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NOTE AND CORRESPONDENCE

THE NONLOCAL DIFFUSION EQUATION; A UNIFYING MODEL OF K-THEORY AND STATISTICAL THEORY OF TURBULENT DIFFUSION OF POLLUTANTS

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Abstract: In this paper we show that the nonlocal diffusion equation is a unified form of the two basic theories in turbulent diffusion: K-theory and statistical theory. Here we present a unidimensional form of our previous results.We show that the turbulent diffusion coefficient (from K- theory) and the Lagrangian correlation function (from statistical theory) can be expressed by using the generalized diffusion coefficient. The generalized diffusion coefficient exhibits the characteristic that turbulent diffusion has space-time memory.

K-Theory is based on the analogy with molecular diffusion processes. Consequently, the one dimensional diffusion equation is:

$$\frac{\partial \overline{C}}{\partial t} = K \frac{\partial^2 \overline{C}}{\partial x^2} \tag{1}$$

where: $\overline{\mathrm{C}}$ (x,t) is the ensemble mean concentration of an instantaneously released pollutant (t=0) at x=0; and K is the turbulent diffusion coefficient.

In this case $\overline{\mathrm{C}}$ (x,t) can also be interpreted as the transition probability density P(x,t) for one particle released at t=0 from x=0 (see, e.g. , Romanof, 1988). Equation (1) is based on the hypothesis that the molecules act independently in the diffusion process of one substance.

Unlike in molecular diffusion, the turbulent diffusion is the result of a memory process in which the substance is scattered by eddies of various dimensions correlated in space and time.

The statistical theory describes turbulence diffusion as a stochastic process with memory, in which pollutant dispersion is described by Taylor's formula:

$$\overline{x^2(t)} = \int x^2 P(x,t)dx = 2\overline{u'^2} \int_0^t d\tau \int_0^\tau R^L(\xi)d\xi \tag{2}$$

where x(t) is the coordinate of a particle released at t=0 from x=0, u' is the velocity fluctuation and $R^L(\xi)$ is the Lagrangian correlation function.

Both theories are described e.g. in Pasquill (1974). In this paper we emphasize that both theories, K-theory and statistical theory, can be explained by the nonlocal diffusion equation (see, e.g. Romanof, 1988). Thus, the space-time nonlocal diffusion equation unifies the two theories.

In the one dimensional case the nonlocal diffusion equation is:

$$\frac{\partial \overline{C}}{\partial t}(x,t) = \frac{\partial}{\partial x}\int dx' \int_0^t dt' D(x-x', t-t') \frac{\partial \overline{C}(x', t')}{\partial x'} \tag{3}$$

where D is the generalized diffusion coefficient. This particular form of D as a function of the differences x-x' and t-t' is for the special case of homogeneous and stationary turbulence.

A series of results obtained by using the nonlocal diffusion equation were previously presented (see Romanof 1986, 1987, 1988, 1989, 1994). Other works which use nonlocal diffusion equations are e.g. Berkowicz, 1979, Fiedler, 1984, Stull, 1993.

After applying a Fourier tranform and a Laplace transform to Equation (3) one gets the Taylor's formula (2), (see Romanof ,1988):

$$\overline{x^2}(t) = 2\int_0^t d\tau \int_0^\tau \tilde{D}(0,\xi) d\xi \tag{4}$$

where $\tilde{D}$(k,ξ) denotes the Fourier tranform of D(x,ξ), see Annex A.
From Equations (2) and (4) we get:

$$\tilde{D}(0,\xi) = \overline{u'^2} R^L \tag{5}$$

Equation (5) shows the Lagrangian statistical significance of the generalized diffusion coefficient.

If the spatial scale of turbulence is finite, then at large times (asymtotically, t→∞) it is expected that the values of concentration gradient at points (x', t') and (x,t) are nearly equal, and hence the asymptotic form of equation (3) (see Romanof 1988) is just the classical diffusion equation:

$$\frac{\partial \overline{C}}{\partial t} = K \frac{\partial^2 \overline{C}}{\partial x^2} \tag{6}$$

where the turbulent diffusion coefficient K is given by

$$K = \int dx \int_0^\infty D(x,\tau) d\tau = \overline{u'^2} T^L \tag{7}$$

where T^L is the Lagrangian temporal scale of turbulence:

$$T^L = \int_0^\infty R^L(\xi) d\xi \tag{8}$$

The method of getting equation (6) from equation (3) appears to be valid only for the special limiting case of near-zero gradient and near-zero curvature of C everywhere. But equation (1) is valid for a wide range of C gradients.

There are also other nonlocal equations whose asymptotic behavior is of the type of the K equation (Roberts, 1961; Saffman, 1969; Berkowicz and Prahm, 1979).

There are additional situations for which the asymptotic behavior of turbulent diffusion can be described as a classical diffusion process.

If the dispersion of a pollutant cloud behaves asymptotically as
$\overline{x^2} = 2Kt$ then after maximizing the cross-entropy, one obtains a Gaussian transition probability density which satisfies the K equation with the diffusion coefficient K (Romanof 1986,1988).

Another situation is the asymptotic study of the motion of a particle in a turbulent flow. It can be shown that asymptotically one obtains a classical diffusion process (Romanof 1988).

We also mention the known result on the asymptotic behavior (t→∞) of dispersion (4), x^2(t) = 2Kt, where the diffusion coefficient K is expressed as a space-time integral of the generalized diffusion coefficient (7).

In conclusion, both the turbulent diffusion coefficient K and the Lagrangian correlation function are related to the generalized diffusion coefficient (Equations (5) and (7)).
Both theories of turbulent diffusion, i.e. the K-theory and statistical theory, are related to the nonlocal diffusion equation (3).

The nonlocal equation and the generalized diffusion coefficient reflect that the turbulent diffusion process has space-time memory, whose measure is given by the dependence of the generalized diffusion coefficient D(x-x', t-t') on space and time, see Equation (3).

ANNEX A

Fourier and Laplace Transforms

The Fourier transform of a function f(x) is defined as:

$$Ff(x) = \tilde{f}(k) = \int e^{ikx} f(x)dx \qquad \text{(A1)}$$

If in the equation above f(x) is a probability density, then $\tilde{f}(k)$ is the characteristic function. The inverse relation of (A1) is

$$F^{-1}\tilde{f}(k) = f(x) = \frac{1}{2\pi}\int e^{-ikx}\tilde{f}(k)dk \qquad \text{(A2)}$$

By definition, the Fourier convolution of the given functions f(x) and g(x) is given by:

$$h(x) = \int f(x-x')g(x')dx' \qquad \text{(A3)}$$

It can be shown that (see e.g. Ditkine and Proudnikov, 1978)

$$\tilde{h}(k) = \tilde{f}(k)\tilde{g}(k) \qquad \text{(A4)}$$

We also have:

$$F\frac{df'}{dx} = -ik\tilde{f}(k) \qquad \text{(A5)}$$

The Laplace transform of a function f(t) is defined as:

$$Lf(t) = \tilde{f}(s) = \int_0^\infty e^{-st} f(t)dt \qquad \text{(A6)}$$

By definition, the Laplace convolution of the given functions f(t) and g(t) is given by:

$$h(t) = \int_0^t f(t-t')g(t')dt' \qquad \text{(A7)}$$

The following equation holds:

$$\tilde{h}(s) = \tilde{f}(s)\tilde{g}(s) \qquad \text{(A8)}$$

We also have:

$$L\int_0^t f(\tau)d\tau = \frac{\tilde{f}(s)}{s} \qquad \text{(A9)}$$

and

$$L\frac{df}{dt} = s\tilde{f}(s) - f(0) \qquad \text{(A10)}$$

Consider now the equation (3). We notice that equation (3) can be obtained by Fourier and Laplace convoluting of functions D and $\frac{\partial \overline{C}}{\partial x}$.

According to the above mentioned properties, after performing Fourier and Laplace transform on equation (3) we get

$$s\tilde{\tilde{C}}(k,s) - \tilde{C}_0(k) = -k^2\tilde{\tilde{D}}(k,s)\tilde{\tilde{C}}(k,s) \tag{A11}$$

where

$$\tilde{\tilde{C}}(k,s) = LF\overline{C}(x,t), \tag{A12}$$

$$\tilde{\tilde{D}}(k,s) = LFD(x,t), \tag{A13}$$

and

$$\tilde{C}(k) = F\overline{C}(x,0). \tag{A14}$$

From equation (A11) it follows that:

$$\tilde{\tilde{C}}(k,s) = \frac{\tilde{C}_0(k)}{s + k^2\tilde{\tilde{D}}(k,s)} \tag{A15}$$

After performing the inverse transforms we get

$$\overline{C}(x,t) = L^{-1}F^{-1}\tilde{\tilde{C}}(k,s) \tag{A16}$$

where L^{-1} and F^{-1} are the inverse operators of Laplace and Fourier operators, L and F respectively.

Consider now an instantaneous source. Then we have $\overline{C}(x,t) = P(x,t)$, where $P(x,t)$ is the transition probability density for a particle released at $t = 0$ in $x = 0$. We also have

$$\overline{C}(x,0) = \delta(x) \tag{A17}$$

where δ is the Dirac function.
In this case:

$$\tilde{C}(k,0) = \tilde{C}_0 = 1 \tag{A18}$$

Dispersion is defined by:

$$\overline{x^2}(t) = \int x^2 P(x,t)dx \tag{A19}$$

The characteristic function is:

$$\tilde{P}(k,t) = \int e^{ikx}P(x,t)dx \tag{A20}$$

From equation (A20) it follows:

$$\overline{x^2}(t) = -\frac{\partial^2}{\partial k^2}\tilde{P}(k,t) \quad / k = 0 \tag{A21}$$

By using the initial condition (A17) and equation (A15) we have:

$$\tilde{\tilde{P}}(k,s) = LFP(x,t) = \frac{1}{s + k^2\tilde{\tilde{D}}(k,s)} \tag{A22}$$

Applying the Laplace operator to equation (A21) yields:

$$L\overline{x^2}(t) = -\frac{\partial^2}{\partial k^2}\tilde{\tilde{P}}(k,s) \quad / k = 0 \tag{A23}$$

By taking into account equation (A22) we have:

$$L\overline{x^2}(t) = 2\frac{\tilde{\tilde{D}}(0,s)}{s^2} \tag{A24}$$

By using equation (A9)

$$L\int_0^t f(\tau)d\tau = \frac{\tilde{f}(s)}{s} \tag{A9}$$

and (A24) the Taylor’s formula (equation (4)) follows:

$$\overline{x^2}(t) = 2\int_0^t d\tau\int_0^\tau \tilde{D}(0,\xi)d\xi \tag{A25}$$

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