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On the spectral turbulent diffusivity theory for homogeneous turbulence

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The spectral turbulent diffusivity (STD) theory, originally deduced from a spectral generalization of the gradient-transfer theory (Berkowicz & Prahm 1979), is here derived from a basic concept of turbulent mixing for the case of homogeneous turbulence. The turbulent mixing is treated in a way similar to Prandtl's mixing-length concept. The contribution to the turbulent flux from eddies of different length is represented by a linear superposition. The spatial variation of the concentration distribution is described in terms of Fourier series. This procedure results in the spectral diffusivity formulation, which is Eulerian and scale dependent. If the concentration distribution is approximated by a truncated Taylor expansion instead of an exact representation by the Fourier series, the gradient-transfer approximation is retrieved.

The turbulent energy density, as function of the eddy length, is related to the eddy transport velocity and a probability of the occurrence of the eddies. The eddy transport velocity, derived from the relation between the energy spectrum and the Lagrangian correlation function, is used for computation of the spectral turbulent diffusivity. The turbulent energy spectrum is approximated by the inertial sub-range form ($-\frac{5}{3}$ law). The STD coefficient obtained here has, for large wavenumbers, a slope of $k^{-\frac{4}{3}}$ as predicted previously.

1. Introduction

In spite of more than 50 years' history, the problem of diffusion in a field of turbulent motion still does not have any unique solution. Even in the most simple case of homogeneous and stationary turbulence, the problem is far from a trivial one. Theoretical analyses of the diffusion of material in a turbulent flow have developed along two main lines: the statistical theory and the gradient-transfer (K-theory) approach.

The statistical theory, as formulated by Taylor (1921), is based on the statistical treatment of particle motion in a turbulent flow. It gives answers in terms of the standard deviation of particle displacement. Many of the properties of turbulent diffusion can be resolved by this statistical approach; however, difficulties arise when modelling of turbulent dispersion under more general conditions is attempted.

Studies of transport of atmospheric pollutants often require treatment of non-homogeneous and non-stationary flows. Also emission from several sources and physical and chemical transformations must be accounted for. Such problems are difficult or even impossible to model in terms of Taylor's statistical theory, and description based on an Eulerian model is more suitable.

In recent years, several sophisticated methods for description of turbulent diffusion have been proposed, for example methods based on the so-called higher-order closure approximation (Lewellyn & Teske 1976), direct-interaction approximation (Roberts 1961), random-walk model (Monin & Yaglom 1965) or renormalized perturbation methods (Phythian & Curtis 1978). These theories, however, are not frequently applied in practical studies of diffusion, e.g. in air pollution modelling, possibly because of their high level of complexity. However, one should note the first attempts to formulate a spectral diffusivity equation by Monin (1955, 1956) and later by Schönfeld (1962).

The aim of the present research is to formulate a theory of turbulent diffusion for practical applications in air pollution modelling, a theory which reveals the essential features of turbulent diffusion, but which as far as possible preserves the simplicity and flexibility of the K-theory formulation.

2. K-theory approach

The most widely used Eulerian description of turbulent diffusion is based on K-theory. The transport of pollutant concentration is given by the continuity equation

$$\frac{\partial c}{\partial t} = -\operatorname{div}(\mathbf{v}.c) + \operatorname{div}(\mathbf{K}.\operatorname{grad} c) + S + Q \tag{1}$$

where $\mathbf{v}$ is the vector of the mean flow velocity, $\mathbf{K}$ the eddy diffusivity tensor and S and Q are terms describing sinks and sources, including physical and chemical processes.

The second term on the right-hand side of (1) describes the turbulent diffusion and results from the so-called gradient-transfer approximation. The gradient-transfer approximation is based on the hypothesis of a turbulent flux proportional to the gradient of the concentration. The earliest attempts to use the gradient-transfer approximation for atmospheric diffusion are due to Schmidt (1925) and, since then, numerous studies have been undertaken (for a review, see, for example, Pasquill 1974).

Because of its flexibility, the K-theory approach is widely used for modelling atmospheric dispersion. The use of the K-theory, however, is limited by serious restrictions. The theory is based on the analogy of turbulent diffusion to molecular diffusion (Fick's law); this analogy is, in fact, a very poor one. Molecular diffusion is caused by microscale motion. Turbulent diffusion, on the other hand, is produced by eddies of usually a broad range of sizes. If the size of the turbulent eddies responsible for the diffusion is small compared with the length scale of the diffusing distribution, the K-theory approximation is appropriate. In the case of eddy diffusion in the atmospheric boundary layer, horizontal motions with a length scale of 100 m to 1000 m can dominate the diffusion process and use of the K-theory approach for a narrow distribution is not valid. From the statistical theory, it is known that the size of a plume, defined by the standard deviation of the concentration distribution, increases initially linearly with the time of travel. Taking only the diffusion term of (1) and considering a one-dimensional and homogeneous case, we have

$$\frac{\partial c}{\partial t} = K\frac{\partial^2 c}{\partial y^2}. \tag{2}$$

The solution of (2) for an instantaneous point source of a strength Q at $y = 0$ is the well-known Gaussian distribution

$$C(y,t) = \frac{Q}{(2\pi)^{\frac{1}{2}}\sigma}\exp\left(-\frac{1}{2}\frac{y^2}{\sigma^2}\right) \tag{3}$$

where the standard deviation σ is given by

$$\sigma = (2Kt)^{\frac{1}{2}}. \tag{4}$$

Thus, the use of the K-theory approximation results in a distribution with a standard deviation proportional to the square root of the travel time. This is in contradiction to the linear initial plume growth predicted from the statistical theory. A linear growth of the horizontal dimensions of a narrow plume can be obtained if K is allowed to be a linear function of the time of travel or distance from the source. However, such a diffusivity cannot be treated as a physical parameter of the turbulent flow, because a stationary and homogeneous turbulence must be characterized by time- and space-independent parameters. The time-dependent diffusivity can be used as a modelling tool only for simulation of dispersion in very simplified cases. An attempt to solve the problem of turbulent diffusion was given by Richardson (1926). He introduced the idea of diffusivity depending on separation of particles. The approach proposed by Richardson and valid for diffusion of puffs results in a solution which does not give an unique concentration distribution, and the solution is not coupled to an advection–diffusion equation of the type given by (1).

3. The spectral turbulent diffusivity concept

The main problem arising in the modelling of turbulent diffusion is the proper description of scale dependence of the diffusion process. In two recent papers (Berkowicz & Prahm 1979; Prahm, Berkowicz & Christensen 1979), a new theory has been formulated, the spectral turbulent diffusivity (STD) theory, which makes it possible to apply the diffusivity formulation for turbulent diffusion taking the scale dependence into account, but without losing the Eulerian properties. The theory has been formulated on the basis of a phenomenological understanding of the physics of turbulent diffusion. In this section, a short résumé of the STD theory is given and, in the following section, a new and more direct derivation is presented.

We will here restrict the discussion to a one-dimensional homogeneous diffusion. A direct derivation of the non-homogeneous case needs some further studies, and the work is in progress.

The Fourier transform of (2) is

$$\frac{\partial \tilde{c}(k,t)}{\partial t} = -k^2K\tilde{c}(k,t), \tag{5}$$

where $\tilde{c}(k,t)$ is the amplitude of the Fourier mode with wavenumber k. The scale dependence of the turbulent diffusivity results from the varying size of eddies which are effective in the diffusion process in relationship to changes in the size of the concentration distribution. Only small eddies are effective for diffusion of a narrow distribution, while larger eddies become active when the distribution becomes broader. The scale of the concentration distribution depends on the relative strength of Fourier modes of different wavenumbers. A narrow distribution is characterized by all modes, also those with high wavenumbers, while a broad distribution can be described by Fourier modes only with relatively small k-values. In order to account for the scale dependence of the turbulent diffusivity, we have postulated that the eddy diffusivity K in (5) is different for different Fourier modes of the concentration distribution. We have introduced the spectral turbulent diffusivity coefficient $K(k)$. The equation corresponding to (5) is now

$$\frac{\partial \tilde{c}}{\partial t}(k,t) = -k^2 K(k)\,\tilde{c}(k,t). \tag{6}$$

The STD coefficient $K(k)$ is a physical parameter as it depends only on the state of the turbulent flow. Equation (6) can be converted to real space, resulting in an integro-differential equation

$$\frac{\partial c}{\partial t}(y,t) = \frac{\partial}{\partial y}\int_{-\infty}^{\infty} D(y-y')\,\frac{\partial c}{\partial y'}(y',t)\,dy', \tag{7}$$

where the turbulent diffusivity transfer (TDT) function is given by

$$D(y-y') = \frac{1}{2\pi}\int_{-\infty}^{\infty} K(k)\exp\left(ik(y-y')\right)dk. \tag{8}$$

Equation (17) is derived for the case of homogeneous turbulence. For the non-homogeneous case, the TDT function is not only a function of the difference of space co-ordinates, but also dependent on the position in space (Berkowicz & Prahm 1979). In contradiction to the gradient-transfer formulation as given by (2), (7) describes a process which is non-local in space. This is a characteristic property of turbulent transport caused by the finite size of the turbulent eddies. When the STD coefficients or the TDT function is specified, (6) or (7) is easy to apply in numerical modelling.

The gradient-transfer formulation, as given by (2), appears as a special case of the more general formulation given by (7), because, when $K(k) = \text{const.}$, (7) converts to (2).

On the basis of empirical considerations, Richardson (1926) proposed that the relative diffusivity coefficient introduced by him depends on the particle separation l as $l^{4/3}$. Because the characteristic length scale in the formulation by Richardson is the particle separation, and the characteristic length scale in the STD theory is the wavelength of the concentration Fourier modes, we postulate by analogy that $K(k) \sim k^{-4/3}$ for large values of k. For small wavenumbers, however, the STD coefficients should converge towards a constant value, say K_0. The following form of $K(k)$ is therefore proposed (Berkowicz & Prahm 1979)

$$K(k) = \frac{K_0}{1+Bk^{4/3}}, \tag{9}$$

where B is a parameter to be estimated. Because the scale of the turbulence depends on the size of the long, most energetic eddies, it is reasonable to assume that $B \propto k_m^{-4/3}$,

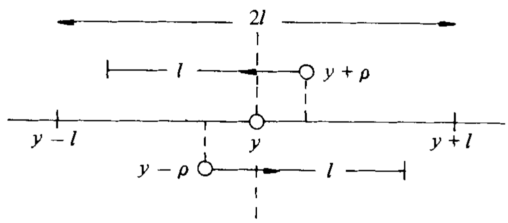

FIGURE 1. Diagram illustrating the contribution of eddies of length l to the eddy flux at point y. Eddies starting from points $y+\rho$ and $y-\rho$ are shown. Only eddies originating in the region $(y-l, y+l)$ contribute.

where k_m is the wavenumber corresponding to the largest turbulent eddies. As pointed out (Berkowicz & Prahm 1979), the form given by (9) has been proposed as a working hypothesis. In the next chapter, we present a more direct derivation of $K(k)$, and it appears that (9) is quite a good estimate.

The application of the STD theory for plume dispersion was treated by Prahm *et al.* (1979). In order to model a time-averaged concentration in a plume, one has to take into account the 'meandering' of the plume owing to action of eddies larger than the size of the plume. Such an effect can be ascribed to phase fluctuation of Fourier modes of the transversal cross-section of the plume. In order to describe these turbulent fluctuations, we have introduced a spectral phase diffusivity coefficient. For detailed discussion of the plume model, the reader is referred to the original paper. Discussion of the geometry and rate of growth predicted by the STD theory is also given there. The rate of growth is in accordance with the main findings of the statistical theory, but the shape of a narrow distribution appears in general to be non-Gaussian.

4. Derivation of the spectral turbulent diffusivity

In this section, we present a direct derivation of the spectral turbulent diffusivity formulation. The procedure presented here is, to some extent, similar to that applied by Prandtl (1925) when he formulated his famous 'mixing length' concept. Further development of his procedure, avoiding some essential simplifications, leads directly to the concept of the spectral turbulent diffusivity.

We start again with considering a turbulent mixing of a one-dimensional distribution in a field of homogeneous and stationary turbulence. An eddy of a length l is able to transport material (or another property, e.g. momentum) at a distance equivalent to or less than its length. The turbulent mixing is a stochastic process and one can consider this as a linear superposition of the transport caused by eddies of all lengths. Let the probability density of occurrence of an eddy of length l be $F(l)$.

We consider the contribution of eddies of a given length l to the turbulent flux at a point y. Only those eddies which are situated in the region $(y-l, y+l)$ can thus contribute to the flux at y (figure 1). Those of the eddies originating at an infinitesimal interval $d\rho$ inside the region, appear with the weight $F(l)\,d\rho/l$. We denote the characteristic velocity of the eddy by $v(l)$. The flux at y caused by eddies with starting points at $y+\rho$ and $y-\rho$ can now be expressed as

$$-v(l)\,c(y+\rho)\,F(l)\,d\rho/l + v(l)\,c(y-\rho)\,F(l)\,d\rho/l. \tag{10}$$

In order to find the total flux at y, we integrate with respect to ρ (from 0 to l), and next integrate over all values of l. The flux at y can now be written as

$$f(y) = \int_0^\infty \left(\int_0^l \frac{v(l)\,F(l)}{l} \{c(y-\rho) - c(y+\rho)\}\,d\rho \right) dl. \tag{11}$$

From the continuity equation, we have

$$\frac{\partial c}{\partial t} = -\frac{\partial}{\partial y} f(y) \tag{12}$$

and, after differentiation with respect to y and integration with respect to ρ, we obtain

$$\frac{\partial c}{\partial t} = \int_0^\infty \frac{v(l)\,F(l)}{l} \{c(y+l) - c(y) + c(y-l) - c(y)\}\,dl. \tag{13}$$

Equation (13) is an integro-differential equation and thus non-local in space; however, it is still local in time. It is obvious that this is a simplification which is justified when the eddy transport is so fast that one may neglect the concentration variation in time, during a one-eddy 'passage'. Time delay for transport through the single eddies can be accounted for in (10) by substituting $c(y+\rho, t-\rho/v(l))$ and $c(y-\rho, t-\rho/v(l))$ for $c(y+\rho)$ and $c(y-\rho)$, respectively. This would result in a diffusion equation which is non-local in time. Introduction of the time non-locality is not complicated from a mathematical point of view, but gives serious difficulties in numerical modelling. In the following, we will neglect the time non-locality because the averaging times used in many practical studies of turbulent diffusion are longer than an eddy transport time, and it appears that introduction of the space non-locality alone explains many features of the turbulent diffusion.

We will proceed further with discussion of (13). The space differences of the concentration distribution appearing in (13) can be evaluated by expanding the concentrations in Taylor series

$$\left.\begin{aligned} c(y+l) &= c(y) + l\frac{\partial c}{\partial y} + \tfrac{1}{2}l^2\frac{\partial^2 c}{\partial y^2} + \dots, \\ c(y-l) &= c(y) - l\frac{\partial c}{\partial y} + \tfrac{1}{2}l^2\frac{\partial^2 c}{\partial y^2} + \dots. \end{aligned}\right\} \tag{14}$$

If the concentration distribution is relatively smooth, we may restrict the expansion to second-order terms with respect to l. With this approximation, (13) becomes

$$\frac{\partial c}{\partial t} = \left[\int_0^\infty v(l)\,lF(l)\,dl\right]\frac{\partial^2 c}{\partial y^2}. \tag{15}$$

One can immediately see that (15) is identical with (2) if

$$K = \int_0^\infty v(l)\,lF(l)\,dl. \tag{16}$$

Thus a second-order approximation of the concentration distribution leads to the gradient-transfer formulation with the diffusivity given by (16). This approximation, however, is not valid when the distribution changes strongly on the length scale for which the turbulence is still significant. In order to evaluate (13) exactly, we apply now a Fourier series expansion to the concentration distribution in (13):

$$c(y) = \int_{-\infty}^{\infty} \tilde{c}(k) \exp(iky)\, dk. \tag{17}$$

The Fourier transform of (13) is

$$\frac{\partial \tilde{c}(k)}{\partial t} = -k^2 \left[\int_0^{\infty} v(l)\, lF(l) \frac{\sin^2 \frac{1}{2}kl}{(\frac{1}{2}kl)^2}\, dl \right] \tilde{c}(k). \tag{18}$$

One can see that (18) is now identical with (6) if

$$K(k) = \int_0^{\infty} v(l)\, lF(l) \left(\frac{\sin \frac{1}{2}kl}{\frac{1}{2}kl} \right)^2 dl. \tag{19}$$

Comparing (19) with (16), we can see that the STD coefficient results from application of a low-pass filter to the integral expression in (16). Only eddies of a size $l < 2\pi/k$ contribute significantly to mixing of a Fourier mode with a wavenumber k.

The derivation of the STD theory presented here is based on Prandtl's concept of 'mixing length', but where Prandtl uses an approximation for the concentration variation in space by a truncated Taylor expansion, we use an exact evaluation by means of infinite Fourier series.

5. Eddy energy density and transport velocity

The main idea of the STD theory appears from (18) and (19). The turbulent diffusion can be modelled by an Eulerian diffusion equation with a k-dependent diffusivity $K(k)$. In order to determine $K(k)$, both $F(l)$ and $v(l)$ have to be specified. However, neither $F(l)$, the probability of occurrence of eddies of length l, nor $v(l)$, the effective transport velocity associated with eddies of length l, can be measured or determined directly. Therefore, we have to find a way in which these quantities can be related to other available quantities.

(*a*) *The eddy energy density*

The contributions of eddies of length l, $l+dl$ to the total variance σ_v^2 of velocity fluctuations can, by means of $v(l)$ and $F(l)$, be expressed as

$$\Delta_l(\sigma_v^2) = \tfrac{1}{2}v^2(l)\, F(l)\, dl, \tag{20}$$

where

$$\tfrac{1}{2}v^2(l)\, F(l) = \epsilon(l) \tag{21}$$

is the energy density of eddies of length l. On the other hand, we can express the contribution to σ_v^2 of turbulent fluctuations by means of the energy spectrum $E_v(\kappa)$, where κ is the wavenumber,

$$\Delta_\kappa(\sigma_v^2) = E_v(\kappa)\, d\kappa. \tag{22}$$

An eddy of the length l is related to a spectral component with a wavenumber $\kappa = \pi/l$ because the period of velocity fluctuations in such an eddy must be $2l$. With this and relations (20) and (22) in mind, we obtain

$$\tfrac{1}{2}v^2(l)\, F(l) = \frac{\pi}{l^2} E_v(\pi/l). \tag{23}$$

We have now established the relation between $v^2(l)\,F(l)$ and the energy spectrum $E_v(\pi/l)$. In the expression (19) for the spectral turbulent diffusivity, the product $v(l)\,F(l)$, however, appears. We have thus to find a way to determine the eddy transport velocity $v(l)$.

(b) *The eddy transport velocity*

Comparing (19) with (16), we see that the spectral diffusivity $K(k)$ converges to the constant value K for $k \to 0$. This is the diffusivity that characterizes dispersion of a concentration distribution after a long time of diffusion. For the long time limit, we can use the expression for diffusivity obtained from Taylor's statistical theory (Taylor 1921; Batchelor & Townsend 1956),

$$K = \int_0^\infty R_L(t)\,dt = \sigma_v^2 \tau_L, \tag{24}$$

where $R_L(t)$ is the Lagrangian correlation function and τ_L is the integral time scale.

In (16), the diffusivity K is expressed in form of contribution from eddies of all lengths. In (20), the contribution of eddies of length l to the variance σ_v^2 is given. This suggests that also $R_L(t)$ can be expressed in form of contribution from all eddies. Comparing (24) with (16), we can put forward the following relation†

$$R_L(t) = \int_0^\infty \tfrac{1}{2} v^2(l)\,F(l)\,\eta(l,t)\,dl, \tag{25}$$

where $\eta(l,t)$ is the correlation coefficient associated with an eddy of the length l and which has the integral time scale equal to $2l/v(l)$, i.e.

$$\int_0^\infty \eta(l,t)\,dt = 2l/v(l). \tag{26}$$

In § 4, we have assumed that the transport in an eddy of length l takes place with a constant velocity $v(l)$ for the distance l. As the transport is equally probable in both directions, i.e. for the distance $2l$, it means that there is a perfect correlation for a time $2l/v(l)$. This suggests the following form for $\eta(l,t)$:

$$\eta(l,t) = \begin{cases} 1 & \text{for} \quad t \leqslant 2l/v(l), \\ 0 & \text{for} \quad t > 2l/v(l). \end{cases} \tag{27}$$

Substituting (27) into (25), we obtain

$$R_L(t) = \int_l^\infty \tfrac{1}{2} v^2(l')\,F(l')\,dl' = \sigma_v^2 - \int_0^l \epsilon(l')\,dl', \tag{28}$$

where

$$t = 2l/v(l). \tag{29}$$

If $R_L(l)$ and the energy of the eddies $\epsilon(l)$ are known, we can by means of (28) and (29) determine $v(l)$.

† This relation was drawn to our attention by Dr M. W. Reeks, resulting in significant improvement in the paper.

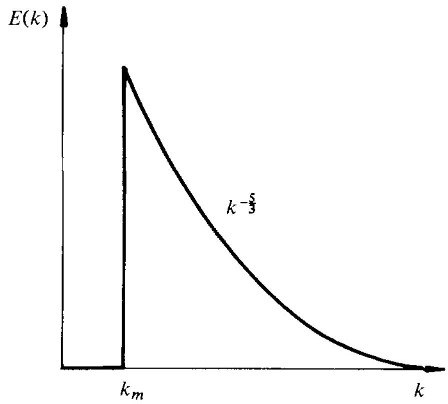

FIGURE 2. Schematic representation of the energy spectrum $E(\kappa)$. The inertial sub-range form ($\kappa^{-\frac{5}{3}}$) is extended from k_m to infinity; k_m is the wavenumber at which the turbulent energy is produced. No energy is assumed to be transferred to wavenumbers smaller than k_m.

(c) *The inertial sub-range relations*

We adapt a simple form of the energy spectrum and the correlation function. It is known that in the inertial sub-range the energy spectrum is proportional to $\kappa^{-\frac{5}{3}}$. We have decided to extend the $\kappa^{-\frac{5}{3}}$ dependence to the whole spectrum. The energy spectrum applied here is shown schematically in figure 2. We assume that the turbulent energy is supplied at a wavenumber $k_m = \pi/l_m$, where l_m is the length of the longest eddies, and the energy is transferred toward the shorter eddies according to the $\kappa^{-\frac{5}{3}}$ law, but no energy is transferred to eddies longer than l_m. From (23) we thus obtain

$$\epsilon(l) = \begin{cases} \frac{2}{3}\sigma_v^2 l_m^{-\frac{2}{3}} l^{-\frac{1}{3}} & \text{for} \quad l \leqslant l_m, \\ 0 & \text{for} \quad l > l_m. \end{cases} \tag{30}$$

The inertial sub-range is in fact not valid for very small eddies. In this range, the so-called dissipation range, the transfer of the turbulent energy to heat becomes the dominating process and $E(\kappa)$ is known to decrease faster than κ^{-2} (Hinze 1975). The molecular diffusion dominates here, and in practical studies of atmospheric diffusion such small scales are usually of no importance.

A finite lower limit of the eddy sizes in fact exists as a result of action of the viscous forces on the eddy motion. Because this size is much smaller than l_m, we can usually assume it to be zero. However, further on in this section, we make use of this finite lower limit when the dissipation rate is evaluated.

Substituting (30) into (28), we obtain

$$R_L(2l/v(l)) = \begin{cases} \sigma_v^2[1-(l/l_m)^{\frac{2}{3}}] & \text{for} \quad l \leqslant l_m, \\ 0 & \text{for} \quad l > l_m. \end{cases} \tag{31}$$

We have decided to use here a linear form for $R_L(t)$, namely

$$R_L(t) = \begin{cases} \sigma_v^2\left(1-\frac{1}{2}t\frac{v_m}{l_m}\right) & \text{for} \quad t \leqslant 2\frac{l_m}{v_m}, \\ 0 & \text{for} \quad t > \frac{l_m}{v_m}, \end{cases} \tag{32}$$

where v_m is the velocity associated with eddies of length l_m. The integral time scale of $R_L(t)$ given by (32) is

$$\tau_L = \frac{1}{\sigma_v^2}\int_0^\infty R_L(t) = l_m/v_m. \tag{33}$$

From (31) and (32), we obtain

$$v(l) = v_m(l/l_m)^{\frac{1}{3}}. \tag{34}$$

Equation (34) establishes the relation between $v(l)$ and l which we have been looking for. A relation similar to (34) has been reported early by Inoue (1950). He introduced the concept of turbulons as being elements of the turbulent motion and in fact equivalent to what is usually understood by eddies. The turbulons are characterized by a length scale l and a velocity associated with them $v(l)$. Inoue makes the assumption that the lifetime of the turbulons is proportional to $l/v(l)$. After this time, the turbulons lose all the energy, which is transferred to smaller turbulons. Inoue furthermore assumes that the energy dissipation rate ε is constant for all the turbulons. As the energy of a turbulon is proportional to $v^2(l)$, he obtains

$$\varepsilon \sim v^2(l)/(l/v(l)) = v^3(l)/l = \text{const.} \tag{35}$$

Inoue (1950) shows furthermore that, assuming a perfect correlation for turbulons for a period of time equal to the lifetime and with $v(l)$ given by (35), a linear Lagrangian correlation function is obtained.

A simple interpretation can be given of the idea of the constant dissipation rate. In the inertial sub-range neither production nor energy loss takes place within the total range of eddies. The energy is only transported from large to small eddies through a cascade process. Assuming that only interaction between eddies of neighbouring size can occur, we can conclude that the dissipation rate is constant for eddies (turbulons) of different size inside the inertial sub-range.

(*d*) *The relation between v_m and σ_v*

The idea of relating $v(l)$ to the rate of dissipation can be used in order to establish a relation between v_m, the maximum eddy transport velocity, and σ_v. It is known that the dissipation rate can be expressed as (Hinze 1975)

$$\varepsilon = 2\nu \int_{k_m}^{k_d} \kappa^2 E(\kappa)\, d\kappa, \tag{36}$$

where ν is the kinematic viscosity, and k_d is introduced as the upper limit of the wave-numbers of the energy spectrum. This is equivalent to the assumption that above k_d a total dissipation of the turbulent energy takes place due to the viscous forces. With the $\kappa^{-\frac{5}{3}}$ law for the energy spectrum in the range from k_m to k_d, we obtain

$$\varepsilon \simeq \nu\sigma_v^2 k_m^{\frac{2}{3}} k_d^{\frac{4}{3}}. \tag{37}$$

In evaluation of the integral in (36), we have made use of the fact that $k_d \gg k_m$. Following the concept of Inoue (1950), we can also write

$$\varepsilon = \frac{1}{4}\frac{v_m^3}{l_m} = (4\pi)^{-1} v_m^3 k_m. \tag{38}$$

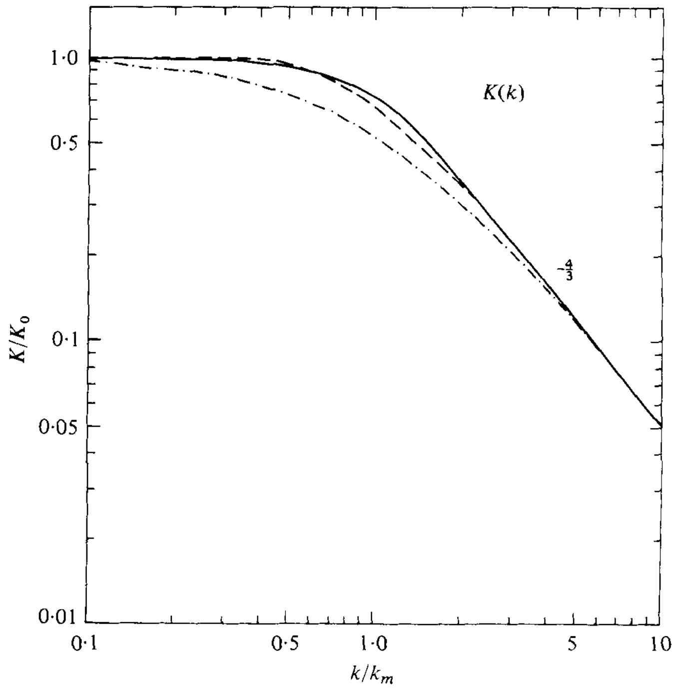

FIGURE 3. The spectral turbulent diffusivity $K(k)$ estimated from (44). Note that $K(k)$ decreases like $k^{-\frac{4}{3}}$ for large k values. The expression given by (9) is plotted with $B = 0{\cdot}87k_m^{-\frac{4}{3}}$. $K(k)$ is shown to be well approximated by the simple exponential expression (48), also with $B = 0{\cdot}87k_m^{-\frac{4}{3}}$. ——, equation (44); –·–·–, equation (9); ––––, equation (48).

In (38), we have put the energy of the eddies equal to $\frac{1}{2}v^2$ and the lifetime to $2l/v$, in accordance with our previous assumptions.

The kinematic viscosity is governed by motions of the scale $l_d = \pi/k_d$ with velocities $v(l_d) = v_d$. From dimensional reasoning, we can get

$$\nu = v_d l_d = \pi v_d/k_d. \tag{39}$$

On the other hand, according to Inoue, we have

$$\epsilon = \frac{1}{4}\frac{v_d^3}{l_d} = \frac{1}{4\pi} v_d^3 k_d. \tag{40}$$

From (37), (39) and (40), we obtain

$$\epsilon = 2\pi^2\sigma_v^3 k_m. \tag{41}$$

The relationship (41) can be put forward from dimensional arguments (Pasquill 1974) and there exists some experimental evidence confirming this relationship for the vertical component of wind velocity fluctuations (Hanna 1968). The numerical constant reported in the literature is quite different from that in (41), but k_m^{-1} refers here to a length scale appropriate to the turbulent fluctuations under consideration, while the length scales reported in the literature are estimated from time-series energy spectra by means of Taylor's hypothesis (Pasquill 1974) thus yielding in fact the longitudinal (along the main wind direction) scale.

Comparing (41) with (38), we obtain

$$v_m = 2\pi\sigma_v. \tag{42}$$

This relationship has already been postulated by Prahm *et al.* (1979) and compares very well with the experimental observations by Markee (1963) if v_m is interpreted as the maximum velocity fluctuation. However, the relationship between v_m and σ_v given by (42) depends on the rather crude estimation of the kinematic viscosity given by (39). Therefore (42) should be considered with caution.

(*e*) *The STD coefficient*

The spectral turbulent diffusivity can now be computed:

$$K(k) = \int_0^\infty \frac{2\epsilon(l)\,l}{v(l)} \left(\frac{\sin\frac{1}{2}kl}{\frac{1}{2}kl}\right)^2 dl. \tag{43}$$

We recall (23) where $\epsilon(l) = (\pi/l^2)\,E(k)$. By using the expression (34) for $v(l)$, (30) for $\epsilon(l)$ and (42) for v_m, we obtain

$$K(k) = \frac{2}{3\pi}\,\sigma_v\, l_m^{-\frac{1}{3}} \int_0^{l_m} l^{\frac{1}{3}} \left(\frac{\sin\frac{1}{2}kl}{\frac{1}{2}kl}\right)^2 dl. \tag{44}$$

The special turbulent diffusivity, $K(k)$, from (44), is plotted in figure 3.

(*f*) *Turbulent diffusivity transfer function*

The turbulent diffusivity transfer function can be computed by substituting in (8) for $K(k)$ from (44). From the identity

$$\int_0^\infty \left(\frac{\sin\frac{1}{2}kl}{\frac{1}{2}kl}\right)^2 \cos(ks)\,dk = \begin{cases} \dfrac{\pi}{l}\left(1 - \dfrac{|s|}{l}\right) & \text{for} \quad |s| \leqslant l, \\ 0 & \text{for} \quad |s| > l, \end{cases} \tag{45}$$

we obtain

$$D(s) = \frac{2}{3\pi}\,\sigma_v\, l_m^{-\frac{1}{3}} \int_{|s|}^{l_m} l^{-\frac{2}{3}} \left(1 - \frac{|s|}{l}\right) dl = \begin{cases} \dfrac{2}{\pi}\,\sigma_v \left[1 + \dfrac{1}{2}\dfrac{|s|}{l_m} - \dfrac{3}{2}\left(\dfrac{|s|}{l_m}\right)^{\frac{1}{3}}\right] & \text{for} \quad |s| \leqslant l_m, \\ 0 & \text{for} \quad |s| > l_m, \end{cases}$$

where $s = y - y'$.

It is interesting to note here that the turbulent diffusivity transfer function is zero for $|y-y'| \geqslant l_m$. This is the consequence of the fact that the turbulent energy has a sharp cut-off for eddies of the length l_m.

6. Discussion

The spectral diffusivity coefficient given by (44) is based on the assumptions we have made about the energy spectrum and the relation between the Lagrangian correlation function and correlation coefficient for separate eddies. Some conclusions about the behaviour of $K(k)$ can be drawn from (44).

(a) The small wavenumber limit of K(k)

For $k = 0$, we have

$$K(0) = K_0 = \frac{1}{2\pi}\sigma_v l_m. \tag{46}$$

This result could also have been obtained already from (24) with the Lagrangian correlation function given by (32) and relation (42) for v_m. As pointed out by Prahm *et al.* (1979), the expression (45) for K_0 is in good agreement with the semi-empirical formula for the vertical diffusivity reported by Smith (1977); K_0 is the diffusivity which describes diffusion in the case of a concentration distribution with the characteristic length scale much longer than the scale of turbulence (l_m). Such conditions are usually satisfied in the case of the vertical diffusion from ground sources. Therefore, the interpretation of the vertical diffusion results, in terms of the gradient-transfer theory, as done by Hanna (1968) and Smith (1977), can be used for estimation of the diffusivity K_0.

(b) The large wavenumber limit of K(k)

Within the limit of $k \gg k_m$, we may replace in (44) the term $([\sin \frac{1}{2}kl]/\frac{1}{2}kl)^2$ by a low-pass box filter of width approximately equal to $2\pi/k$, and as a consequence obtain

$$K(k \gg k_m) \sim (k/k_m)^{-\frac{4}{3}}. \tag{47}$$

For $k \gg k_m$, we thus obtain again the $k^{-\frac{4}{3}}$ shape which was previously postulated by Berkowicz & Prahm (1979) on the basis of mainly dimensional arguments. In figure 3, $K(k)$ is plotted according to the simple formula (9) with the coefficient $B = 0{\cdot}87k_m^{-\frac{4}{3}}$. The agreement with the curve corresponding to (44) is very good for $k > 3k_m$. The somewhat larger disagreement for smaller wavenumbers is, however, not important because the product $k^2K(k)$ appears in the diffusion expressions, making the deviation less significant. In practical applications, the simple formula given in (9) could thus be used. Several simple analytical expressions can approximate (44) very well. An example is

$$K(k) = K_0[1-\exp(-B^{-1}(k_m/k)^{\frac{4}{3}})]. \tag{48}$$

The curve corresponding to (48) is also shown in figure 3.

(c) Relation to the Lagrangian correlation function

The expression for $K(k)$ given by (44) is obtained using the specific form for the Lagrangian correlation function and the energy spectrum. For more general cases, (43) can be used, with $v(l)$ computed by means of (28) and (29). The value of K_0 is determined by the integral time scale of the Lagrangian correlation function. The shape of $K(k)$ for $k \gg k_m$ depends, however, on the shape of $R_L(t)$ for $t \to 0$ and the shape of the energy spectrum in the inertial sub-range. With the $\kappa^{-\frac{5}{3}}$ law for the energy spectrum, any Lagrangian correlation function with a linear shape at $t \to 0$ will result in the $k^{-\frac{4}{3}}$ behaviour of $K(k)$ for $k \gg k_m$. A direct relation between the Lagrangian correlation function and the spectral turbulent diffusivity can be given using (28) and (29) to determine $\epsilon(l)$.

$$K(k) = \int_0^{\tau_m} R_L(\tau)\frac{d}{d\tau}\left[\tau\frac{\sin^2\frac{1}{4}kv\tau}{(\frac{1}{4}kv\tau)^2}\right]d\tau, \tag{49}$$

where

$$\tau_m = 2l_m/v_m$$

and v is expressed as a function of τ according to (29).

Equation (49) can be compared with the expression for the time-dependent diffusivity which is used in Lagrangian diffusion models

$$K(t) = \int_0^t R_L(\tau)\,d\tau. \tag{50}$$

By comparing (49) and (50), it can be seen that the k-dependent diffusivity corresponds to the use of a correlation function modified by a k-dependent filter. In the expression (50) for the time-dependent diffusivity, the upper limit of the time integral determines the diffusivity.

(d) Heisenberg's spectral eddy viscosity

The idea of a spectral diffusivity is known in theories of the turbulent energy transport. According to the hypothesis of Heisenberg (1948), the amount of energy, $W(k)$, transferred per unit time from disturbances with wavenumber smaller than k to the other disturbances (called the spectral energy-transfer function) can be expressed as

$$W(k) = 2\nu(k)\int_0^k \kappa^2 E(\kappa)\,d\kappa, \tag{51}$$

where $\nu(k)$ is the spectral eddy viscosity which plays a role similar to the eddy diffusivity in turbulent transport of a passive contaminant. Heisenberg assumed that the contribution to the eddy viscosity due to the velocity disturbances with a wavelength $l = 2\pi/\kappa$ is proportional to the product of the corresponding 'mixing length', $l_\kappa \propto 1/\kappa$, and the characteristic 'velocity scale' v_κ of the disturbances. Using this idea together with dimensional considerations, Heisenberg postulates the following formula:

$$\nu(k) = \gamma_H \int_k^\infty (E(\kappa)\,\kappa^{-3})^{\frac{1}{2}}\,d\kappa,$$

where γ_H is a dimensionless constant. It can easily be shown that, in the inertial subrange, where $E(\kappa) \propto \kappa^{-\frac{5}{3}}$, $\nu(k)$ behaves as $k^{-\frac{4}{3}}$, i.e. like the spectral turbulent diffusivity.

7. Applications of the STD theory

The STD theory was developed to model puff and plume dispersion in homogeneous turbulence (Berkowicz & Prahm 1979; Prahm *et al.* 1979). The results are in agreement with predictions of the statistical theory but, in general, the STD theory gives non-Gaussian distributions. This is an interesting feature which should be investigated experimentally.

A preliminary study seems to indicate a non-Gaussian shape (Prahm & Berkowicz 1979), but a final experimental proof still remains to be demonstrated. Such studies are difficult because of the non-stationarity and non-homogeneity of the real atmosphere. These problems might be overcome in laboratory studies which are now initiated. The theoretical interpretation of experimental data should preferably be performed in terms of Fourier analysis as previously discussed (Prahm *et al.* 1979, § 9).

Presently, the theory is being applied to model transport of pollutants on a global scale in a two-dimensional meridional troposphere–stratosphere model (Berkowicz, Prahm & Louis 1979). Use of a proper, scale-dependent diffusivity is here of importance. The scale of eddies ranges from a hundred to several thousand kilometres and application of a conventional K-theory is, in this case, very doubtful. The STD theory was in the latter study adapted for non-homogeneous turbulence, but in a somewhat primitive way. A more detailed presentation of the non-homogeneous case is in preparation.

The STD theory is especially easy to apply in modelling turbulent transport when a numerical technique based on the so-called pseudospectral method is used to evaluate the space derivatives occurring in the transport equation. The pseudo-spectral technique has been applied with success for modelling of transport of air pollution (Christensen & Prahm 1976; Prahm & Christensen 1977; Berkowicz & Prahm 1978).

8. Résumé and conclusions

The spectral turbulent diffusivity theory is derived on a simple mixing-length concept using Fourier expansion of the concentration distribution. It is shown that the k dependence of the diffusivity results from the hypothesis that the turbulent mixing is caused by the effect of a linear superposition of transport by eddies of different length. The gradient-transfer approximation appears as a special case of the spectral turbulent diffusivity theory when the size of the turbulent eddies is small compared with the size of the diffusing distribution. The shape of the spectral turbulent diffusivity is computed using a simplified form of the turbulent energy spectrum, namely $\kappa^{-\frac{5}{3}}$ dependence for the whole spectrum above k_m, where k_m is the wavenumber at which the turbulence is produced. A sharp cut-off of the energy spectrum is assumed for wavenumbers below k_m. The spectral turbulent diffusivity exhibits, for large k, a slope of $k^{-\frac{4}{3}}$ in accordance with predictions from previous studies. The theoretical value of $K_0 = K(0)$ is also found to agree with empirical results and previous theoretical estimates. It is shown that the turbulent diffusivity transfer function, (7), is zero for $|y-y'| \geqslant l_m$, a consequence of the assumption that the maximum size of eddies is l_m.

The spectral turbulent diffusivity theory should be used in cases where it is important to account for the scale dependence of the diffusivity and a simple and practical Eulerian model is required.

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REFERENCES

Batchelor, G. K. & Townsend, A. A. 1956 Turbulent diffusion. *Surveys in Mechanics* (ed. G. K. Batchelor & R. M. Davies), pp. 352–399. Cambridge University Press.

Berkowicz, R. & Prahm, L. P. 1978 Pseudospectral simulation of dry deposition from a point source. *Atmos. Environ.* **12**, 379–387.

Berkowicz, R. & Prahm, L. P. 1979 Generalization of K-theory for turbulent diffusion. Part I. Spectral turbulent diffusivity concept. *J. Appl. Met.* **18**, 266–272.

Berkowicz, R., Prahm, L. P. & Louis, J.-F. 1979 Global 2-D spectral dispersion model. *Proc. WMO Symp. on the long-range transport of pollutants and its relation to general circulation including stratospheric–tropospheric exchange processes, Sofia. WMO Rep.* no. 538.

CHRISTENSEN, O. & PRAHM, L. P. 1976 A pseudospectral model for dispersion of atmospheric pollutants. *J. Appl. Met.* **15**, 1284–1294.

HANNA, S. R. 1968 A method of estimating vertical eddy transport in the planetary boundary layer using characteristics of the vertical velocity spectrum. *J. Atmos. Sci.* **25**, 1026–1032.

HEISENBERG, W. 1948 Zur statistischen Theorie der Turbulenz. *Z. Phys.* **124**, 628–657.

HINZE, J. O. 1975 *Turbulence.* 2nd edn. McGraw-Hill.

INOUE, E. 1950 On the turbulent diffusion in the atmosphere (I). *J. Met. Soc. Japan* **28**, 444–455.

LEWELLYN, W. S. & TESKE, M. E. 1976 Second-order closure modelling of diffusion in the atmospheric boundary layer. *Boundary-Layer Met.* **10**, 69–90.

MARKEE, E. H. 1963 On the relationships of range to standard deviation of wind fluctuations. *Mon. Weath. Rev.* **91**, 83–87.

MONIN, A. S. 1955 Equation of turbulent diffusion. *Dokl. Akad. Nauk S.S.S.R.* **105**, 256–259.

MONIN, A. S. 1956 Horizontal mixing in the atmosphere. *Izv. Akad. Nauk S.S.S.R., Ser. Geofiz.* **3**, 327–345.

MONIN, A. S. & YAGLOM, A. M. 1965 *Statistical Fluid Mechanics, Mechanics of Turbulence. Part I.* Washington: Trans-Joint Publication Research Service.

PASQUILL, F. 1974 *Atmospheric Diffusion.* 2nd edn Chichester: Ellis Norwood. Wiley.

PHYTHIAN, R. & CURTIS, W. D. 1978 The effective long-time diffusivity for a passive scalar in a Gaussian model fluid flow. *J. Fluid Mech.* **89**, 241–250.

PRAHM, L. P., BERKOWICZ, R. & CHRISTENSEN, O. 1979 Generalization of K-theory for turbulent diffusion. Part II. Spectral diffusivity model for plume dispersion. *J. Appl. Met.* **18**, 273–282.

PRAHM, L. P. & CHRISTENSEN, O. 1977 Long-range transmission of pollutants simulated by the 2-D pseudospectral dispersion model. *J. Appl. Met.* **16**, 896–910.

PRANDTL, L. 1925 Bericht über Untersuchungen zur ausgebildeten Turbulenz. *Z. angew. Math. Mech.* **5**, 136–139.

RICHARDSON, L. F. 1926 Atmospheric diffusion shown on a distance-neighbour graph. *Proc. Roy. Soc.* A **110**, 709–737.

ROBERTS, P. M. 1961 Analytical theory of turbulent diffusion. *J. Fluid Mech.* **11**, 257–283.

SCHMIDT, W. 1925 Der Massenhaustausch in freier Luft und Verwandte Erscheinungen. In *Probleme der Kosmischen Physic.* Hamburg: Von Henri Grand.

SCHÖNFELD, J. C. 1962 Integral diffusivity. *J. Geophys. Res.* **67**, 3187–3199.

SMITH, F. B. 1977 Application from field programmes to estimation of K-profiles and vertical dispersion. *British Met. O.* **14**, *Turbulence and Diffusion Note* no. 86 (unpublished).

TAYLOR, G. I. 1921 Diffusion by continuous movements. *Proc. London Math. Soc. Ser.* 2, **20**, 196–211.