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NON-LOCAL MODELS FOR DIFFUSION IN ATMOSPHERIC CALM

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Summary

The non-local diffusion equation in space and time previously determined is applied to the particular case of diffusion in calm. Non-local diffusion models are presented in relation to the non-markovian character of turbulent diffusion. A space-time non-local one-dimensional model is used to show that non-local models are consistent with the statistical theory of turbulent diffusion, even without the introduction of virtual diffusion coefficients (K). A series of non-local models for continuous and instantaneous sources are derived and the consequences of these models compared to K-theory are discussed.

1. INTRODUCTION

Non-local diffusion models are obtained by generalization of local diffusion theory. They avoid some of the limitations of local eddy-diffusion (K) theory, which was based on a flux-gradient relation similar to molecular diffusion.

Molecular diffusion is the outcome of several scattering processes taking place independently in space and time. This random process has independent increments; consequently, the equation for the transition probability P is local in space and time. $P(x, t; x_0, t_0)$ is the transition probability for a marked particle located in x_0 at t_0 to reach x at t.

Turbulent diffusion is a non-markovian process with space-time memory due to the fact that vortices operate in space-time correlation. Hence, the turbulent diffusion equation must be non-local in space and time.

A number of non-local models have been described in the literature: the non-linear diffusion equation, non-local in space and time, obtained by the direct interaction approximation (Roberts, 1961); the non-local equation in time found with the Wiener-Hermite expansions method in the Gaussian approximation applied to homogeneous and stationary turbulence (Saffman, 1969); the K-spectral equation, non-local in space obtained by generalizing the diffusion coefficient (Berkowicz and Prahm, 1979); the non-local diffusion in space and time determined by the orthonormal expansions for random functions (Romanof, 1984, 1988); and transilient theory (Stull, 1993). A particular form for the generalized diffusion tensor was used for the estimation of the flatness-factor by Romanof (1994).

2. THEORETICAL BACKGROUND

Using space coordinates denoted by $x = (x_1, x_2, x_3)$, the non-local diffusion equation is:

$$\frac{\partial \overline{C}}{\partial t} + \frac{\partial}{\partial x_i}\left(\overline{u_i C}\right) = \frac{\partial}{\partial x_i}\int_0^t dt' \int dx' D_{ij}\left(x, t : x' t'\right) \frac{\partial \overline{C\left(x', t'\right)}}{\partial x'_j} + \rho \qquad (2.1)$$

where D_{ij} is the generalized diffusion tensor; $\overline{C}$ stands for the ensemble mean concentration; $\overline{u}_i$ represent the mean velocity components, and ρ is the source term.

Some special cases of this equation can be examined. If $\rho = \delta(x - x_0)\,\delta(t - t_0)$ (δ is the Dirac function), then $\overline{C}$ = (x, t; x_0, t_0) = P(x, t; x_0, t_0). If $D_{ij} = K_{ij}$ (x, t) δ (x – x’) δ (t – t’), then the equation for K-theory is obtained with the diffusion coefficients K_{ij}. This points to the introduction of several non-local models by substituting the Dirac functions for certain functions dependent upon the space and time scales of turbulence which tend to the Dirac function, when space-time scales tend to zero.

By way of example, δ (x – x’) can be replaced by D(x – x’) = $= \frac{1}{\sqrt{2\pi}\, L_x} \exp\left[-\frac{(x - x')^2}{2L_x^2}\right]$ where L_x stands for the space scale corresponding to the velocity components on the x axis. If $L_x \to 0$ and D(x – x’) $\to \delta$ (x-x’), then the local K-theory equation is obtained for the x variable.

Asymptotically (large times in comparison with the Lagrangian time scale) the eddy-diffusion equation can be obtained with the coefficients:

$$K_{ij}(x, t) = \int_0^\infty dt' \int dx' D_{ij}(x, t; x', t') \qquad (2.2)$$

Similarly, the Lagrangian correlation function (for the special case of homogeneous and stationary turbulence) can be found (Romanof, 1987) as:

$$B_{ij}^L(t) = \int D_{ij}(x, t)\, dx \qquad (2.3)$$

In this case, D_{ij} depends upon x - x’; t - t’ only; hence, one may write D_{ij} (x, t).

Equation (2.1) was devised without approximations; however, explicit expressions for D_{ij} were obtained with the Gaussian approximation (Romanof, 1988). Particular forms of the generalized diffusion tensor D_{ij} leads us to the diffusion equations in the specialized literature (Romanof, 1988), as described in the next two sections.

3. INSTANTANEOUS SOURCES

With instantaneous sources, the non-local model should be space-temporal; thus, an agreement may be obtained with the statistical theory of turbulent diffusion. The case of homogeneous and stationary turbulence is envisaged. Let P(x, t) be the transition probability for a marked particle moving in the turbulent fluid, which at t = 0 is located in x = 0. Note that P has a Gaussian distribution and satisfies the equation (Monin, Iaglom, 1965):

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial x_i}\left[K_{ij}(t) \frac{\partial P}{\partial x_i}\right] \qquad (3.1)$$

where K_{ij} (t) are the virtual (eddy) diffusion coefficients:

$$K_{ij} = \frac{1}{2}\frac{dD_{ij}(t)}{dt} = \frac{1}{2}\int_0^t \left[B_{ij}^L(\tau) + B_{ji}^L(\tau)\right] d\tau \tag{3.2}$$

In this expression, D_{ij} is the dispersion tensor, and B_{ij}^L is the Lagrangian correlation function:

$$D_{ij}(t) = \int_0^t dt_1 \int_0^t dt_2\, B_{ij}^L(t_2 - t_1) \tag{3.3}$$

$$B_{ij}^L(t_2 - t_1) = \langle V_i(t_1) V_j(t_2) \rangle \tag{3.4}$$

where V_i stands for the instantaneous components of the particle velocity, and $(\overline{V}_i = \overline{u}_i = 0)$ for calm conditions. With an instantaneous source, the transition probability coincides with the mean concentration P(x, t) = $\overline{C}$(x, t), thus equation (2.1) becomes:

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial x_i}\int_0^t dt' \int dx' D_{ij}(x - x'; t - t')\frac{\partial P}{\partial x_j^{'}} \tag{3.5}$$

Therefore, instead of the virtual diffusion coefficients $K_{ij}(t)$ introduced for establishing an agreement between K – theory and the statistical theory, we change the form of the K equation, rendering it non-local. This is a theoretically deduced result, without hypotheses except for the conditions of homogeneous stationary turbulence in a calm mean-wind situation.

The non-local equation leads to results concordant with the statistical theory. For instance, to get the one-dimensional case, one can choose:

$$D(x, t) = Q(x, t)\, B(x, t) \tag{3.6}$$

where B is the Eulerian space-time correlation function. Q stands for a certain probability density which, for special physical situations, could be parameterized as:

$$Q(x,t) = \frac{1}{\sqrt{2\pi t \sigma_u}} e^{-\frac{x^2}{2t^2\sigma_u{}^2}}$$

$$\sigma_u^2 = \overline{u^2}$$

For B, the expression below is proposed:

$$B = \overline{u^2}\; e^{-\frac{|x| + t\cdot\sigma_u}{L_x}}, \quad t > 0 \tag{3.8}$$

$\overline{u^2} = 1$ *and* $L_x = 1$ *was chosen* for numerical simulation.

This is equivalent with using non-dimensional variables x/L_x and t/T_x, where $T_x = L_x/\sigma_u$.

By means of the relations (2.3), (3.6), (3.7) and (3.8) the Lagrangian correlation functions $B^L(t)$ can be estimated (Fig. 1). The result derived is consistent with numerical simulations (Romanof, 1989; Romanof, Pescaru, 1984) of B_n^L (t), also plotted in Fig. 1.

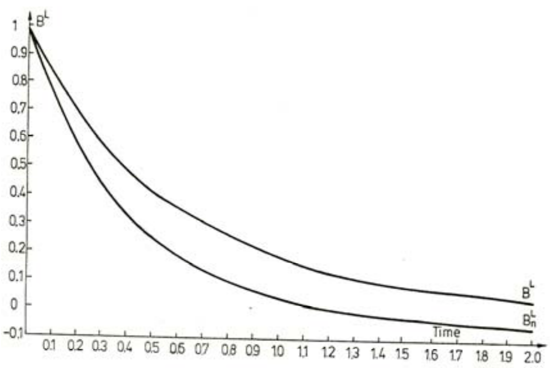

Figure 1. The Lagrangian correlation function B^L derived analytically compared with previously reported numerical simulations B_n^L.

At small times, B $\to\cong$ 1 ($\overline{u^2}$ = 1 was chosen); hence D (x, t) = Q (x, t), B^L (t) $\cong\to$ 1 and $\overline{x^2} = \overline{u^2}\ \ t^2$ in the keeping with statistical theory. The form of function Q has little influence on the Lagrangian correlation function; however, the flatness factor F = $\dfrac{\overline{x^4}}{3\left(\overline{x^2}\right)^2}$ is quite sensitive to the form of Q.

Let $\tilde{Q}(k,t)$ be the Fourier transform of Q (x, t).

$$\tilde{Q}(k,t) = \int e^{ikx}\, Q(x,t)\, dx$$

In the case of expression (3.7) we have:

$$\tilde{Q}(k,t) = e^{-\frac{k^2\ t^2 \sigma_u{}^2}{2}}$$

One can hypothesize that this expression can be generalized to be

$$\tilde{Q}(k,t) = e^{-\frac{\alpha k^2 t^2 \sigma_u{}^2}{2}} \qquad \alpha > 0$$

where parameter α can be determined so that the solution to equation (3.5) approaches a flatness factor of F = 1 at small times. This corresponds to a Gaussian distribution in agreement with statistical theory.

By making the Fourier transform of the equation (3.5) and taking account of the fact that the n order moment is related to the characteristic function by

$$\overline{x^n} = \frac{1}{i^n}\frac{\partial \tilde{P}(k,t)}{\partial k}\Big|_{k=0} \qquad \text{we get:}$$

$$F = \frac{\overline{x^4}}{3\left(\overline{x^2}\right)^2} = \frac{\alpha+1}{3}$$

$$F = 1 \Rightarrow \alpha = 2$$

For this case $\tilde{Q}$(k, t) = $e^{-k^2 t^2 \sigma_u^2}$ is identical to the universal function numerically determined by the condition that the solution to the equation (3.5) should be Gaussian at small times (Romanof, 1987). Hence, the hypothesized expression may be employed also for other estimates on account of the fact that it describes accurately the behaviour of dispersion σ^2 and the distribution of P with small times.

Suppose that the velocity variance and the space and time scales of turbulence (or the maximum frequency in the spectrum) are of great significance for characterizing turbulent diffusion. Then the velocity variance gives local influence and the space and time scales determine the non-locality degree. Within this hypothesis, the vertical turbulent flux $\overline{w'C'}$ in the boundary layer may be non-locally modelled as:

$$\overline{w'C'} = -\int_0^t dt' \int_0^\infty dz' \,\overline{w'^2}\, e^{-\frac{\pi(t-t')^2}{4T_z^2}} \frac{1}{\sqrt{2\pi}\, L_z} e^{-\frac{(z-z')^2}{2L_z^2}} \frac{\partial \overline{C}(z';t')}{\partial z'} \qquad (3.9)$$

where T_z is the Eulerian temporal scale and L_z stands for the space scale.

From (3.9) and (2.3), it follows that the Lagrangian correlation function is:

$$B_{33}^L(t) = \overline{w'^2}\, e^{-\frac{\pi t^2}{4T_z^2}}$$

To pass to the limit, we multiply and divide it with T_z and find the Dirac function.

If $T_z \to 0$, $L_z \to 0$ and $\overline{w'^2}\ T_z \to K_z$ ($\overline{w'^2} \to \infty$, just as with the white noise case) then the diffusion equation corresponding to the flux given by (3.9) becomes (see Annex A):

$$\frac{\partial \overline{C}}{\partial t} = \frac{\partial}{\partial z}\left(K_z \frac{\partial \overline{C}}{\partial z} \right) \tag{3.10}$$

where: $\overline{w'^2}$, T_z, L_z, K_z are functions of z.

For boundary layer problems, see e.g. Stull (1988) and for white noise problems see e.g. Hida (1980).

Equation (3.10) is a local expression; namely, it is identical to the K-equation for an instantaneous surface source. The analysis of spectra of the vertical velocity shows that T_z and L_z are functions increasing with height, and also increasing from stable to unstable conditions (Pasquill, 1974).

4. CONTINUOUS SOURCES

In this case the equation (2.1) becomes non-local with space coordinates only:

$$\frac{\partial}{\partial x_i}\int dx' D^c_{ij}(x,x')\frac{\partial \overline{C}(x')}{\partial x'_j} + \rho(x) = 0 \tag{4.1}$$

$$D^c_{ij}(x,x') = \int_0^\infty D_{ij}(x,x',\tau)\, d\tau \tag{4.2}$$

The continuous sources are characterized by the source term ρ(x). Turbulence is assumed to be stationary, so that $\overline{C}$ depends upon x only.

If a continuous surface source is considered (for instance, the emissions of radon and thoron at the ground surface) into a horizontally homogeneous boundary layer, the concentration will depend upon z only,

$$\frac{d}{dz}\int_0^\infty D^c_{33}(z,z')\frac{d\,\overline{C}(z)}{dz'}dz' + Q\,\delta(z) - \lambda\overline{C} = 0 \tag{4.3}$$

where λ is the radioactive decay constant and

$$D^c_{33}(z,z') = \iint dxdy\, D^c_{33}(z,z';x,y) \tag{4.4}$$

Also, because of horizontal homogeneity, the equation above used

$$D^c_{33}(z,z';x,x';y,y') = D^c_{33}(z,z';x-x';y-y')$$

From (4.3) it follows

$$\overline{w'C'} = -\int_0^\infty D^c_{33}(z,z')\frac{d\overline{C}(z')}{dz'}dz' \tag{4.5}$$

A similar relation was considered by Fiedler (1984). Thus, relation (4.5) can be related to general equation (2.1).

For $D^c_{33}(z,z')$ an expression of the type below may be envisaged:

$$D^c_{33}(z,z') = \frac{\sigma_w}{\sqrt{2\pi}} e^{-\frac{(z-z')^2}{2\lambda_m^2(z)}} \tag{4.6}$$

where $\lambda_m(z)$ is the wave length having maximum intensity in the vertical velocity spectrum. If $\lambda_m \to 0$, $\sigma_w \to \infty$ and $\sigma_w\lambda_m \to K_z$ then the equation (4.3) becomes the K-theory equation

$$\frac{d}{dz}K_z\left(\frac{d\overline{C}}{dz}\right)+Q\,\delta(z)-\lambda\,\overline{C}=0 \qquad (4.7)$$

As in the case of equation (3.9), we multiplied and divided by λ_m and found the Dirac function.

The analysis of vertical spectra points to the fact that $\lambda_m(z) = \alpha z$ (Pasquill, 1974) α is a constant increasing from stable to unstable conditions. Since λ_m defines the non-locality degree, it follows that it increases with height and is greater under non-stable conditions that under stable ones.

5. CONCLUSIONS

1. In the case of the instantaneous point source, instead of the diffusion coefficients, a non-local expression in space and time is inserted, expressing the turbulent flux function of the mean concentration gradient, with the help of the generalized diffusion tensor.

2. In the one-dimensional case, a particular expression is chosen for the generalized diffusion tensor, on the basis of which the Langragian correlation function is estimated. The estimation is in accordance with the result obtained with a numerical simulation.

3. In the case of the instantaneous surface source, K equation is obtained, as a limit-case of the non-local model.

4. In the case of the continuous surface source, a non-local expression is proposed for the vertical turbulent flux, leading at the limit, to the K equation.

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ANNEX A

Deducing equation K from the non-local equation, when the space and time scales tend to zero.

In the case of the instantaneous surface source, using the non-local expression (3.9) for the vertical turbulent flux, we find the non-local diffusion equation:

$$\frac{\partial \overline{C}}{\partial t} = \frac{\partial}{\partial z} \int_0^t dt' \int_0^\infty dz' \, \overline{w'^2} \, e^{-\frac{\pi (t-t')^2}{4T_z^2}} \frac{1}{\sqrt{2\pi} L_z} e^{-\frac{(z-z')^2}{2L_z^2}} \frac{\partial \overline{C}(z';t')}{\partial z'} \tag{A1}$$

We observe that:

$$T_z = \int_0^\infty e^{-\frac{\pi t^2}{4T_z^2}} \, dt \tag{A2}$$

Consider z > 0, then:

$$\frac{1}{\sqrt{2\pi} L_z} e^{-\frac{(z-z')^2}{2L_z^2}} \xrightarrow[L_z \to 0]{} \delta(z-z') \tag{A3}$$

From (A1) and (A3), there results:

$$\frac{\partial \overline{C}}{\partial t} = \frac{\partial}{\partial z} \int_0^t dt' \int_0^\infty dz' \, \overline{w'^2} \, e^{-\frac{\pi (t-t')^2}{4T_z^2}} \frac{\partial \overline{C}(z,t')}{\partial z} \tag{A4}$$

Applying a Laplace transform (L) to equation (A4) and taking into account that the right side of equation (A4) is a Laplace convolution, it suffices to compute:

$$L \, \overline{w'^2} \, e^{-\frac{\pi t^2}{4T_z^2}} = \overline{w'^2} \int_0^\infty e^{-st} \, e^{-\frac{\pi t^2}{4T_z^2}} dt = \overline{w'^2} T_z \, e^{-\frac{s^2 T_z^2}{\pi}} \left[1 - \Phi\left(\frac{s T_z}{\sqrt{\pi}}\right) \right] \tag{A5}$$

where:

$$\Phi\left(\frac{s T_z}{\sqrt{\pi}}\right) = \frac{2}{\sqrt{\pi}} \int_0^{\frac{sT_z}{\sqrt{\pi}}} e^{-t^2} \, dt \tag{A6}$$

When $T_z \to 0$, $\overline{w'^2} \to \infty$ (white noise case), $\overline{w'^2}\ T_z \to K_z$
and taking into account (A5) and (A6), the non-local equation becomes equation K:

$$\frac{\partial \overline{C}}{\partial t} = \frac{\partial}{\partial z}\left(K_z \frac{\partial \overline{C}}{\partial z} \right) \tag{A7}$$

i.e. equation (3.10). This limit-case corresponds to molecular diffusion or Brownian motion. $\overline{w'^2}$, T_z, L_z, K_z are functions of z. For boundary layer problems, see e.g. Stull (1988) and for white noise problems see e.g. Hida (1980).

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