Note on Spectral Diffusivity Theory

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ABSTRACT

The diffusion equation with a wavenumber-dependent diffusivity is derived as an approximation to the statistical theory of plume dispersion from a continuous point source. The travel time explicitly appearing in the statistical theory is implicitly included in the wavenumber-dependent diffusivity $K(k)$. By suitable choice of this function it is possible within a few percent to reproduce the centerline concentration. Due to the approximate nature of the method, however, it yields a non-Gaussian concentration shape close to the source.

Results for the case of a crosswind extended source are compared to other commonly used methods for this problem. Some considerations are presented on the proper choice of averaging time for the concentration field.

1. Introduction

In two recent papers (Berkowitz and Prahm, 1979; Prahm et al., 1979) a spectral diffusivity theory was presented. In these papers this theory is proposed for the description of dispersion of instantaneous puffs and of time-averaged plumes, and appropriate expressions for the diffusivity for each Fourier mode of the concentration distribution is proposed on the basis of a heuristic picture of turbulent dispersion. In a commentary note (Troen et al., 1980) we have pointed out certain inherent difficulties in the approach chosen by Prahm et al. (1979). A more satisfactory treatment was presented by Schönfeld (1962) who present the same diffusion equation with a wavenumber-dependent diffusivity and also considers the effect of the finite transport velocity of the turbulence. In Deardorff (1978) it is shown that the problem of a "memory" equivalent to the explicit travel time appearing in the statistical theory of dispersion is not remedied in Eulerian models by employing a higher order closure and it is suggested that a possible solution to this problem is to include the time dependency implicitly from knowledge of the shape of the concentration distribution. In the following we derive such an approximate method. For simplicity we restrict ourselves to two dimensions and consider the crosswind (y direction) dispersion of a plume being advected by the mean wind $u$ along the $x$ axis.

2. Theory

For a continuous point source in a field of homogeneous and stationary turbulence the statistical theory yields for the second moment $\sigma$ of the concentration distribution the familiar result

$$\frac{d}{dt} \sigma^2 = u \frac{\partial}{\partial x} \sigma^2 = 2 \sigma \frac{\partial}{\partial \xi} \int_0^t R_2(\xi)d\xi, \quad (1)$$

where $t$ is travel time ($=x/u$), $\sigma$ is the variance of the cross-wind turbulent fluctuations and $R_2$ is the Lagrangian velocity correlation function.

The time dependency of $\sigma$ as given by (1) can be reproduced by a diffusion equation with a time-dependent diffusivity $K(t)$ defined by

$$K(t) = \frac{1}{2} \frac{d}{dt} \sigma^2 = \frac{\partial}{\partial \xi} \int_0^t R_2(\xi)d\xi. \quad (2)$$

Equivalently, the travel time $t$ can be formally eliminated in (2) by using (1) to yield a scale-dependent diffusivity $K(\sigma)$ defined by

$$K(\sigma) = K(t_0), \quad (3a)$$

with $t_0$ determined by

$$\sigma^2 = 2 \sigma \frac{\partial}{\partial \xi} \int_0^{t_0} R_2(\xi)d\xi dt. \quad (3b)$$

The resultant diffusion equation then takes the form

$$\frac{\partial}{\partial t} c(y,t) = K(\sigma) \frac{\partial^2}{\partial y^2} c(y,t). \quad (4)$$

As shown by Batchelor (1949) Eq. (4) yields the correct $\sigma$ at all distances; moreover, the resulting concentration distribution is Gaussian.

The Gaussian shape is supported by a number of experimental studies which indicate that the turbulent fluctuations conform to Gaussian statistics with the result that the concentration distribution

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very close to the source must be closely Gaussian. At large distances the Gaussian distribution can be argued to result from a large number of weakly coupled processes by application of the central-limit theorem (see Monin and Yaglom, 1971, 540–542). Also, at intermediate distances the Gaussian distribution seems to describe experimental results very well and there is no indication of a systematic departure from this shape (Pasquill, 1974, 178–179).

Eq. (4) is Eulerian in form, i.e., it does not contain an explicit travel-time dependency; however, this is obviously a formal property and (4) has no greater generality than (1). Transforming (4) into Fourier space yields

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

(5)

with

$$c(y,t) = \pi^{-1} \int_0^\infty \cos(ky)c(k,t)dk,$$

(6)

where we have assumed $c$ to be a symmetrical distribution. With $c(y,t)$ Gaussian the Fourier transform $c(k,t)$ is also Gaussian. The change in time of the $k$th component $c(k,t)$ is then given by

$$\frac{\partial}{\partial t} c(k,t) = -\tilde{K}(\sigma) k^2 c_0 \exp(-\frac{1}{2}k^2\sigma^2),$$

(7)

where we have introduced $c_0 = c(k,0)$, a constant for a point source. For a given value of $\sigma$ this expression has a global maximum for $k\sigma = \sqrt{2}$ and is zero in the limits zero and infinity. Assuming $\tilde{K}(\sigma)$ to be a function which does not vary too rapidly with $\sigma$, we can with some approximation substitute a function $K(k)$ for $\tilde{K}$ in (5), where

$$K(k) = \tilde{K}(\delta k),$$

(8)

resulting in a set of decoupled ordinary differential equations for the Fourier modes of the concentration distribution:

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

(9)

In Eq. (8) we have introduced a geometrical factor $\delta$ since a value which differs from $\sqrt{2}$ might give a better approximation as a consequence of the function $K(k)$ not being constant.

If the spread $\sigma$ is given by a power law we can easily show that the spectral model (9) yields an evolution of the plume width following the same power law:

Assuming $\sigma \propto t^\gamma$ the first equality in (2), (3a) and (8) implies $K(k) = a k^{(1/2\gamma-3)}$, where $a$ is constant. The solution of (9) in this case is

$$c(k,t) = c_0 \exp(-ak^{1/2}\gamma t) = c_0 \exp\{-[k(at)^{1/\gamma}]^\gamma\},$$

(9a)

which shows that the distribution at different times is the same except for a scaling of $k$ by $(at)^{-\gamma}$. Thus the concentration distribution has a self-similar development and any width follows the $\gamma$-power law.

The quality of the approximation depends on the relative change of the function $K(k)$ across the region where the function $k^2 \exp(-\frac{1}{2}k^2\sigma^2)$ has its main support. This width is easily seen to be inversely proportional to $\sigma$; with the use of (8) we see that the approximation is the better the less $\tilde{K}$ varies with $\sigma$. Eq. (9) is obviously identical with (5) for $\tilde{K}$ constant. Close to the source it will be shown that $\tilde{K}$ is proportional to $\sigma$, and we should expect the largest error to occur in this region.

We can determine $\delta$ by the requirement that the rms difference between results from Eqs. (3) and (9) of the concentration distribution close to the source is minimum. Eq. (9) is easily solved to yield

$$c(k,t) = c_0 \exp(-k^2K(k)t)$$

(10)

or, by substitution in (6):

$$c(y,t) = \frac{c_0}{\pi} \int_0^\infty \cos(ky) \exp(-k^2K(k)t)dk.$$  

(11)

Close to the source (i.e., for small $t$, $t_0$, $R_t \approx 1$ and Eqs. (2) and (3) imply that $K'(t) = \sigma^2 t$, $\sigma = \sigma t$, and hence $\tilde{K}(\sigma) = A\sigma$ with $A^2 = \sigma^2 t^2$. Eq. (8) therefore yields $K(k) = A(\delta k)$ for large $k$. Close to the source the concentration distribution is dominated by contributions $c(k,t)$ from large $k$. The solution of (9) in the near region is therefore approximately given by (11) with $K(k) = A(\delta k)$:

$$c_\delta(y,t) = \frac{c_0}{\pi} \int_0^\infty \cos(ky) \exp(-kA\delta t)dk$$

$$= \frac{c_0}{\pi} \frac{A\delta t}{[(A\delta t)^2 + y^2]},$$

(12)

and from (5) and (6) we obtain the usual Gaussian solution

$$c_\sigma(y,t) = \frac{c_0}{\sqrt{2\pi At}} \exp\left[-\frac{1}{2} \frac{y^2}{(At)^2}\right].$$

(13)

The requirement of minimum rms difference between $c_\delta$ and $c_\sigma$ is then

$$\int_{-\infty}^{\infty} [c_\delta(y,t) - c_\sigma(y,t)]^2dy = \text{minimum}.$$ 

(14)

Inserting the expressions (12) and (13) into Eq. (14) and evaluating the integral numerically, the minimum can be found to occur with the value $\delta \approx 0.76$. We could also determine $\delta$ by the requirement that the center line concentrations from (12) and (13) be equal, i.e.,
\[ c_0 \left( \frac{1}{\pi A t} \right) = c_0 \frac{1}{\sqrt{2 \pi} \sigma t/L} \quad \text{or} \quad \delta = \sqrt{\frac{2}{\pi}} \approx 0.80. \quad (15) \]

The two estimates of \( \delta \) are nearly equal; in the following we use the value 0.80 (see Fig. 1). We still have not specified \( K(k) \), and from Eqs. (8), (3a) and (2) we see that in order to do this we must specify the Lagrangian autocorrelation function \( R_L \) and \( \sigma^2 \).

A simple choice for \( R_L \) is an exponential function

\[ R_L(\xi) = \exp(-\xi t_L), \quad (16) \]

where \( t_L \) is the Lagrangian time scale

\[ t_L = \int_0^\infty R_L(\xi) d\xi. \quad (17) \]

It has been shown by Neumann (1978) that with suitable choice for \( \sigma^2 \) and \( t_L \) this form of \( R_L \) yields results in good agreement with the recently updated experimentally determined Hosker-Briggs-Gifford-Pasquill graphs of horizontal plume dispersion (Hosker, 1974).

Using (16) Eqs. (2) and (3a) yield

\[ \tilde{K}(\sigma) = \sigma^2 t_L \left[ 1 - \exp(-t_\sigma/t_L) \right], \quad (18) \]

with \( t_\sigma \) given by (3b), i.e.,

\[ \sigma^2 = 2\sigma^2 t_L \left[ 1 - \exp(-t_\sigma/t_L) \right]. \quad (19a) \]

Defining \( \tau = t_\sigma/t_L \) and \( \alpha = (\sigma/\sigma_0 t_L) \) we have

\[ \frac{1}{2} \alpha^2 = \tau + \exp(-\tau) - 1. \quad (19b) \]

which we must solve for \( \tau \). In order to arrive to an explicit expression for \( \tau \) we approximate the function \( \tau + \exp(-\tau) \) by \((1 + \tau^2)^{1/2}\) with less than 5% relative error. The solution to Eq. (19b) is then

\[ \tau = \left( (1 + \frac{1}{2} \alpha^2)^2 - 1 \right)^{1/2}. \quad (20) \]

The final expression for \( \tilde{K}(\sigma) \) then reads

\[ \tilde{K}(\sigma) = \sigma^2 t_L \left[ 1 - \exp\left[-\alpha \sqrt{(4 \alpha^2 + 1)/2} \right] \right]. \quad (21) \]

From Eq. (8) \( K(k) \) becomes

\[ K(k) = K_0 \left[ 1 - \exp\left[-\frac{k t_L}{k_L} \left( \frac{k t_L}{4} + 1 \right)^{1/2} \right] \right], \quad (22) \]

where we have defined the far-field diffusivity \( K_0 = \sigma^2 t_L \) and the wavenumber scaling \( k_L = 2\delta \sigma_0 t_L \). In the far-field wavenumbers for which \( k \ll k_L \) dominate, \( K(k) = K_0 \). Fig. 2 shows a plot of \( K(k)/K_0 \) vs \( k/k_L \). And for comparison we have included a plot of the spectral diffusivity function proposed by Prabh et al. (1979).

With \( K(k) \) given by (22) we can solve (9) for a point source. The result is given by (11).

Fig. 3a shows a plot of the resultant centerline concentration normalized by the value for a Gaussian distribution \( 1/\sqrt{2 \pi} \sigma \) with \( \sigma \) taken from (19a). We see that the agreement is very good with a maximum deviation of less than 5%.

3. Solution for cross-wind extended sources

The general solution to (9) is given by

\[ c(y,t) = \pi^{-1} \int_0^\infty c(k,0) \cos(ky) \exp(-k^2 K(k) t) dk, \quad (23) \]

where \( c(k,0) \) is proportional to the \( k \)th Fourier mode of the source distribution. We investigate the result for extended sources by assuming the source distribution to be given by a Gaussian with variance \( \Sigma^2 \).
The source is located at \( x = 0 \), oriented crosswind; the strength is thus given by

\[
Q(y) = \frac{M}{\sqrt{2\pi\Sigma}} \exp\left(-\frac{y^2}{2\Sigma^2}\right),
\]  

(24)

where \( M \) is total mass emitted per unit time. As a result we have

\[
c(k,0) = Mu^{-1} \exp(-\frac{1}{2}k^2\Sigma^2).
\]  

(25)

We can compare the result (23) with those from two other methods which can be employed in this case:

1) Regarding the source as being made up of a superposition of point sources, solving (1) for each individually and summing to obtain the total con-
centration. Assuming again a Gaussian distribution from each individual point source, the result is again a Gaussian with the variance given by \( \Sigma^2 + \sigma^2 \), i.e.,

\[
c(y,t) = \frac{Mu^{-1}}{\sqrt{2\pi\sqrt{\Sigma^2 + \sigma^2}}} \exp\left(-\frac{1}{2} \frac{y^2}{\Sigma^2 + \sigma^2}\right), \tag{26}
\]

This result can be argued to be the correct answer provided \( c \) is the time-averaged concentration and the averaging time is sufficiently long in the same sense as the averaging time necessary for a point source in order to have stable statistics on the concentration distribution.

2) Another commonly used method for the extended source problem is the virtual source approach. In this case we associate a "virtual" point source upwind which gives the concentration distribution \( Q(y)u^{-1} \) at \( x = 0 \). The distribution downstream from \( x = 0 \) is then given by

\[
c(y,t) = \frac{Mu^{-1}}{\sqrt{2\pi\sigma^*(t)}} \exp\left[-\frac{1}{2} \frac{y^2}{\sigma^*(t)}\right], \tag{27}
\]

with \( \sigma^*(t) \) given by

\[
\sigma^*(t) = 2\sigma_v^2 \int_0^{t+T} \int_0^{t'} R(t,\xi)d\xi dt' \tag{28a}
\]

and

\[
\Sigma^2 = \sigma^*(0) = 2\sigma_v^2 \int_0^T \int_0^{t'} R(t,\xi)d\xi dt'. \tag{28b}
\]

The virtual point source is thus located at \( x = -uT \).

Fig. 3 shows the relative concentrations for the methods considered as function of time of travel normalized by \( t_L \), defined in (17), with the result from the superposition of point sources (26) used as normalization. In this figure we have also included the result of using a constant diffusivity \( K_0 = \sigma^2 t_L \).

The concentrations are shown at centerline \( y = 0 \) and at \( y = y_1 = [\Sigma^2 + \sigma^2(t)]^{1/2} \).

For the point source (\( \Sigma = 0 \) and \( T = 0 \) so that \( \sigma^* = \sigma \)) the virtual source is identical to the actual source. The spectral method gives less than 5% deviation at centerline. However, as expected from Fig. 1 of the near-field concentration shape, the concentration at \( y = y_1 \), is lower than for the Gaussian distribution. The constant \( K \) diffusion shows the well-known \((t/t_L)^{1/2}\) dependency of the spread close to the source.

For extended sources we can understand the initial decrease at centerline by considering the virtual source result. In this case, for \( t \ll T \), defined by Eq. (28bb), we obtain the following expression for the spread, by making a Taylor series expansion of \( \sigma^*(t + T) \) at \( t = 0 \):

\[
S_v = \Sigma + \left(\frac{d\sigma^*}{dt}\right)_T \cdot (1 + \beta t/T), \tag{29}
\]

with \( \beta = \frac{T}{\Sigma} \left(\frac{d\sigma^*}{dt}\right)_T = \frac{d \ln \Sigma}{d \ln T} \),

where the second equality results by differentiating (28a) with respect to \( t + T \) and evaluating at \( t = 0 \), which gives the same result as differentiating (28b) with respect to \( T \). We note that \( 0.5 \leq \beta \leq 1 \) (Fig. 4). For \( t \ll T_L \) the superposition method [Eq. (26)] gives

\[
S = (\Sigma^2 + \sigma^2)^{1/2} = \Sigma + O((t/t_L)^2), \tag{31}
\]

where we have used a Taylor series expansion of the spread in the superposition method \( s(t/t_L) \) noting that \( \sigma(0) = 0 \). The relative concentration at centerline may then be written

\[
\frac{c_v}{c_\Sigma} = \frac{S_v}{S_\Sigma} \approx 1 - \beta t/T + O((t/T)^2) + O((t/t_L)^2). \tag{32}
\]

The largest initial decrease thus occurs for small \( T \) (i.e., the virtual source is close to \( x = 0 \)). From Fig. 4 this can be seen to correspond to \( \Sigma < \sigma v t_L \), where the slope \( \beta = 1 \). We see this effect both in the virtual source result and in the result from the spectral method. For sources with \( \Sigma \) smaller than the example shown in Figs. 3c–3d, the minimum moves closer to \( t = 0 \) but the minimum value is unchanged.

The spectral method yields a better estimate at centerline. Off the centerline the shape of the distribution at some distance downstream from the initially Gaussian source again tends to have a shape similar to the one shown in Fig. 1; this decreases the relative concentration at \( y = y_1 \) and the spectral method is somewhat less accurate than both the virtual source method and the constant \( K \)-method off centerline some distance downwind.

4. Averaging time dependency

In order to include the concentration dependency of the receptor averaging time in diffusion calcula-
Inserting the spectrum [Eq. (34)] and performing the integration results in
\[ \frac{\sigma^2_v}{\sigma^2_{v_m}} = r(T) = 1 - 2 \left( \frac{1}{n} \right) [n - (1 - e^{-n})], \] (36)
where \( n = T/t_L \). By (36) the function \( f(T', T) \) in (33) can be found as \( f(T', T) = r(T')/r(T) \).

Fig. 5 shows a plot of \( r(T) \) together with the relation \( \sigma_v \propto T^{1/2} \) recommended by Turner (1970). The functions are seen to approximate each other fairly within the limited range \( 1 < T/t_L < 15 \).

We next consider the Gaussian plume model. The effect on averaging time as introduced by Eq. (33) results here in a simple scale relation between the concentrations \( c' \) and \( c \) corresponding to the two different averaging times:
\[ c'(y, t) = \alpha c(\alpha y, t), \] (37)
where \( \alpha = 1/f(T', T) \). Now turning to the spectral method, we note that the wavenumber scaling and the far-field diffusivity corresponding to the two different averaging times are then related through
\[ k_L' = \frac{\delta}{\sigma_v'^{L}} = \frac{\delta}{\sigma_{v_L}} = \alpha k_L, \] (38)
and
\[ K_v' = \sigma_v'^{L} = \alpha^{-2} \sigma_{v_L} = \alpha^{-2} K_v. \] (39)
Inserting these expressions into Eqs. (22) and using the substitution \( k = \tilde{k}/\alpha \), we may write Eq. (11) in the form
\[ c'(y, t) = \frac{\alpha}{\pi} \int_0^{\infty} \cos(\tilde{k}y) \exp \left[ -\tilde{k}^2 K_v \right] \times \left[ 1 - \exp \left[ -\frac{k_L}{\tilde{k}} \left( \frac{1}{4} \frac{k_L}{\tilde{k}} + 1 \right) \right] \right] d\tilde{k} \]
\[ = \alpha c(\alpha y, t), \] (40)
which is equivalent to (37).

The expression (36) enables us to compute the appropriate value of the variance \( \sigma_v'^2 \) in the expression for \( K(k) \) [Eq. (22)] for use in a numerical dispersion model. In such a model the slowest wind fluctuations are explicitly accounted for by the terms describing advection by a mean wind defined over some averaging time \( T_w \). In order to be consistent with the statistical plume model, the receptor averaging time must be at least the time scale of the slowest fluctuations in the turbulence. This means that \( T \) in (36) must be chosen so that \( T \gg T_w \). Setting \( T \gg T_w \) means that the fluctuations in the mean wind incorrectly enters twice and, consequently, we must have \( T \approx T_w \).

5. Conclusions

We have presented a method by which the known travel-time dependency on plume spread can be in-
incorporated within the framework of numerical modeling. By a suitable choice for the geometrical factor $\delta$ [Eq. (8)], the resultant centerline concentration downstream from a point source will (within a few percent) reproduce the result from statistical theory. Close to the source, however, the concentration distribution deviates significantly from a Gaussian shape and relative errors can exceed 50%. For extended sources the model yields results similar to those obtained by associating a virtual point source to the actual source distribution, and the time-averaged concentration will be underestimated close to the source (Fig. 3).

Compared to the common use of a constant diffusivity $K_0$ to parameterize the effect of horizontal dispersion in numerical models, the extra degree of freedom introduced by the possibility of specifying the diffusivity to be a function of wavenumber in the Fourier expansion of the concentration field improves the approximation to the statistical theory. The method presented here should be considered as a systematic way of using this extra degree of freedom in models where the spectral information is readily available, as in the case of spectral and pseudospectral models of dispersion (Orszag 1971; Christensen and Prahm, 1976).

We have utilized a particularly simple form for the Lagrangian autocorrelation function, but the general procedure outlined here can be employed with any correlation function.

In view of the very complicated nature of turbulent dispersion, and the incompleteness with which the detailed physical processes are known, the fitting of the relevant functions to experimental data of plume dispersion is the most natural and most feasible method for practical dispersion calculations.

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