COMMISSION OF THE EUROPEAN COMMUNITIES

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1976

EUR 5564 e

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Published by the

COMMISSION OF THE EUROPEAN COMMUNITIES
Directorate-General
' Scientific and Technical Information
and Information Management '
Bâtiment Jean Monnet - Kirchberg

LUXEMBOURG

Printed in Belgium

Abstract

Pollutant dispersion is brought about primarily by the relative motions of individual masses of polluted air migrating along random paths. The linear Boltzmann equation represents an adequate description of the polluted eddy transport. The gradient-transfer approach is a first order approximation to it. Analytical solutions and a numerical integration procedure are presented.

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Diffusion Models

for Air Pollutants

A. Gaussian Models

1. Introduction

An inspection of smoke diffusing near the ground gives the impression that the dispersion is brought about primarily by the relative motion of individual masses of air, which drift with the wind but otherwise seem to move at random. An examination of the record of wind speed shows that the oscillations are caused by the passage of whirls and vortices which, like molecules, appear to have distinct identities. Such an air parcel, called eddy, is large compared with a molecule but is of an unspecified size. As it moves it carries with it a content of mass, heat, pollution etc. typical of the locus of its generation. On reaching a new "level" it may be assumed to mix with the surrounding air, and in this way a much-enhanced diffusion process becomes possible.

Turbulence has the effect of hastening the mixing of pollutants with ambient air. It is obvious that it is a key factor in air pollution meteorology. It is evident that a given volume of suspended material will be acted upon by the whole spectrum of turbulent fluctuations. Clearly only those fluctuations which are spatially small compared with the existing distribution of material can be expected to exert an action representable in "mixing length". The fluctuations which are on a scale similar to or greater than that of the material distribution (puff) itself will exert actions ranging over convolution, systematic distortion and bodily movement of the volume. These effects obviously cannot be represented as a simple diffusion process except in the most superficial and formal way.

In view of the lack of a general theory of turbulence that can be applied to the prediction of the eddy diffusion of atmospheric contaminants, it may not be surprising that simple, empirical methods have been sought. The idea that molecular formalism can describe in an empirical fashion the transport of pollutants within a turbulent atmosphere is taken for granted by many researchers even though there is no proof that this is generally justifiable. Whether this approximation is appropriate can be judged only on the basis of the particular application.

The growth of the volume over which a given amount of suspended material spreads has been conventionally regarded as a result of an exchange process analogous to molecular diffusion. In reality, the growth arises from a process of distortion, stretching and convolution whereby a compact "puff" of material is distributed in an irregular way over an increasing volume. The probability of encountering material at all will progressively have a less concentrated distribution in space and the corresponding average concentration over the larger volume containing the distorted puff will be less.

Much information is available from surveys which have been made of the actual distribution of effluent concentration, downwind of individual stacks. These provide a valuable practical basis in examining the extent to which simple models of dispersion provide a satisfactory basis for generalization.

Whatever formal mathematical approach is adopted its ultimate value rests on the physical validity of the entire concept of diffusivity. Lacking this, any prediction of concentration distributions and generalizations from observed distributions provided in this way are reduced to nothing more than rather arbitrary formula-fitting.

Theoretical analysis of the diffusion of material in turbulent flow has developed along three main lines: the gradient-transfer approach, the statistical theory of turbulent velocity fluctuations and similarity considerations. In the first a particular physical model of mixing is implied. The statistical theory is essentially a kinematic approach in which the behaviour of marked elements of the turbulent fluid is described in terms of given statistical properties of the motion. In the similarity theory the controlling physical parameters are postulated and laws relating the diffusion of these parameters are then derived on a dimensional basis. Diffusion models mean application of the gradient-transfer approach. Here, it is assumed that turbulence causes a net movement of material down the gradient of material concentration, at a rate which is proportional to the magnitude of the gradient.

Any complete expression for the spatial distribution of airborne material released at a point must contain three features:

(1) The shape of the distributions of concentration at any given time or down-wind position; i.e. the manner in which the concentration varies across wind, vertically and along wind.

(2) The dimensions of the diffusing cloud in these directions.

(3) An expression of the so-called continuity (or conservation) condition which will here be restricted to the case when no material is lost by deposition or decomposition.

It is useful to consider certain convenient expressions which may be looked upon either as formal solutions or as empirical equations in which to substitute features (2) and (3) above, the former of these being provided either in a purely empirical way or on the basis of statistical treatments.

It is essential to have a realistic view of the complications arising from various features, such as the aerodynamic effects of buildings both in an individual sense and collectively in an urban area, the control exerted by natural topography and the influence of the "heat island" effect created by a modern city.

Experiences have shown that the diffusion theory runs into difficulties under the following circumstances:

(a) when the airflow is indefinite (calm conditions)

(b) when there are marked local disurbances in the airflow, e.g. in the immediate vicinity of buildings and obstacles, unless the diffusing cloud has already grown to a size considerably greater than the disturbances,

(c) when the airflow is channelled or when it contains circulations or drainage set up by the heating or cooling of undulating or hilly terrain.

Even in these complex conditions however it may often be possible to speculate usefully on the sense and extent of the changes which the complexities are likely to impose on the diffusion, but clearly such cases need to be given special consideration.

In any case, even if the conditions of terrain and weather approach the ideal of uniformity and steadiness, the estimates which may be made correspond to an ensemble average, from which there may be appreciable deviations on individual occasions.

Great care must be taken in applying these models to real situations, however, because the surface of the earth is very irregular, and furthermore, the weather sometimes changes even from hour to hour. In general, reliable predictions of dilution rates cannot be obtained by simply applying formulas obtained from engineering handbooks. This is not because the formulas are wrong but because they cannot be safely extrapolated when the experimental situation has not been exactly duplicated.

2. Eddy diffusion

Flying balloons or tetroons move along polygonial trajectories, i.e. straight paths interrupted by instantaneous deviations. The same transport mechanism is also assumed to be valid for the eddy transport. Because of this, an adequate description for a diluted eddy gas is given by the linear Boltzmann equation+):

+) $\mathfrak{S}$ denotes a superposition, e.g. a discrete summation $\sum$ or a continuous integration $\int$

(1) $$\left(\frac{\partial}{\partial t} + \vec{v}\cdot\mathrm{grad}\right)N = -\alpha N + \underset{\vec{v}'}{S}\,\beta(\vec{v}'\rightarrow\vec{v})N(\vec{v}') + S$$

(1) (2) (3) (4)

This is a balance equation. The left-hand side (1) is the substantial derivative of N, e.g. the number of eddies per phase-space volume element, whereas the right-hand side represents the sum of gains and losses: firstly the loss (2) due to combined scattering and absorption, then the gain (3) due to scattering from other velocities, and finally the gain or loss (4) due to sources or sinks. α is the "total interaction coefficient" and $\ell = 1/\alpha$ the "mean free path"; β is the "differential scattering coefficient". For a more detailed explanation see, for instance, DAVISON (1957).

The transport equation may be stated in slightly different forms if the eddy distribution is expressed by the "flux" $\phi = \vec{v}\,N$ or by the "collision density" $\psi = \alpha N$.

The space-time dependent number of eddies, i.e. eddy density

(2) $$M = \underset{\vec{v}}{S}\,N(\vec{v})$$

satisfies the differential equation

(3) $$\mathrm{div}\,(\mathbb{D}\,\mathrm{grad})M = a\,M + \frac{\partial M}{\partial t} + T\frac{\partial^2 M}{\partial t^2} + \sum_{k=3}^{\infty}\mathcal{E}_k\frac{\partial^k M}{\partial t^k}$$

where $\mathcal{E}_k$, the absorption coefficient a, the relaxation time T and the eddy diffusion tensor $\mathbb{D}$ depend on α, β, $\vec{v}$ and space-time $(\vec{r},t)$.

In addition, one can still classify N with regard to eddy size or mass m of pollutant carried with, e.g. $\overline{N}(m,\vec{v})$. The corresponding transport equation thus has the form:

(4) $$\left(\frac{\partial}{\partial t} + \vec{v}\cdot\mathrm{grad}\right)\overline{N} = -\alpha\overline{N} + \underset{m'}{S}\,\underset{\vec{v}'}{S}\,\beta(m',\vec{v}'\rightarrow m,\vec{v})\,\overline{N}(m',\vec{v}')$$

The distribution

$$\bar{M}(m) = \sum_{\vec{v}} \bar{N}(m,\vec{v}) \tag{5}$$

satisfies the equation

$$\operatorname{div}(\mathbb{D}\operatorname{grad})\bar{M} = a\bar{M} + \frac{\partial \bar{M}}{\partial t} + T\frac{\partial^2 \bar{M}}{\partial t^2} + \sum_{k=3}^{\infty} \varepsilon_k \frac{\partial^k \bar{M}}{\partial t^k} + \sum_{m'} b(m'-m)\bar{M}(m') \tag{6}$$

To keep the mathematical effort within reasonable bounds, we shall, in the first step, confine ourselves to the so-called "hyperbolic approximation" characterized by

$$\varepsilon_k \equiv 0 \qquad \text{for} \qquad k \geq 3 \tag{7}$$

Only when it becomes evident that this approximation is not sufficient for the interpretation, shall we also take higher time derivatives into consideration.

The hyperbolic approximation leads to classical equations of the mathematical physics. In the past, numerous integration approaches have been developed; we can use them (e.g. FRANK-v. MISES (1961)).

3. Hyperbolic approximation

Equation (6) degenerates, for n different types of eddies, to the set of wave equations

$$T_i \frac{\partial^2 \bar{M}_i}{\partial t^2} + \frac{\partial \bar{M}_i}{\partial t} + \sum_{j=1}^{n} b_{ij}\bar{M}_j = \nabla\cdot(\mathbb{D}_i \nabla)\bar{M}_i \tag{8}$$

with $a_i = b_{ii}$ and $i = 1,2,\ldots n$.

Since the solution M_i^{as} of the parabolic equation, i.e. the diffusion equation

$$(9) \qquad \frac{\partial \overline{M}_i^{as}}{\partial t} + \sum_{j=1}^{n} b_{ij} \overline{M}_i^{as} = \nabla \cdot (\mathbb{D}_i \nabla) \overline{M}_i^{as}$$

converges, for increasing t, to M_i, i.e.

$$(10) \qquad \overline{M}_i^{as} \approx \overline{M}_i \qquad \text{for} \qquad t > T,$$

we shall also test the solutions of (9) by experiments, with regard to their practical usefulness.

From it follows that

$$(11) \qquad T \frac{\partial^2 M}{\partial t^2} + \frac{\partial M}{\partial t} + aM = \nabla \cdot (\mathbb{D} \nabla) M$$

and for the asymptote M^{as}

$$(12) \qquad \frac{\partial M^{as}}{\partial t} + a M^{as} = \nabla \cdot (\mathbb{D} \nabla) M^{as}$$

There are several justifications for the application of both the wave equations (8)(11), and the diffusion equations (9)(12) (e.g. MONIN (1959), LAMB-SEINFELD (1973), PASQUILL (1974)).

In the past, several computer codes for solving the parabolic equations (9)(12) have been developed and applied, mainly in the reactor physics. In this field, they are known as "multi-group diffusion codes" (e.g. MENELEY et al.(1971)). The expert should be acquainted with the present state of the art.

We are currently considering several analytical solutions of (8)(11) and (9)(12), since such solutions represent the basis of the most widely used dispersion models for air pollutants today. Our discussion deals mainly with cases (11) and (12).

4. Green's function

For a punctiform "puff", $Q \sim \delta(r)\,\delta(t)$, in an infinite $\vec{r}$-space we call the Green's function belonging to quation (11)

$$M = G(\vec{r},t)$$

Different weather situations require different dispersion characteristics $(T,a,\mathbb{D})$. One, via a weather index λ , introduces a linear weather classification, i.e.

$$(T,a,\mathbb{D}) \longrightarrow G(\vec{r},t,\lambda),$$

and calls the mean

$$(13) \qquad \Gamma_1 = \sum_{\lambda} F(\lambda) G(\vec{r},t,\lambda) \qquad \text{with} \sum_{\lambda} F(\lambda) = 1$$

a "climatological model", where $F(\lambda)$ denotes the frequency distribution of the different weather situations which occured during the time period under consideration.

Linear superpositions of the type

$$(14) \qquad \Gamma_2 = \sum_{\vec{\rho}} \sum_{\tau} Q(\vec{\rho},\tau)\, G(\vec{r}-\vec{\rho}, t-\tau)$$

weighted with the space-time dependent source-distribution Q, extend the set of solutions of (11). The Green's functions to (11) both for the half-space and the parallel-layer can be constructed by the classical mirror-method (e.g. FRANK-v.MISES (1961)).

The accumulated eddy distribution

$$(15) \qquad \Gamma_3 = \int_{-\infty}^{+\infty} G(\vec{r} - \vec{\rho}(\tau), \tau)\, d\tau$$

generated by a puff migrating along the trajectory $\vec{r} = \vec{\rho}\,(t)$ is called a "plume".

A puff moving with a velocity $\vec{u}(t)$ satisfies the somewhat generalized equation

$$(16) \qquad T\frac{\partial^2 M}{\partial t^2} + \frac{\partial M}{\partial t} + aM + \vec{w} \cdot \nabla M = \nabla \cdot (\mathbb{K} \nabla) M$$

The dispersion characteristic is now $(T, a, \vec{w}, \mathbb{K})$. The transformation $\vec{\rho} = \vec{r} - \int \vec{u}\,(\tau) d\tau$ reduces eq. (16) to an equation of type (11). $\vec{w}$ and $\vec{u}$, resp. $\mathbb{K}$ and $\mathbb{D}$ are coupled by the relations

$$\vec{w} = \vec{u} + T\frac{d\vec{u}}{dt} \qquad\qquad \mathbb{K} = \mathbb{D} - u^2 T$$

All information presented in this chapter is also valid for the puff $M = G^{as}$ corresponding to eq. (12).

Considerable practical importance has been conceded to the solutions of the stationary equation

$$(17) \qquad \vec{u} \cdot \nabla M + aM = \nabla \cdot (\mathbb{K} \nabla) M$$

Here too, one appropriately starts with Green's functions belonging to the source $Q \sim \delta(r)$ in an infinite $\vec{r}$-space and constructs rather general classes of solutions for (17) by linear superpositions.

The method of mirror-sources can also be applied here. There are climatological models.

Now that the more formal considerations are done with, we will proceed to concrete examples.

5. Analytical solutions

A class of solutions for eq. (17) frequently studied in the past is characterized by a = 0; $\mathbb{K} = \{ K_{ij} \cdot \delta_{ij} \}$ and

(18)
$$\begin{cases} u_1 = u_0(\lambda) z^m & u_2 = u_3 = 0 \\ K_{11} = 0 \quad K_{22} = k_2(x,\lambda) z^m & K_{33} = k_3(x,\lambda) z^n \end{cases}$$

Its kernel is the Green's function $M = G_1(\vec{r}, \lambda)$ for eq. (18) and an infinite $\vec{r}$-space:

(19)
$$\begin{cases} G_1(\vec{r},\lambda) = \kappa_2^{-1/2} \kappa_3^{-s} \exp\left(- \dfrac{u_0 y^2}{4 \kappa_2} - \dfrac{u_0 z^r}{r^2 \kappa_3} \right) \\ \kappa_i = \displaystyle\int_0^x k_i(\xi,\lambda) d\xi \qquad r = m - n + 2 \qquad s = \dfrac{m+1}{r} \end{cases}$$

(e.g. ROBERTS (1923, BOSANQUET-PEARSON (1936), SUTTON (1943, 1947), CALDER (1949, 1952), DEACON (1949), DAVIES (1950), ROUNDS (1955), SMITH (1957), BARAD-HAUGEN (1959)).

Another class well suited to practical purposes corresponds to the convective diffusion equation

(20)
$$\frac{\partial M}{\partial t} + \vec{u} \cdot \nabla M = \nabla \cdot (\mathbb{K} \nabla) M$$

It is characterized by

$$(21)\quad \begin{cases} \vec{u} = \vec{u}(t,\lambda) \\ K_{11} = k_1(t,\lambda) \qquad K_{22} = k_2(t,\lambda) \qquad K_{33} = k_3(t,\lambda)\, z^n \end{cases}$$

Its kernel is the Green's function $M = G_2(\vec{r}, t, \lambda)$ for an infinite $\vec{r}$-space:

$$(22)\quad \begin{cases} G_2(\vec{r}, t, \lambda) = (\kappa_1 \kappa_2)^{-1/2} \kappa_3^{-1/r} \exp\left[-\dfrac{(x-\rho_1)^2}{4\kappa_1} - \dfrac{(y-\rho_2)^2}{4\kappa_2} - \dfrac{(z-\rho_3)^2}{4\kappa_3} \right] \\ \kappa_i = \displaystyle\int_0^t k_i(\tau,\lambda)\,d\tau \qquad \vec{\rho} = \int_0^t \vec{u}(\tau,\lambda)\,d\tau \qquad r = 2-n \end{cases}$$

(e.g. FRENKIEL (1952), SUTTON (1953), CSANADY (1973)).

For the sake of completeness, we mention here the special case of the so-called "telegraphers equation":

$$(23)\quad T\frac{\partial^2 M}{\partial t^2} + \frac{\partial M}{\partial t} + aM = K\Delta M$$

The corresponding Green's function $M = G_3(\vec{r}, t, \lambda)$ for an infinite $\vec{r}$-space is

$$(24)\quad \begin{cases} M \sim \exp(-t/2T) \cdot I_1(q\xi) \cdot \varepsilon(\xi^2)/\xi \\ \xi^2 = Kt^2/T - r^2 \qquad q^2 = 1/4KT - a/K \end{cases}$$

(e.g. GOLDSTEIN (1950), MONIN (1959), PASQUILL (1974)).

Using linear superpositions of solutions such as (19)(22)(24), in the sense of (13)(14)(15), one constructs rather flexible classes of solutions for (23). Thus, for instance, the classical mirror method generates the Green's functions for the half-space corresponding to G_1, G_2 and G_3:

$$G_4' = G(z-h) + \varepsilon\, G(z+h)$$

I_1 = Bessel function, ε = step function which satisfy the boundary condition

$$z = 0 \qquad \begin{matrix} G \\ \\ \frac{\partial G}{\partial z} \end{matrix} = 0 \qquad \text{for} \quad \varepsilon = \begin{matrix} - \\ 1 \\ + \end{matrix}$$

The Green's functions corresponding to the parallel layer with similar boundary conditions can be found by a superposition of an infinite set of linearly arranged discrete mirror sources.

For purposes of illustration, we select from the different possibilities of a continuous superposition only some typical solutions constructed from

$$G = x^{-a} \exp\left(-\frac{by^2}{x^p} - \frac{cz^r}{x^q}\right) \tag{25}$$

which is obviously a subset of (19). (see fig. 1)

Source type	distribution	density
line	$-\infty < \xi \leq x$	$\chi_1(y,z) = \Gamma\left(\frac{a-1}{p}\right) p^{-1} (by^2 + cz^r)^{-1}$
line	$-\infty < \eta \leq y$	$\chi_2(x,z) = \sqrt{\frac{\pi}{b}}\, x^{-\lambda} \exp\left(-\frac{cz^r}{x^q}\right)$
area	$-\infty < \xi \leq x$ $-\infty < \eta \leq y$	$\chi_3(z) = \sqrt{\frac{\pi}{b}}\, q^{-1}\, \Gamma\left(\frac{\lambda}{q}\right) (cz^r)^{-1}$

$$\lambda = 1 - a + p/2$$

A study of the current literature shows that the diffusion models most widely used today are special cases of the classes listed above (e.g. LUCAS (1958), TURNER (1964), MILLER-HOLZWORTH (1967), KOGLER et al. (1967), MARSH-WITHERS (1969), ROBERTS et al. (1969), JOHNSON et al. (1969), FORTAK (1970), GIFFORD-HANNA (1971)).

A description of pollutant dispersion, by far more flexible and better adapted to real problems than the analytical solutions mentioned, is given by the so-called Galerkin method.

With this one reduces the initial equation

(26) $$\mathcal{D} M = Q$$

where $\mathcal{D}$ denotes a linear differential-operator, to a system of equations acting on a space of lower dimension. The particle number M is exactly expressible as an expansion

(27) $$M = \sum_{k=1}^{K} \varphi_k \psi_k$$

into a complete system of functions ψ_k of one or more of the basic variables, e.g. $\psi_k(x,y)$ or more briefly $\psi_k(\eta)$. The remaining variables, here (z,t), are represented by the symbol ξ. While the ψ_k are well-known functions, the $\varphi_k(\xi)$ are still to be determined. Inserting the representation (27) into the starting equation (26), η becomes a free parameter with a continuous range of values. The resulting equation, can via

(28) $$\int_{\eta_{min}}^{\eta_{max}} (\mathcal{D} M - Q) \psi_k \, d\eta = 0 \qquad k = 1,2,\ldots K$$

be gradually replaced by an equivalent set of equations governing the coefficients φ_k. These sets will be referred to as the "reduced dispersion equations". Their mathematical structure is uniquely and completely fixed by the distribution of the variables between ξ and η.

Example:

$\psi_k = x^m y^n$ complete on $(-\infty < {x \atop y} < +\infty)$ reduces eq. (20) via (28) to the system

(29) $$\frac{\partial \varphi_k}{\partial t} = \frac{\partial}{\partial z}\left(K_3 \frac{\partial \varphi_k}{\partial z}\right) + \sum_k c_k \varphi_k + q_k$$

(e.g. SAFFMAN (1962), SMITH (1965), MÜLLER (1974)).

B. Trajectory Models

1. Puffs

They attach their coordinate system to an air volume which moves with the advective wind. The model of ESCHENROEDER-MARTINEZ (1972) is based on the concept of a fictitious vertical air column that must maintain its integrity as it moves through the atmosphere. Due to the fact that in the planetary boundary layer, both the magnitude and the direction of wind vary with height, it is impossible for an air column to remain vertical as it is being advected by the wind over time periods commonly of interest. One, therefore, will study the advection of an expanding "puff" instead of a vertical column.

Suppose we have a puff of pollutant of known concentration distribution $\chi(\vec{r},t_o)$ at time t_o. In absence of chemical reactions and other sources, and if we assume molecular diffusion to be negligible, the concentration distribution $\chi(\vec{r},t)$ at some later time $t > t_o$ is described by the so-called advective equation

$$\frac{\partial \chi}{\partial t} + div(\vec{u}\chi) = 0 \tag{30}$$

If we solve this equation with $\vec{u} = \vec{u}_{mean}$, and compare the solution with observations we would find in reality that the material spreads out more than predicted. The extra spreading is, in fact, what is referred to as "turbulent diffusion" and results from the influence of the stochastic component $\vec{u}'$ which we have ignored. Implying that we knew the velocity field $\vec{u} = \vec{u}_{mean} + \vec{u}'$ precisely at all locations and times, there would be no such phenomenon as turbulent diffusion.

Thus, turbulent diffusion is an artifact of our lack of knowledge of the true velocity field. Consequently, one of the fundamental tasks in turbulent diffusion theory is to define the deterministic component $\vec{u}_{mean}$ and the stochastic component $\vec{u}'$ of the velocity field $\vec{u}$.

Knowing finally this field one could try to construct the trajectory followed by the moving puff. But there are other difficulties.

A first-order approach would be, to assume the puff is Gaussian puff, expanding with time.

To take care of $\vec{u}'$ one could interpret the puff as a realization of an ensemble of identically expanding puffs moving along stochastic trajectories.

In the case of a significantly varying wind shear, the lower parts of the puff will be slower than the upper ones. One could pay regard to that, at least partially, assuming each puff to be composed of horizontal layers, each of them following its own dispersion characteristics, $\lambda(z)$. The corresponding formalism is given by

$$0 < t \leq t_1 \qquad \chi_1(\vec{r},t) = \chi(\vec{r},t,\lambda(h))$$

(31)

$$t_n < t < t_{n+1} \qquad \chi_{n+1}(\vec{r},t) = \sum_{\vec{\rho}} \chi_n(\vec{\rho},t_n)\chi(\vec{r}-\vec{\rho},t-t_n,\lambda(\zeta))$$

where z = h is the emission height and $\vec{\rho} = (\xi, \eta, \zeta)$. The χ's measure the pollutant concentrations in consecutive time intervals. The superpositions can properly be performed by the so-called stochastic integration approach

2. Plumes

The continuous stream or "plume" of effluent gas stretching from an industrial chimney may be thought of as a succession of elementary sections which behave somewhat like individual puffs. The trajectories of these sections are not identical, but are irregularly displaced by the larger scale fluctuations in the flow. The result is a progressive broadening of the cross-wind front over which material is spread at a given distance downwind of the source, and the same process is also effective in the vertical. Thus, the average concentration produced downwind of a point source not only diminuishes with distance from the source but also with the time of exposure. It is important to realize that this property of time mean concentration is a consequence of the existence of dispersive motions on a scale larger than the plume cross section itself.

3. Stochastic integration

We now present another stochastic approach in order to describe the pollution dispersion during stagnant weather situations as well.

The linear Boltzmann equation

$$(32) \quad \frac{1}{v}\frac{\partial f}{\partial t} + \vec{\Omega}\cdot\nabla f = -\alpha f + \frac{\beta}{4\pi}\int f(\vec{r},\vec{v}',t)\,d\vec{\Omega}' \qquad \vec{v}=v\vec{\Omega}$$

is the Eulerian description of particle transport in a homogeneous isotropic material, taking account of the "free path" (SODAK, 1962) and so it is the corresponding modification of the Liouville-equation. The term

$(-\alpha f)$ measures the absorption and the so-called "collision integral" on the right-hand side of (32) describes the interaction mechanism. The integro-differential eq. (32) can be solved by a random walk approach ($\longrightarrow$ Monte Carlo technique, e.g. SODAK, 1962). The "flux" caused by a point source isotropically emitting into an infinite extended space satisfiés the Peierls equation

$$(33) \quad \begin{cases} \chi(\vec{r},t) = \dfrac{\beta}{4\pi} \displaystyle\int d\vec{r}\,' \, \dfrac{e^{-\alpha|\vec{r}\,'-\vec{r}|}}{|\vec{r}\,'-\vec{r}|^2} \, \chi(\vec{r}\,',t') \\ t' = t - |\vec{r}\,'-\vec{r}|/v \end{cases}$$

A Laplace transformation $\chi(\vec{r},t) \longrightarrow \phi(\vec{r},p)$ with respect to time t and a subsequent Taylor expansion of the integrand leads to the equation

$$\phi = \beta \sum_{k=0}^{\infty} \frac{\nabla^{2k}\phi}{(2k+1)\,\gamma^{2k+1}} \qquad \gamma = \alpha + \frac{p}{v}$$

the differential operator of which degenerates to a Helmholtz-operator $(\nabla^2 + B^2)$, if the cross-sections α and β are coupled by

$$(34) \qquad \frac{1}{\alpha + p/v} = \frac{1}{B} \tan \frac{B}{\beta}$$

In this case, the transformed flux ϕ, obviously, satisfies the second order differential equation

$$(35) \qquad (\nabla^2 + B^2)\,\phi = 0$$

and, because of this, the flux χ satisfies a differential equation of the type

$$\left(\nabla^2 - \sum_{k=0}^{\infty} \varepsilon_k \frac{\partial^k}{\partial t^k}\right)\chi = 0 \quad ,$$

The so-called "hyperbolic approximation" to it is given by the "telegrapher's equation"

$$(36) \qquad D\,\nabla^2\chi = \frac{D}{c^2}\frac{\partial^2\chi}{\partial t^2} + \frac{\partial\chi}{\partial t} + b\chi$$

the coefficients of which are approximately connected with those of the transport equation via

$$(37) \qquad D = \frac{v}{3(2\alpha-\beta)} \qquad c = \frac{v}{\sqrt{3}} \qquad b = \frac{v\alpha(\alpha-\beta)}{2\alpha-\beta}$$

It should be mentioned here that the parabolic equation

$$(38) \qquad D\,\nabla^2\chi = \frac{\partial\chi}{\partial t} + b\chi$$

corresponds to the asymptotic case $r^2/c^2t \rightarrow 0$. All this, demonstrated above, appears very useful, since one can now also solve both the telegrapher's equation (36) and the diffusion equation (38) by a random walk approach (e.g. MÜLLER, 1976).

The convection by air flow requires nothing but an addition of the local wind vector to the actual eddy velocity.

4. Conclusion

At this point it must be admitted that, due to purely mathematical difficulties during the determination of suitable classes of solutions of the above equations, some people occupied in air quality management simply take available solutions, which are sometimes less than adequate for the physical-chemical problem to be treated. Obviously, one is always able to gain a certain adaption to the reality by a fitting, i.e. a suitable choice of the free parameters, which leads finally to a more or less suitable description of the dispersion behaviour of a pollutant. This fact makes the transferability of a dispersion model, up to now successful in a certain region and with certain weather conditions, to another region and situation somewhat doubtful. Success is not necessarily simultaneously transferable - a fact that a models user must never forget.

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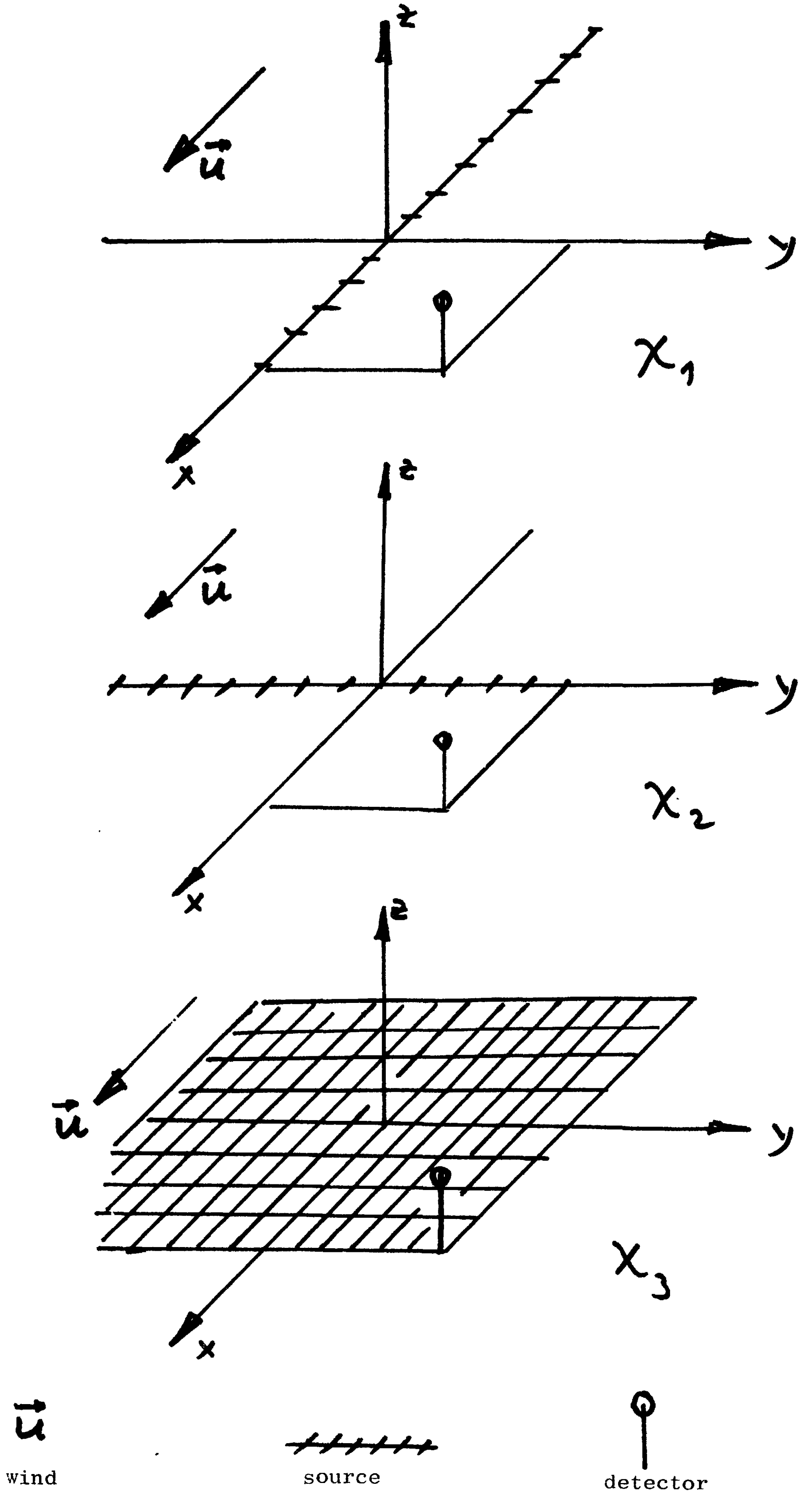
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fig. 1

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