)w-\frac{1}{\sigma_{u/w}}\left(\frac{\partial\sigma_{u/w}}{\partial t}+w\frac{\partial\sigma_{u/w}}{\partial z}\right)(u-\rho w)\ ,
\end{aligned}
\tag{2.15}
$$

and

$$
a'_v(t,z,u,v,w)=-\left(\frac{C_0\varepsilon}{2\sigma^2_v}-\frac{1}{\sigma_v}\frac{\partial\sigma_v}{\partial t}\right)v+\frac{1}{2}\frac{\partial\sigma^2_v}{\partial z}\frac{vw}{\sigma^2_v}\ . \tag{2.16}
$$

Note that in the stationary case these expressions can be simplified to

$$
\begin{aligned}
a'_u(t,z,u,w) = & -\frac{C_0\varepsilon(1+\rho^2)}{2\sigma^2_{u/w}}(u-\rho w)+\frac{\rho\,C_0\varepsilon}{2\sigma^2_w}w+\frac{\rho}{2}\frac{\partial\sigma^2_w}{\partial z}\left(\frac{w^2}{\sigma^2_w}+1\right) \\
& -\frac{\partial\rho}{\partial z}w^2-\frac{1}{\sigma_{u/w}}\frac{\partial\sigma_{u/w}}{\partial z}(u-\rho w)w\ ,
\end{aligned}
\tag{2.17}
$$

$$
a'_v(t,z,u,v,w)=-\frac{C_0\varepsilon}{2\sigma^2_v}v+\frac{1}{2}\frac{\partial\sigma^2_v}{\partial z}\frac{vw}{\sigma^2_v}\ , \tag{2.18}
$$

$$
a'_w(t,z,w)=-\frac{C_0\varepsilon}{2\sigma^2_w}w+\frac{1}{2}\frac{\partial\sigma^2_w}{\partial z}\left(\frac{w^2}{\sigma^2_w}+1\right). \tag{2.19}
$$

3 Comparison with other models and measurements

3.1 Comparison with measurements in ideally-neutral surface layer (INSL)

In this section we analyse some quantities in the case of turbulent dispersion in a stationary, horizontally homogeneous, ideally-neutral surface layer (i.e., the Obukhov-Monin length L equals to infinity).

We have calculated the following dimensionless Lagrangian characteristics:

$$A(t) = \frac{\sqrt{\langle Z^2(t)\rangle}}{u_* t}, \; B(t) = \frac{\langle Z(t)\rangle}{u_* t}, \; C(t) = \frac{z_0}{u_* t} \exp\left\{\frac{\kappa\langle X(t)\rangle}{u_* t} + 1\right\}, \tag{3.1}$$

and the ratio $pr(z) = k_\mu(z)/k_z(z)$, where κ is the von Karman constant, $k_\mu = \kappa u_* z$ is the molecular diffusivity, and k_z is the vertical eddy diffusivity coefficient defined through the Boussinesque hypothesis:

$$\overline{c'w'}(z) = -k_z(z)\frac{\partial \bar{c}(z)}{\partial z}. \tag{3.2}$$

Importance of the characteristics $A(t), B(t)$ and $C(t)$ is that these functions tend, as $t \to \infty$, to some universal constant values a, b and c, respectively, provided h_s and z_0 are much less than $u_* t$ (e.g., see Bysova et al., 1991, p.77). Here h_s is the height at which the Lagrangian trajectory starts. As to the ratio $pr(z)$, for values z much larger than the source height, it tends to the Prandtl constant Pr; its universal character is well known and is in the literature often approximately taken equal to unity (e.g., see Monin and Yaglom, 1971, Section 8.2).

Since all the four quantities $A(t), B(t), C(t)$, and $pr(z)$ do not depend on the crosswind dispersion, we use the 2D stochastic models to simulate the dispersion:

$$\begin{aligned} dX &= (U' + \bar{u}(Z,t))dt, \; dZ = W'dt, \\ dU' &= a'_u(Z, U', W')dt + \sqrt{C_0\varepsilon}\, dB_u(t), \\ dW' &= a'_w(Z, U', W')dt + \sqrt{C_0\varepsilon}\, dB_w(t), \end{aligned} \tag{3.3}$$

where for the ISNL, the vertical profiles of ε and $\bar{u}$ can be taken as follows (e.g., see Monin and Yaglom, 1971)

$$\varepsilon(z) = \frac{u_*^3}{\kappa z}, \quad \bar{u}(z) = \frac{u_*}{\kappa}\ln\left(z/z_0\right),$$

and z_0 is the roughness height. The calculations were carried out by Thomson's, Reynolds', Flesch and Wilson's, and ours models. Thomson's 2D model in this case is specified by

$$a'_u(z,u,w) = -\frac{C_0\varepsilon(z)}{2\Delta}\left(\sigma_w^2 u + u_*^2 w\right), \quad a'_w(z,u,w) = -\frac{C_0\varepsilon(z)}{2\Delta}\left(\sigma_u^2 w + u_*^2 u\right),$$

where σ_u and σ_w are given by $\sigma_u = b_u u_*$, $\sigma_w = b_w u_*$ with $u_*^2 = -\overline{uw} = const$; $\Delta = \sigma_u^2\sigma_w^2 - \overline{uw}^2$, b_u and b_w are universal constants. Following Panofsky and Dutton (1984), and Stull (1988) we have taken $b_u = 2.5$, $b_w = 1.25$. These parameters enter all the models specified below.

The drift terms of the model due to Flesch and Wilson (1992) can be written in the case of INSL as follows

$$a'_u(z,u,w) = -\frac{C_0\varepsilon(z)}{2}\frac{\partial \ln p'_E}{\partial u} = -\frac{C_0\varepsilon(z)}{2\sigma^2_{u/w}}(u-\rho w),$$

$$a'_w(z,u,w) = -\frac{C_0\varepsilon(z)}{2}\frac{\partial \ln p'_E}{\partial w} = \frac{C_0\varepsilon(z)\rho}{2\sigma^2_{u/w}}(u-\rho w) - \frac{C_0\varepsilon(z)}{2\sigma^2_w}\,w,$$

where $\sigma_{u/w} = \sqrt{\Delta}/\sigma_w$, $\rho = \overline{uw}/\sigma^2_w$.

The model of Reynolds (1998) in our case of ideally-neutral surface layer is specified by

$$a'_u(z,u,w) = -\left(\frac{C_0\varepsilon}{2} + C_1 u_*^2\frac{d\bar{u}}{dz}\right)\frac{\sigma^2_w u + u^2_* w}{\Delta}\ ,$$

$$a'_w(z,u,w) = -\frac{C_0\varepsilon(z)}{2\Delta}\left(\sigma^2_u w + u^2_* u\right) + C_1\sigma^2_w\frac{d\bar{u}}{dz}\frac{\sigma^2_w u + u^2_* w}{\Delta}\ , \tag{3.4}$$

with $C_1 = 3$ chosen by Reynolds (1998) to fit the experimental results of Legg (1983).

Our model (2.14)-(2.15) (in what follows we call it a KS model) in the case of INSL is specified by

$$a'_u(z,u,w) = -\frac{C_0\varepsilon(z)(1+\rho^2)}{2\sigma^2_{u/w}}(u-\rho w) + \frac{\rho\, C_0\varepsilon(z)}{2\sigma^2_w}w,$$

$$a'_w(z,w) = -\frac{C_0\varepsilon(z)}{2\sigma^2_w}w. \tag{3.5}$$

Note that if we choose the parameter C_1 in (3.4) as $C_1 = C_0/2b_w^4$, then it reduces to our model (3.5) (see Appendix B). Reynolds however suggests in his model $C_1 = 3$, and in all comparisons below, when referring to Reynolds' model, we take $C_1 = 3$.

In all models, the calculations were carried out for $z_0 = 0.01\ m$, the trajectories started at $h_s = 0.02\ m$, $u_* = 0.4\ m\ s^{-1}$, the number of trajectories was $N = 10^5$ in the case of a, b and c calculations, and $N = 10^6$ for the constant Pr. The vertical eddy diffusivity k_z was calculated from the relation (3.2) where a finite-difference approximation of the calculated mean concentartion was used to find the mean concentration derivative. A stationary source was uniformly distributed on the plane $z = z_s = 0.02\ m$.

The stochastic differential equations were solved by the explicit Euler scheme, with the varying time step $\Delta t = \alpha\tau_L(z)$, where $\tau_L(z) = 2\sigma_w/C_0\varepsilon(z)$ is the Lagrangian time scale; to reach stable numerical results, we found that $\alpha = 0.02$ was sufficient. At the boundary, a perfect reflection is made after the trajectory hits the layer $\{z < z_0\}$, z_0 being the roughness height.

The results of calculations and experimental data are presented in Table 1. The calculations were carried out for different values of C_0 since the constant C_0 is known to be scattered in the interval $(2, 8)$, (e.g., see Pope, 1994). The results for all four constants a, b, c and Pr show that our model is in a good agreement with Thomson's, Flesch and Wilson's models and experimental results, but in a poor agreement with the results obtained by Reynolds' model. As to the best fit to the experimental data, our model reaches it at $C_0 = 4$ while Thomson's and Flesch and Wilson's models fit best at

$C_0 = 5$. Concerning the Reynolds model, it should be mentioned that as C_0 becomes larger, the discrepancy between the results obtained by his model and measurements slightly decreases, but even for $C_0 = 7$ it remains too large. Calculations for $C_0 = 10$ (in the Table not shown) gave almost the same results as for $C_0 = 7$.

Table 3.1. Universal constants a, b, c and Pr calculated by different Lagrangian models, compared against experimental results.

Model	C_0	a	b	c	Pr
Thomson (1987)	3.	0.85	0.65	0.25	0.47
	4.	0.71	0.54	0.22	0.6
	5.	0.61	0.46	0.2	0.74
	7.	0.48	0.35	0.16	1.
Flesch & Wilson (1992)	3.	0.85	0.65	0.26	0.45
	5.	0.61	0.46	0.2	0.8
	7.	0.48	0.35	0.16	0.9
KS (see (3.5), Section 3.1)	3.	0.73	0.55	0.17	0.64
	4.	0.59	0.44	0.15	0.82
	5.	0.5	0.36	0.14	1.
	7.	0.37	0.27	0.11	1.43
Reynolds (1997)	3.	0.13	0.09	0.04	5.26
	5.	0.18	0.13	0.06	3.3
	7.	0.21	0.15	0.07	2.86
MEASUREMENTS					
Garger & Zhukov (1986)		0.58	0.44	0.19	
Chandhry & Meroney (1973)			0.4		
Rider (1954)					0.83
Gurvich (1965)					1.25

3.2 Comparison with wind-tunnel experiment by Raupach and Legg (1983)

In this section we present a comparison of the same models analysed in the previous section against the data of the wind-tunnel experiment by Raupach and Legg (1983). The vertical profiles of the mean concentration $\bar{c}$, the streamwise and vertical fluxes of concentraion $\overline{c'u'}$, $\overline{c'w'}$ were analysed.

A stationary line source at the height $h_s = 0.06\ m$ directed along the y-axis was considered, and all the profiles were calculated at the downwind distance $x = 7.5\, h_s$.

The problem is governed by 2D equations used in the previous subsection.

In Figure 1 the scaled mean concenrtaion $\bar{c}(x,z)/c_*$ and temperature $\bar{\theta}(x,z)/\theta_*$ profiles are shown for $C_0 = 3$, where

$$c_* = Q/(h_s \bar{u}(h_s)), \quad \theta_* = Q/(\rho c_p h_s \bar{u}(h_s)) \ .$$

Here Q is the line source strength per unit length, ρ the air density and c_p the specific heat of air at constant pressure. The temperature profiles were taken from the paper by Raupach and Legg (1983).

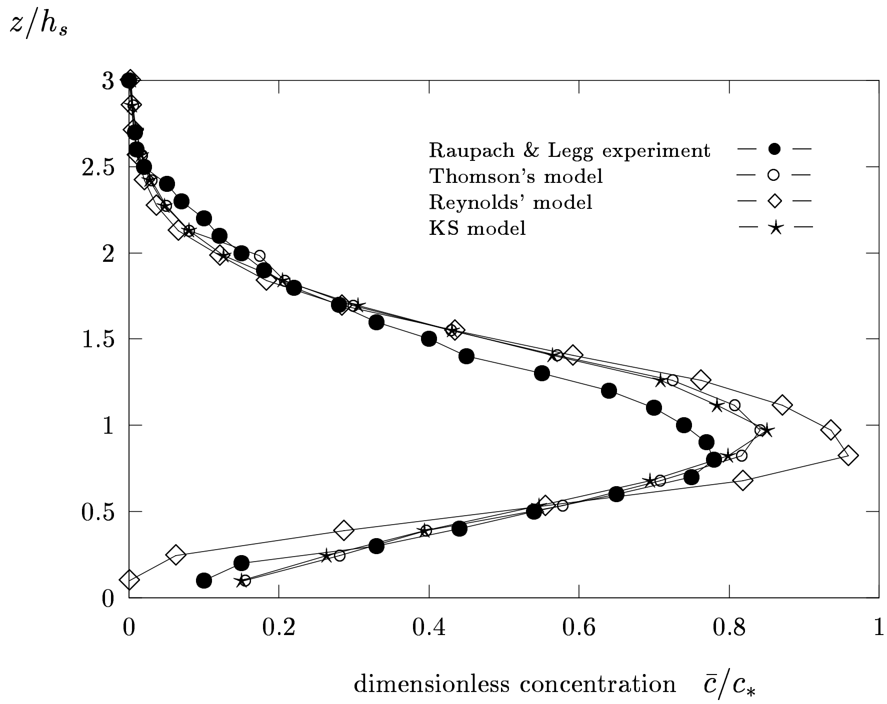

Figure 1. A comparison of three model predictions of vertical profile of mean concentrtaion with Raupach and Legg's measurement, for $C_0 = 3$.

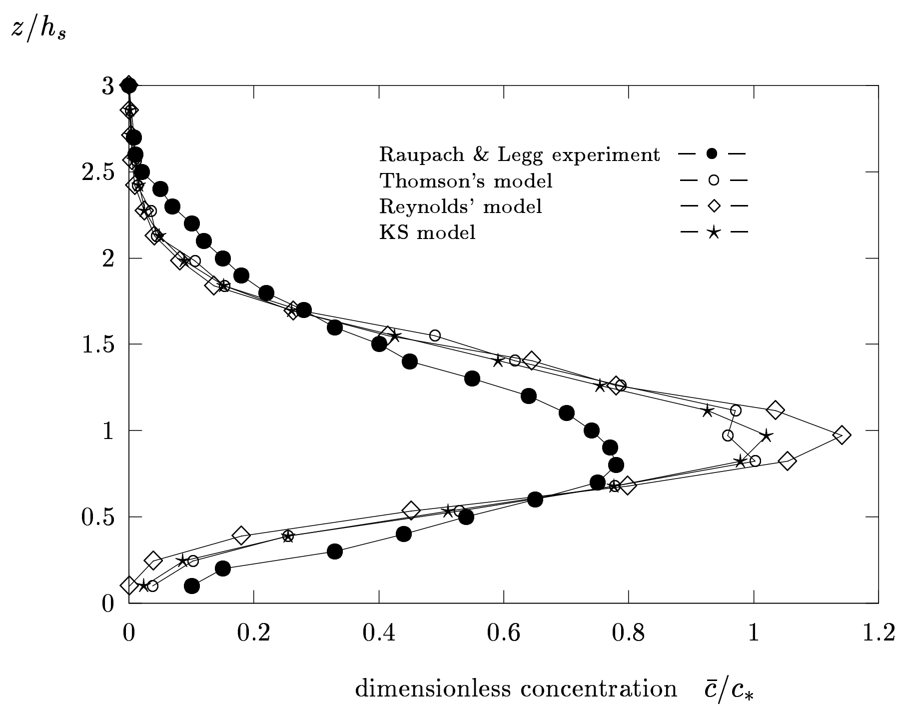

Figure 2. The same as in Figure 1, but for $C_0 = 7$.

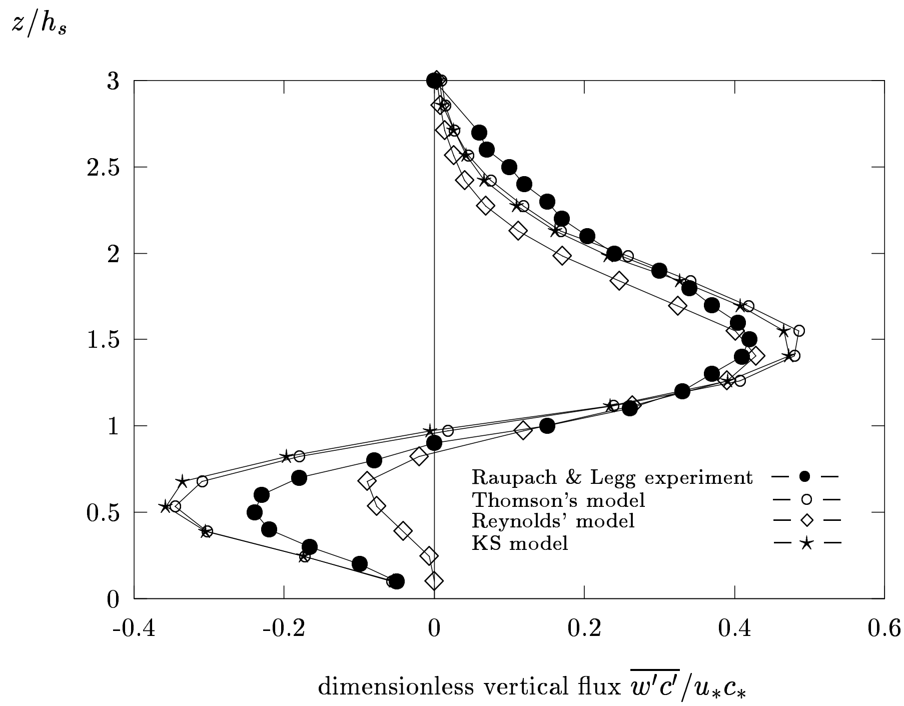

Figure 3. A comparison of three model predictions of the vertical profile of mean vertical flux with Raupach and Legg's measurement, for $C_0 = 3$.

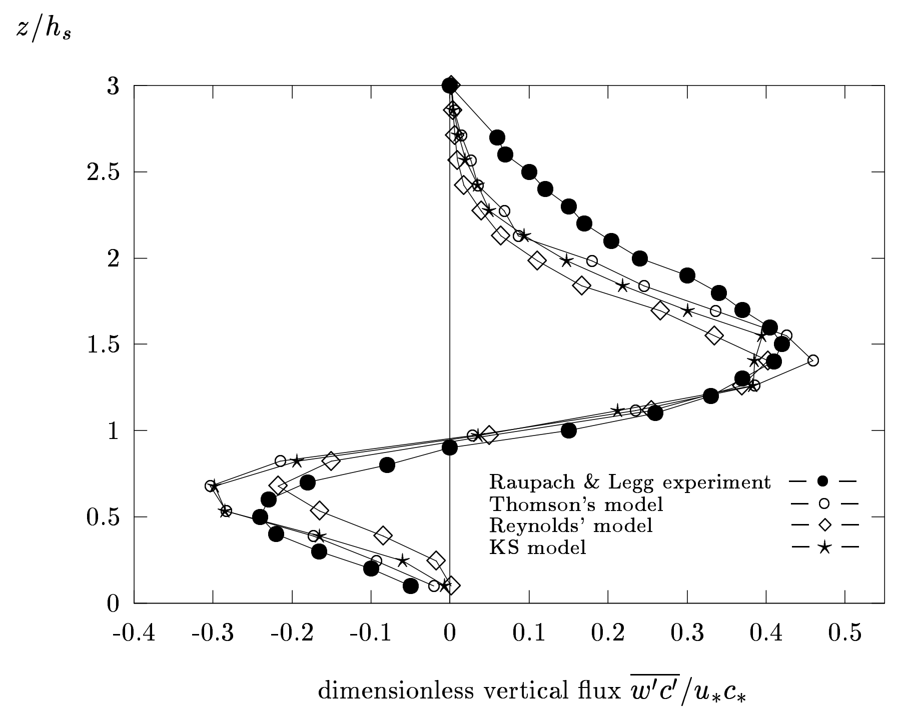

Figure 4. The same as in Figure 3, but for $C_0 = 7$.

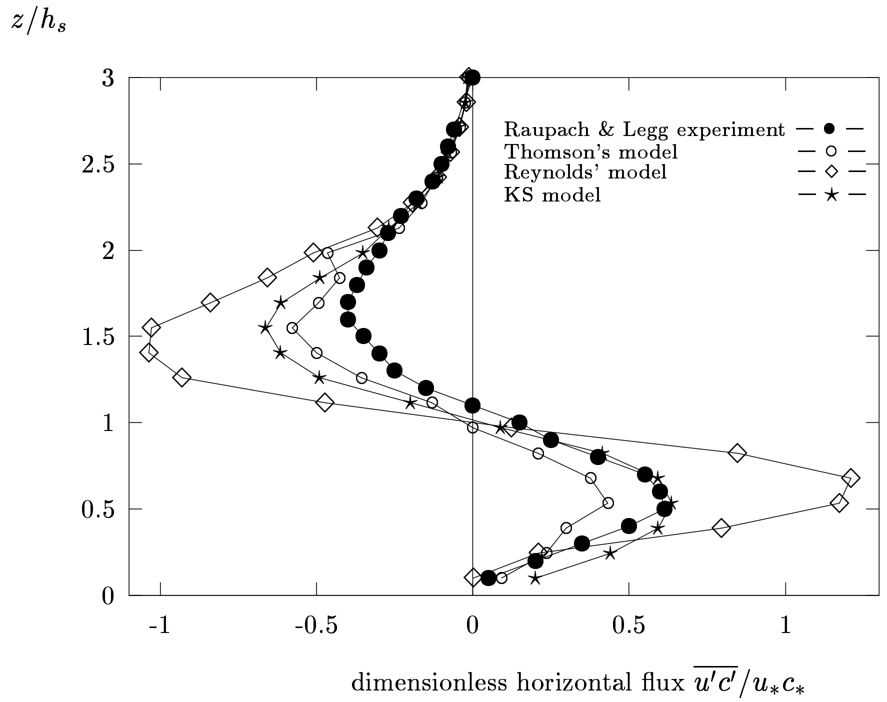

Figure 5. A comparison of three model predictions of the vertical profile of mean streamwise flux with Raupach and Legg's measurement, for $C_0 = 3$.

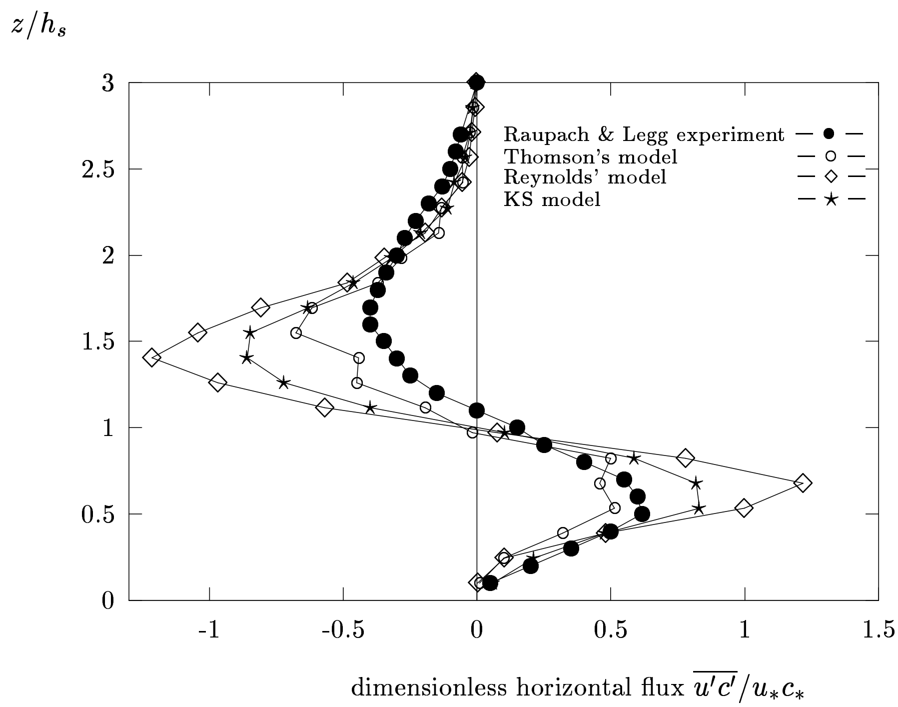

Figure 6. The same as in Figure 5, but for $C_0 = 7$.

All the models predict the experimental results qualitatively well. We mention that the results obtained by Flesch and Wilson's model are very close to the results obtained by Thomson's model, therefore, we do not plot them in our Figures. Above the height $z = 1.75h_s$ all three models agree well with the experimental results.

Below the height $1.5h_s$ Thomson's and KS models give results close to the measurements, while Reynolds's model overestimates the maximum concentration and underestimates the concentration near the ground. As to the sensitivity to the constant C_0, we have made calculations also for $C_0 = 2., 4., 5.$, and 7. The best fit of Thomson's and KS models was found at $C_0 = 3$.

For larger values of C_0 (see Figure 2 for $C_0 = 7.$) all the models overestimate the values at the maximum, and underestimate at small and large heights. In Figure 3 the vertical profile of the vertical flux of concentration is shown for $C_0 = 3$. From this curves, it is clearly seen that at the height $z < z_s$ Thomson's and KS models underestimates, and Reynolds' model overestimates the experimental results. Above the height $z = 1.5z_s$ all three models are in a good agreement with the measurements.

Note that for $C_0 = 7.$ the picture is different (see Figure 4): the models give slightly better predictions for heights $z < 1.5z_s$ In Figures 5 and 6 the vertical profiles of the streamwise flux of concentrtaion are presented for $C_0 = 3.$ and $C_0 = 7.$, respectively. Here the Reynolds' model significantly overpredicts the maximum and underpredicts the minimum values. Thomson's and KS models show better agreement with the measurements. Note however, that the agreement between Thomson's and KS models in this case is not so perfect as in the Figures 1-4. Calculations of the vertical and horizontal fluxes by our model with different values of C_0 have shown that the best fit with the experimental results was around $C_0 = 3.5 \pm 0.5$ (e.g., see Figures 3-6).

4 Convective case

In this section we consider a horizontally homogeneous boundary layer under strong convective conditions, at sufficiently large heights compared to $|L|$. In this case, the velocity fluctuations can be considered as horizontally isotropic (e.g., see Monin and Yaglom, 1971). Therefore, the mean velocity is zero, and the correlation between the vertical and horizontal velocities is zero.

In this section we show that the horizontal isotropy and the dependence supposed in (i) of the Assumption ensure the unique choice of the Lagrangian stochastic model for the convective layer.

To construct the Lagrangian one-particle model in the convective case, we have to specify the Eulerian velocity pdf. For simplicity, we will treat the case when the Eulerian pdf has the form

$$p_E(u, v, w; z, t) = p_E^{\parallel}(w; z, t) p_E^{\perp}(u_\perp; z, t), \tag{4.1}$$

where $u_\perp = \sqrt{u^2 + v^2}$, $p_E^{\parallel}$ is the pdf of the vertical velocity component, and $p_E^{\perp}$ is the pdf of the horizontal velocity components satisfying the relation:

$$\int_{-\infty}^{\infty} du \int_{-\infty}^{\infty} dv p_E^{\perp}(\sqrt{u^2 + v^2}; z, t) = 2\pi \int_0^{\infty} du_\perp \, u_\perp p_E^{\perp}(u_\perp; z, t) = 1.$$

Note that in the convective case, the assumption (4.1) is quite reasonable, because the vertical and horizontal velocity fluctuations can be considered as approximately independent.

Under the horizontally isotropy and assuming that the vertical velocity component is governed as assumed in the Assumption, point (i), the model (2.1) takes the form

$$\begin{aligned} dX &= U dt, \quad dY = V dt, \quad dZ = W dt \ , \\ dU &= U g(t, Z, U_\perp, W) dt + \sqrt{C_0 \varepsilon} dB_u(t) \ , \\ dV &= V g(t, Z, U_\perp, W) dt + \sqrt{C_0 \varepsilon} dB_v(t) \ , \\ dW &= a_w(t, Z, W) dt + \sqrt{C_0 \varepsilon} dB_w(t) \ . \end{aligned} \tag{4.2}$$

Thomson's well-mixed condition implies in our case that

$$\begin{aligned} u_\perp \frac{\partial p_E(u_\perp, w; z, t)}{\partial t} &+ \frac{\partial}{\partial z}(w u_\perp p_E) + \frac{\partial}{\partial u_\perp}(u_\perp^2 g \, p_E) + \frac{\partial}{\partial w}(u_\perp \, a_w \, p_E) \\ &= \frac{C_0 \varepsilon}{2} \Big\{ \frac{\partial}{\partial u_\perp} \Big(u_\perp \frac{\partial p_E}{\partial u_\perp} \Big) + \frac{\partial^2}{\partial w^2} \big(u_\perp p_E \big) \Big\}. \end{aligned} \tag{4.3}$$

This relation follows from (1.7) and from the following simple equalities

$$\frac{\partial}{\partial u}(u g p_E) + \frac{\partial}{\partial v}(v g p_E) = \frac{1}{u_\perp} \frac{\partial}{\partial u_\perp}(u_\perp^2 g p_E),$$

$$\frac{\partial^2 p_E}{\partial u^2} + \frac{\partial^2 p_E}{\partial v^2} + \frac{\partial^2 p_E}{\partial w^2} = \frac{1}{u_\perp} \frac{\partial}{\partial u_\perp} \Big(u_\perp \frac{\partial p_E}{\partial u_\perp} \Big) + \frac{\partial^2 p_E}{\partial w^2}.$$

The well-mixed condition (4.3) can be simplified as follows. Integrate (4.3) over $u_\perp$ and use the relation $2\pi \int_0^\infty p_E(u_\perp, w; z, t) u_\perp du_\perp = p_E^{\|}(w; z, t)$. This yields (assuming $u_\perp^2 p_E$ and $u_\perp \frac{\partial p_E}{\partial u_\perp}$ tend to zero as $u_\perp \to \infty$)

$$\frac{\partial p_E^{\|}}{\partial t} + \frac{\partial}{\partial z}(w p_E^{\|}) + \frac{\partial}{\partial w}(a_w p_E^{\|}) = \frac{C_0 \varepsilon}{2} \frac{\partial^2 p_E^{\|}}{\partial w^2}. \tag{4.4}$$

This is the one-dimensional well-mixed condition (2.4). As in the case (2.4), we can find from (4.4) the coefficient $a_w(t, z, w)$:

$$a_w(t, z, w) = \frac{1}{p_E^{\|}(w; z, t)} \left\{ \frac{C_0 \varepsilon}{2} \frac{\partial p_E^{\|}}{\partial w} - \left(\frac{\partial f_{1E}}{\partial t} + \frac{\partial F_{1E}}{\partial z} \right) \right\}, \tag{4.5}$$

where

$$f_{1E}(w; z, t) = \int_{-\infty}^{w} p_E^{\|}(w'; z, t) \, dw',$$

$$F_{1E}(w; z, t) = \int_{-\infty}^{w} w' p_E^{\|}(w'; z, t) \, dw' \ .$$

To find the function g, we substitute (4.1) in (4.3), which in view of (4.4) yields

$$u_\perp \frac{\partial p_E^\perp}{\partial t} + \frac{\partial}{\partial z}(w u_\perp p_E^\perp) + \frac{\partial}{\partial u_\perp}(u_\perp^2 g\, p_E^\perp) = \frac{C_0\varepsilon}{2}\frac{\partial}{\partial u_\perp}\Big(u_\perp \frac{\partial p_E^\perp}{\partial u_\perp}\Big). \tag{4.6}$$

Integrating (4.6) over $u_\perp$ from 0 to ∞ we get, under the condition $u_\perp^2 g p_E^\perp \to 0$ as $u_\perp \to 0$, that

$$\frac{\partial P_E}{\partial t} + w\frac{\partial P_E}{\partial z} + u_\perp^2 g(t,z,u_\perp,w)p_E^\perp = \frac{C_0\varepsilon}{2} u_\perp \frac{\partial p_E^\perp}{\partial u_\perp}, \tag{4.7}$$

where

$$P_E(u_\perp; z,t) = \int_0^{u_\perp} u p_E^\perp(u;z,t)du.$$

This defines the function g if $p_E^\perp$ is given.

For example, if

$$p_E^\perp(u_\perp) = \frac{1}{2\pi\sigma^2(t,z)}\exp\Big\{-\frac{u_\perp^2}{2\sigma^2(t,z)}\Big\}, \quad P_E(u_\perp) = \frac{1}{2\pi}\Big(1 - \exp\Big\{-\frac{u_\perp^2}{2\sigma^2(t,z)}\Big\}\Big),$$

then,

$$\frac{\partial P_E}{\partial z} = \frac{\partial \ln\sigma_\perp}{\partial z}(u_\perp^2 p_E^\perp), \quad \frac{\partial P_E}{\partial t} = \frac{\partial \ln\sigma_\perp}{\partial t}(u_\perp^2 p_E^\perp), \quad \frac{\partial p_E^\perp}{\partial u_\perp} = -\frac{u_\perp}{\sigma_\perp^2}p_E^\perp,$$

and we get

$$g = \frac{1}{u_\perp^2 p_E^\perp}\Big\{\frac{C_0\varepsilon}{2}u_\perp\frac{\partial p_E^\perp}{\partial u_\perp} - \frac{\partial P_E}{\partial t} - w\frac{\partial P_E}{\partial z}\Big\} = -\frac{C_0\varepsilon}{2\sigma_\perp^2} - \frac{\partial \ln\sigma_\perp}{\partial t} - w\frac{\partial\ln\sigma_\perp}{\partial z}. \tag{4.8}$$

As to the coefficient $a_w(t,z,w)$, it is suggested in Luhar and Britter (1989) for the stationary convective boundary layer.

Remark. *We have assumed here the factorization (4.1), which simplifies the form of g. Generally, when (4.1) is not true, the function g can be found analogously but its structure is more complicated.*

5 Boundary conditions

Note that to complete the description of the Lagrangian stochastic model, we need to define the behaviour of $(X(t), Y(t), Z(t), U(t), V(t), W(t))$, the solution to (1.2) in the neighbourhood of the boundary $\Gamma = \{(x,y,z) : z = 0\}$. We assume that the boundary is impenetrable, i.e., that $w = 0$ at the boundary of Γ. This implies that the true Lagrangian trajectories never reach Γ. Therefore it is reasonable to require that the same property holds for $X(t), Y(t), Z(t)$, the solutions to (1.2). This can be done by special choice of the function $\varepsilon(z,t)$. Indeed, in the neighbourhood of Γ, it is reasonable to consider the flow as ideally neutral stratified. Therefore, $p_E(w)$ is Gaussian, with constant σ_w, and the vertical profile of $\varepsilon(z)$ is given by (e.g., see Monin and Yaglom, 1971):

$$\varepsilon(z) = \frac{u_*^3}{\kappa z}, \quad \kappa \simeq 0.4, \quad z > z_0. \tag{5.1}$$

Here κ is the Karman constant, and z_0 is the roughness height.

The equation of vertical motion then is

$$dZ = W\,dt, \quad dW(t) = -\frac{a}{Z}W(t)dt + \frac{b}{\sqrt{Z}}\,dB(t), \tag{5.2}$$

where

$$a = \frac{u_*^3}{2\kappa\sigma_w^2}, \quad b = \Big(\frac{C_0 u_*^3}{\kappa}\Big)^{\frac{1}{2}}.$$

If we assume that the formula (5.1) is true for all $z > 0$, then all the solutions to (5.2) do not reach the boundary Γ. Indeed, let τ be a random variable (wich depends on the trajectory $Z(t)$) defined by

$$\tau(t) = \int_0^t \frac{ds}{Z(s)}.$$

Then, the vertical velocity in new variable $W(\tau)$ satisfies the equation

$$dW(\tau) = -aW(\tau)d\tau + b\,dB(\tau).$$

Therefore, from

$$\frac{dZ}{d\tau} = \frac{dZ}{dt}\frac{dt}{d\tau} = W(\tau)Z(\tau)$$

we have

$$Z(\tau) = Z(0)\exp\{S(\tau)\}, \quad S(\tau) = \int_0^\tau W(\tau')\,d\tau'.$$

The function $W(\tau)$ is an Uhlenbeck-Ornstein process with continuous samples. Therefore, $|S(\tau)| < \infty$ for all $\tau > 0$ with probability one. This implies that $Z(\tau) > 0$ provided that $Z(0) > 0$. Thus the function $Z(\tau)$ never reaches the boundary Γ. The same is true for $Z(t)$. To show this, it is sufficient to note that $t(\tau) \to \infty$ as $\tau \to \infty$. Let us show this property. We have

$$t(\tau) = \int_0^\tau \frac{dt}{d\tau'}\,d\tau' = \int_0^\tau Z(\tau')\,d\tau' = Z(0)\int_0^\tau \exp\{S(\tau')\}\,d\tau'.$$

In Kurbanmuradov (1995) it is shown that with probablity one,

$$\int_0^\infty \exp\{S(\tau)\}\,d\tau = \infty.$$

This implies that with probability one $t(\tau) \to \infty$ as $\tau \to \infty$.

6 Conclusion

A uniquely defined Lagrangian stochastic model in the class of well-mixed models is constructed from physically plausible assumptions: (i) in the neutrally stratified horizontally homogeneous surface layer, the vertical motion is mainly controlled by eddies whose size is of order of the current height, and (ii), the streamwise drift term is independent of the crosswind velocity fluctuations. The supposition (i) is motivated by the well known property that the vertical motion of vortices whose size is much larger than the current height is damped by the ground surface. Therefore, it is reasonable to assume that the vertical drift term is the same as in the isotropic case: $a'_w = a'_w(t, z, w)$. As to the point (ii), it comes from the assumption that in the special coordinate system where the X-axis is oriented along the mean velocity vector, the crosswind velocity fluctuations are symmetrically distributed with respect to the plane XZ.

In the free convective layer the mean velocity vector vanishes, and the horizontal motion is isotropic. This property is used to define uniquely the model using only the point (i) of the Assumption.

In the model presented the Eulerian pdf p_E may be not Gaussian, as, for instance, in the forest canopy (Wilson and Flesch, 1992). The Gaussian case is analysed in details. The model is compared against the wind-tunnel experiment of Raupach and Legg (1983) and models due to Thomson (1987), Flesch and Wislon (1992) and Reynolds (1998). Numerical experiments have shown a good agreement of our model with the models of Thomson (1987), Flesch and Wilson (1992), and with experimental measurements as well. However there is a large discrepancy of these results with the results obtained by Reynolds' model. Our model shows the best fit to the measurements for $C_0 = 3.5 \pm 0.5$; namely, at $C = 4.$, we found the best agreement between the calculated and measured values of the universal constants a, b, c and Pr; at $C_0 = 3.$, the best agreement with the wind-tunnel experiments by Raupach and Legg (1983) was achieved. It is interesting to note that our model, also being quadratic in velocity (in the Gaussian case), does not belong to the general two-parametric class of models suggested by Reynolds (1997); it is also not in the family of "zero-spin" models introduced by Wilson and Flesch (1997).

It is beleived that the model proposed is well suited for the case of neutrally (or close to) stratified surface layer. For the whole boundary layer with the mean velocity vector varying with height the generalization might be possible, but requires a special study. The same is true for the generalization to compressible flows which is important for studying a stably stratified surface layer.

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Appendix A. Derivation of the coefficients in the Gaussian case.

Here we derive the coefficients (2.14)-(2.16) from (2.8)-(2.10) in the case of Gaussian pdf (2.13). First we remark that from (2.5) and (2.7) it follows

$$p'_{1E}(w; z, t) = \frac{1}{\sqrt{2\pi}\sigma_w} \exp\left\{-\frac{w^2}{2\sigma_w^2}\right\},$$

$$p'_{2E}(u, w; z, t) = \frac{1}{2\pi\sigma_{u/w}\sigma_w} \exp\left\{-\frac{1}{2\sigma_{u/w}^2}(u - \rho w)^2 - \frac{w^2}{2\sigma_w^2}\right\} .$$

Consequently,

$$f_{1E}(w;z,t) = \int_{-\infty}^{\frac{w}{\sigma_w}} \frac{1}{\sqrt{2\pi}} \exp\left(-t^2/2\right) dt = \Phi\left(\frac{w}{\sigma_w}\right),$$

$$F_{1E}(w;z,t) = -\sigma_w^2 p'_{1E}(w;z,t).$$

Note that

$$\frac{1}{p'_{1E}}\frac{\partial p'_{1E}}{\partial w} = -\frac{w}{\sigma_w^2}, \quad -\frac{1}{p'_{1E}}\frac{\partial F_{1E}}{\partial z} = \frac{1}{2}(w^2+1)\frac{\partial \sigma_w^2}{\partial z},$$

and

$$\frac{\partial f_{1E}}{\partial t} = -\frac{w}{\sigma_w^2}\frac{\partial \sigma_w}{\partial t}\dot{\Phi}(w/\sigma_w),$$

where

$$\Phi(\tau) = \int_{-\infty}^{\tau} \frac{1}{\sqrt{2\pi}} \exp\left(-t^2/2\right) dt, \quad \dot{\Phi}(\tau) = \frac{d\Phi}{d\tau}.$$

From (2.8) we find

$$a'_w(t,z,w) = -\left(\frac{C_0\varepsilon}{2\sigma_w^2} - \frac{1}{\sigma_w}\frac{\partial \sigma_w}{\partial t}\right) w + \frac{1}{2}\frac{\partial \sigma_w^2}{\partial z}\left(\frac{w^2}{\sigma_w^2}+1\right).$$

Note that this coincides with Thomson's relevant expression in his 1D model.

By the definition

$$f_{2E}(u,w,z,t) = p'_{1E}(w;z,t)\,\Phi\Big(\frac{u-\rho w}{\sigma_{u/w}}\Big).$$

To find a'_u from (2.9) we need the expressions for

$$\frac{\partial f_{2E}}{\partial t}, \quad \frac{\partial f_{2E}}{\partial z}, \quad \frac{\partial f_{2E}}{\partial w}, \quad \frac{\partial p'_{2E}}{\partial u}, \quad \frac{\partial^2 f_{2E}}{\partial w^2}.$$

By definition we get

$$\begin{aligned}
\frac{\partial p'_{2E}}{\partial u} &= -\frac{(u-\rho w)}{\sigma_{u/w}^2} p'_{2E}, \; \frac{\partial f_{2E}}{\partial t} = f_{2E}\left\{\frac{1}{2\sigma_w^2}\frac{\partial \sigma_w^2}{\partial t}\left(\frac{w^2}{\sigma_w^2}-1\right) + \Psi(\xi)\frac{\partial \xi}{\partial t}\right\}, \\
\frac{\partial f_{2E}}{\partial z} &= f_{2E}\left\{\frac{1}{2\sigma_w^2}\frac{\partial \sigma_w^2}{\partial z}\left(\frac{w^2}{\sigma_w^2}-1\right) + \Psi(\xi)\frac{\partial \xi}{\partial z}\right\}, \\
\frac{\partial f_{2E}}{\partial w} &= f_{2E}\left\{-\frac{w}{\sigma_w^2} - \Psi(\xi)\eta\right\}, \\
\frac{\partial^2 f_{2E}}{\partial w^2} &= f_{2E}\Big\{\Big[-\frac{w}{\sigma_w^2} - \Psi(\xi)\eta\Big]^2 - \frac{1}{\sigma_w^2} + \eta^2\dot{\Psi}(\xi)\Big\},
\end{aligned}$$

where

$$\Psi(\tau) = \frac{d}{d\tau}\ln\Phi(\tau), \; \dot{\Psi}(\tau) = \frac{d\Psi(\tau)}{d\tau}, \; \xi = \frac{u-\rho w}{\sigma_{u/w}}, \; \eta = \frac{\overline{uw}}{\sigma_{u/w}\sigma_w^2}.$$

Substituting these expressions in (2.9) yields

$$a_u' = -\frac{C_0\varepsilon}{2\sigma_{u/w}^2}(u-\rho w) + \frac{1}{p_{2E}'}\left\{-\frac{\partial f_{2E}}{\partial t} - w\frac{\partial f_{2E}}{\partial z} - f_{2E}\frac{\partial a_w'}{\partial w} - a_w'\frac{\partial f_{2E}}{\partial w} + \frac{C_0\varepsilon}{2}\frac{\partial^2 f_{2E}}{\partial w^2}\right\}$$

$$= -\frac{C_0\varepsilon}{2\sigma_{u/w}^2}(u-\rho w) + \frac{f_{2E}}{p_{2E}'}\left\{-\frac{1}{2\sigma_w^2}\frac{\partial\sigma_w^2}{\partial t}\left(\frac{w^2}{\sigma_w^2}-1\right) - \Psi(\xi)\frac{\partial\xi}{\partial t}\right.$$

$$-w\left[\frac{1}{2\sigma_w^2}\frac{\partial\sigma_w^2}{\partial z}\left(\frac{w^2}{\sigma_w^2}-1\right) + \Psi(\xi)\frac{\partial\xi}{\partial z}\right] - \frac{\partial a_w'}{\partial w} - a_w'\left[-\frac{w}{\sigma_w^2} - \Psi(\xi)\eta\right]$$

$$\left. + \frac{C_0\varepsilon}{2}\left[\left(-\frac{w}{\sigma_w^2} - \Psi(\xi)\eta\right)^2 - \frac{1}{\sigma_w^2} + \eta^2\dot{\Psi}(\xi)\right]\right\}. \qquad (A1)$$

Since

$$\frac{f_{2E}\Psi}{p_{2E}'} = \sigma_{u/w}, \quad \dot{\Psi}(\xi) = -\Psi(\xi)(\xi + \Psi(\xi)),$$

we find from (A1)

$$a_u'(t,z,u,w) = -\frac{C_0\varepsilon(1+\rho^2)}{2\sigma_{u/w}^2}(u-\rho w) + \frac{\rho}{2\sigma_w^2}\left(C_0\varepsilon + \frac{\partial\sigma_w^2}{\partial t}\right)w$$

$$+\frac{\rho}{2}\frac{\partial\sigma_w^2}{\partial z}\left(\frac{w^2}{\sigma_w^2}+1\right) - \sigma_{u/w}\left(\frac{\partial\xi}{\partial t} + w\frac{\partial\xi}{\partial z}\right)$$

$$= -\frac{C_0\varepsilon(1+\rho^2)}{2\sigma_{u/w}^2}(u-\rho w) + \frac{\rho}{2\sigma_w^2}\left(C_0\varepsilon + \frac{\partial\sigma_w^2}{\partial t}\right)w + \frac{\rho}{2}\frac{\partial\sigma_w^2}{\partial z}\left(\frac{w^2}{\sigma_w^2}+1\right)$$

$$-\left(\frac{\partial\rho}{\partial t}+w\frac{\partial\rho}{\partial z}\right)w - \frac{1}{\sigma_{u/w}}\left(\frac{\partial\sigma_{u/w}}{\partial t}+w\frac{\partial\sigma_{u/w}}{\partial z}\right)(u-\rho w),$$

Since for the case considered the condition (2.11) is satisfied, we use here the expression (2.12). Substituting

$$\frac{1}{p_{vE}}\frac{\partial p_{vE}}{\partial v} = -\frac{v}{\sigma_v^2}, \; \frac{1}{p_{vE}}\frac{\partial f_{vE}}{\partial t} = -\frac{v}{\sigma_v}\frac{\partial\sigma_v}{\partial t}, \; \frac{1}{p_{vE}}\frac{\partial f_{vE}}{\partial z} = -\frac{v}{\sigma_v}\frac{\partial\sigma_v}{\partial z}$$

into (2.12), we get

$$a_v'(t,z,u,v,w) = -\left(\frac{C_0\varepsilon}{2\sigma_v^2} - \frac{1}{\sigma_v}\frac{\partial\sigma_v}{\partial t}\right)v + \frac{1}{2}\frac{\partial\sigma_v^2}{\partial z}\frac{vw}{\sigma_v^2}.$$

Appendix B. Relation to other models.

Two-parametric class of models due to Reynolds.

Here we analyse Reynolds' two-parametric class of models in the case of horizontally homogeneous turbulence with the mean velocity direction not varying with height. It is also assumed that the X-axis is oriented along the mean velocity vector, and the crosswind velocity fluctuations are symmetric with respect to the plane XZ. Then the two-parametric class of models quadratic in velocity, which satisfies the well-mixed condition for Gaussian p_E, considered by Reynolds (1997), reads

$$dX_1 = (U_1' + \bar{u}(X_3,t))dt, \; dX_2 = U_2'dt, \; dX_3 = U_3'dt,$$

$$dU_1' = a_1'(t, X_3, U_1', U_2', U_3')dt + \sqrt{C_0\varepsilon}\, dB_1(t),$$

$$dU_2' = a_2'(t, X_3, U_1', U_2', U_3')dt + \sqrt{C_0\varepsilon}\, dB_2(t), \qquad (B1)$$
$$dU_3' = a_3'(t, X_3, U_1', U_2', U_3')dt + \sqrt{C_0\varepsilon}\, dB_3(t)\ ,$$

where

$$a_i'(t, z, u_1, u_2, u_3) = -\frac{C_0\varepsilon}{2}\lambda_{ij}u_j + \frac{1}{2}\frac{\partial\sigma_{i3}}{\partial z} + \frac{1}{2}C_2\Big(\frac{\partial\sigma_{i3}}{\partial z} + \sigma_{i3}\sigma_{km}\frac{\partial\lambda_{km}}{\partial z}\Big)$$
$$-\frac{1}{2}\sigma_{im}\frac{\partial\lambda_{jm}}{\partial t}u_j + C_1\Big(\sigma_{i3}\frac{\partial\bar{u}}{\partial z}\lambda_{j1} - \delta_{1i}\delta_{3j}\frac{\partial\bar{u}}{\partial z}\Big)u_j - \frac{1}{2}C_2\sigma_{i3}\frac{\partial\lambda_{jk}}{\partial z}u_ju_k$$
$$-\frac{1}{2}(1 - C_2)\sigma_{im}\frac{\partial\lambda_{km}}{\partial z}u_3u_k, \quad i = 1, 2, 3. \qquad (B2)$$

Here we adopt the summation convention, hence the notation $(X, Y, Z) = (X_1, X_2, X_3)$ and $(U, V, W) = (U_1, U_2, U_3)$ is used; δ_{ij} is the Kronecker symbol, $\sigma_{ij} = (\lambda^{-1})_{ij}$ are the velocity covariances which in the case considered have the form:

$$\sigma_{11} = \sigma_u^2, \quad \sigma_{22} = \sigma_v^2, \quad \sigma_3 = \sigma_w^2, \quad \sigma_{12} = \sigma_{21} = \sigma_{23} = \sigma_{32} = 0, \sigma_{13} = \sigma_{31} = \overline{uw};$$

$$\lambda_{11} = \frac{\sigma_w^2}{\Delta}, \lambda_{22} = \frac{1}{\sigma_v^2}, \lambda_{33} = \frac{\sigma_u^2}{\Delta}, \lambda_{12} = \lambda_{21} = \lambda_{23} = \lambda_{32} = 0, \lambda_{13} = \lambda_{31} = -\frac{\overline{uw}}{\Delta},$$

where σ_u^2, σ_v^2, and σ_w^2 are the variances of velocity components, $\Delta = \sigma_u^2\sigma_w^2 - (\overline{uw})^2$.

Thus the model includes two free parameters C_1 and C_2. Reynolds (1998) has suggested $C_1 = \pm 3$, and $C_2 = 0$ to fit the experimental results for wind-tunnel boundary layer by Legg (1983).

It is interesting to find if there are some values of C_1, C_2 such that the model (B2) reduces to our model (2.14)-(2.16). To this end, it is sufficient to check if the model (B2) satisfies the Assumption of our model (see Section 2.1). It is clear that the point (ii) of the Assumption is satisfied iff $C_2 = 0$, since in the expression for a_1', the dependence on u_2 can be eliminated only if $C_2 = 0$. Thus taking $C_2 = 0$, we analyse the point (i) of the Assumption. In the expression for $a_3'(t, z, u_1, u_2, u_3)$ we are interested in the terms depending on u_1 and u_2, therefore we write it as

$$a_3' = \{\dots\} + C_1\sigma_{33}\frac{\partial\bar{u}}{\partial z}\lambda_{11}u_1 - \frac{1}{2}C_0\varepsilon\lambda_{31}u_1 - \frac{1}{2}\sigma_{3m}\frac{\partial\lambda_{1m}}{\partial z}u_3u_1$$

where $\{\dots\}$ stands for the terms not depending on u_1 and u_2. From this we see that if the term $\frac{\partial\lambda_{1m}}{\partial z}$ is not equal to zero, then the point (i) cannot be satisfied. Note that this term iz zero in the ideally-neutral stratification ($L = \infty$). In this case (i) is satisfied, iff $C_1 = C_0u_*^4/(2\sigma_w^4)$.

From this we conclude that only in the case of ideally-neutral stratification our model belongs to the class of models (B1)-(B2) if $C_2 = 0$, and $C_1 = C_0u_*^4/(2\sigma_w^4)$.

The “zero-spin” property.

Here we show that in our model (for simplicity we consider the stationary turbulence) the average increment $\langle d\theta; z\rangle$ to the orientation $\theta = arctan(w'/u')$ of the Lagrangian velocity fluctuation vector in 2D case is negative, and hence it does not belong to the “zero-spin” class of models.

Wilson and Flesch (1997) showed that

$$\langle d\theta; z\rangle = dt \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{u\phi'_w - w\phi'_u}{u^2+w^2}\, du\, dw \ ,$$

where

$$\frac{\phi'_u}{p'_E} = a'_u - \frac{C_0\varepsilon}{2}\frac{\partial \ln\, p'_E}{\partial u}\ , \quad \frac{\phi'_w}{p'_E} = a'_w - \frac{C_0\varepsilon}{2}\frac{\partial \ln\, p'_E}{\partial w}\ .$$

For our model (see (2.18)) we find

$$\frac{\phi'_u}{p'_E} = w^2\frac{d\rho}{dz} + \frac{1}{\sigma}\frac{d\sigma}{dz}w(u-\rho w) - \frac{C_0\varepsilon\rho^2}{2\sigma^2}(u-\rho w) + \frac{C_0\varepsilon\rho}{2\sigma_w^2}w + \frac{\rho}{2}\frac{d\sigma_w^2}{dz}\Big(1+\frac{w^2}{\sigma_w^2}\Big),$$
$$\frac{\phi'_w}{p'_E} = \frac{1}{2}\frac{d\sigma_w^2}{dz}\Big(1+\frac{w^2}{\sigma_w^2}\Big) - \frac{C_0\varepsilon\rho}{2\sigma^2}(u-\rho w),$$

where we use the notation $\sigma = \sigma_{u/w}$. After some algebra we can find that

$$\langle d\theta; z\rangle = -\, dt\, \frac{C_0\varepsilon\rho}{2} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{p'_E}{u^2+w^2}\Big(\frac{u^2}{\sigma^2} + \frac{\rho^2 w^2}{\sigma^2} + \frac{w^2}{\sigma_w^2}\Big)\, du\, dw < 0\ .$$

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