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16. ABSTRACT

An introductory treatment of the fundamentals of diffusion theory is presented, starting with molecular diffusion and leading up to the statistical methods of turbulent diffusion. The concepts and equations of diffusion are developed on an elementary level, with emphasis on atmospheric applications.

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TABLE OF CONTENTS

		Page
I.	INTRODUCTION	1
II.	BASIC EQUATIONS OF DIFFUSION	2
	A. Stationary Medium	2
	B. Moving Medium	6
	C. Anisotropic Medium	8
III.	SOURCE SOLUTIONS	12
	A. Instantaneous Sources	12
	B. Continuous Sources	31
	C. Source Solutions in a Moving Medium	35
	D. Source Solutions in an Anisotropic Medium	42
IV.	TURBULENT DIFFUSION	48
	A. Taylor's Theorem	48
	B. Example from Brownian Motion	55
	C. Sutton's Formulas for the Dispersion	60
	D. Hay-Pasquill Method for Determining the Dispersion	65
V.	NASA/MSFC MULTILAYER DIFFUSION MODEL	67
	A. Point Source Solutions in a Layer with Impervious Boundaries	67
	B. Summary of the NASA/MSFC Mode'	73
REFERENCES		75

LIST OF ILLUSTRATIONS

Figure	Title	Page
1.	The unit normal and flux vectors at a point on a surface S bounding the volume V	3
2.	The solution for the instantaneous plane source for three values of σ^2, illustrating the spread of the distribution with increasing σ	14
3.	The solution for an instantaneous source of thickness 2a for several values of the dimensionless parameter $\sigma^2/2a^2$	18
4.	The real source and its image, where $\chi = L$ is an impermeable boundary and all quantities are measured relative to a coordinate x whose origin is at the center of the source	21
5.	The geometry for the integration of the point source solution for a spherical source of radius a	28
6.	The continuous point source in a wind and its image	41

TECHNICAL MEMORANDUM 78128

SOME BASIC MATHEMATICAL METHODS OF DIFFUSION THEORY

I. INTRODUCTION

The purpose of this report is to provide an introductory treatment of the basic mathematical aspects of diffusion theory as it applies to the atmosphere, starting with molecular diffusion and leading up to the statistical methods of turbulent diffusion. The scope of the treatment is evident in that hydrodynamical theory, which is a necessary foundation of diffusion theory when applied to a medium as complex as the atmosphere, has been kept to a minimum. The basic concepts and equations of diffusion are developed on an elementary level, with emphasis on the mathematical steps. Many of the derivations given cannot easily, if at all, be found in the literature on diffusion. The report is not meant to be definitive in any sense. It is hoped that sufficient material has been treated to provide a background for further reading to understand today's specialized papers in the field.

II. BASIC EQUATIONS OF DIFFUSION

A. Stationary Medium

Diffusion is the process whereby a substance introduced in a localized region of some medium (e.g., a fluid) spreads throughout the medium either by molecular motion or by turbulence. The basic equations of molecular diffusion are derived first. Turbulent flow will be treated later. If χ denotes the concentration of a diffusing substance, defined as the quantity of substance per unit volume, then relative to a set of rectangular axes the vector rate of transfer of substance through unit area of a section of medium is called the flux $\vec{F}$. In many diffusion problems the assumption made is that $\vec{F}$ is proportional to the concentration gradient normal to the section. That is,

$$F_x = -D\frac{\partial\chi}{\partial x} \quad , \quad F_y = -D\frac{\partial\chi}{\partial y} \quad , \quad F_z = -D\frac{\partial\chi}{\partial z}$$

or in vector form

$$\vec{F} = -D\nabla\chi \tag{1}$$

where $D = D(x, y, z, t, \chi)$ is the diffusivity or coefficient of diffusion which may, in general, be a function of the coordinates, the time, and the concentration. The quantity $\nabla\chi$ is the gradient of the concentration defined by

$$\nabla\chi = \frac{\partial\chi}{\partial x}\vec{i} + \frac{\partial\chi}{\partial y}\vec{j} + \frac{\partial\chi}{\partial z}\vec{k} \quad ,$$

where $\vec{i}$, $\vec{j}$, and $\vec{k}$ are unit vectors along the x, y, and z axes, respectively. The negative sign indicates that the diffusion occurs in the direction of decreasing concentration.

We derive next the equation connecting the time rate of change of the concentration with the spatial rate of change of the concentration at any given point. This is accomplished by considering an arbitrary volume of fluid V, bounded by the surface S, as shown in Figure 1, and applying the principle of continuity to the diffusing substance.

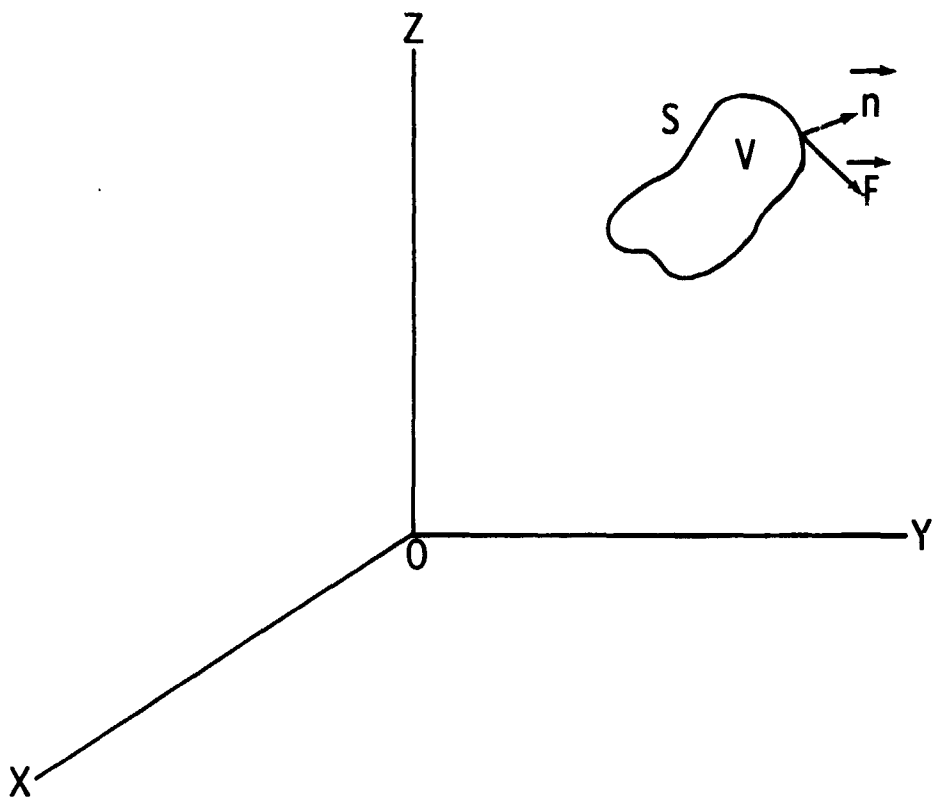

Figure 1. The unit normal and flux vectors at a point on a surface S bounding the volume V.

Let M be the total mass of diffusing substance within V. It is clear that M will be a function of time. From the definition of χ it follows that

$$M(t) = \int_V \chi \, dV \quad . \tag{2}$$

At every point of the surface S there is a flux $\vec{F}$ making some angle with the unit normal $\vec{n}$ at the point. The only flux out of the volume V has to be along the direction of $\vec{n}$, which is just the component of $\vec{F}$ parallel to $\vec{n}$, or $\vec{F} \cdot \vec{n}$. Therefore, the total flux leaving the volume V is obtained by integration over the surface S. The total flux has units of mass per unit time and, therefore, may be called the current, which is denoted by I(t). Thus

$$I(t) = \int_S \vec{F} \cdot \bar{n} \, dS \quad .$$

This surface integral may be converted to a volume integral by use of the divergence, or Gauss', theorem which states that

$$\int_S \vec{F} \cdot \vec{n} \, ds = \int_V \nabla \cdot \vec{F} \, dV$$

and so

$$I(t) = \int_V \nabla \cdot \vec{F} \, dV \quad . \tag{3}$$

Since I is a mass current, we have

$$I(t) = - \frac{\partial M}{\partial t}$$

which, when combined with equations (2) and (3), results in

$$\int_V \nabla \cdot \vec{F} \, dV = - \frac{\partial}{\partial t} \int_V \chi \, dV$$

or

$$\int_V \left(\frac{\partial \chi}{\partial t} + \nabla \cdot \vec{F} \right) dV = 0 \quad .$$

Since the volume is arbitrary, the integrand must vanish, yielding

$$\frac{\partial \chi}{\partial t} = -\nabla \cdot \vec{F} \tag{4}$$

which is simply the expression for the conservation of diffusing matter, namely that the rate of change of the concentration at any point must equal the net flux at the point. The assumption of conservation is valid provided there is no creation or destruction of the diffusing matter.

In rectangular coordinates, equation (4) assumes the form

$$\frac{\partial \chi}{\partial t} = - \frac{\partial F_x}{\partial x} - \frac{\partial F_y}{\partial y} - \frac{\partial F_z}{\partial z} \quad . \tag{5}$$

Substituting equation (1) into equation (4) yields the relation we sought connecting the time rate of change of χ with its spatial rate of change,

$$\frac{\partial \chi}{\partial t} = \nabla \cdot D \nabla \chi \quad , \tag{6}$$

which in rectangular coordinates is

$$\frac{\partial \chi}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial \chi}{\partial x} \right) + \frac{\partial}{\partial y} \left(D \frac{\partial \chi}{\partial y} \right) + \frac{\partial}{\partial z} \left(D \frac{\partial \chi}{\partial z} \right) \quad . \tag{7}$$

Equation (6) is the fundamental equation governing the diffusion process in stationary isotropic media. If D is constant, it reduces to

$$\frac{\partial \chi}{\partial t} = D\nabla^2 \chi \quad , \tag{8}$$

where $\nabla^2\chi \equiv \nabla \cdot \nabla\chi$ is the Laplacian of χ which, in rectangular coordinates, has the form

$$\nabla^2\chi = \frac{\partial^2\chi}{\partial x^2} + \frac{\partial^2\chi}{\partial y^2} + \frac{\partial^2\chi}{\partial z^2} \quad . \tag{9}$$

When D is constant, the diffusion, as expressed by equation (8), is called Fickian diffusion. The formulation given here is strictly phenomenological, resting on the assumption that the flux is proportional to the concentration gradient as expressed by equation (1).

B. Moving Medium

In the case of a fluid moving with a laminar flow velocity $\vec{u}$, as might be the case in the atmosphere when there is a wind, the flow will contribute to the flux by physically transporting the diffusing matter. The additional flux is $\vec{u}\chi$, and the flux equation (1) becomes

$$\vec{F} = \vec{u}\chi - D\nabla\chi \quad . \tag{10}$$

Substitution of equation (10) into equation (4) gives

$$\frac{\partial \chi}{\partial t} = -\nabla \cdot (\vec{u}\chi - D\nabla\chi)$$

$$= -\nabla \cdot (\vec{u}\chi) + \nabla \cdot (D\nabla\chi)$$

$$= -\vec{u}\nabla\chi - \chi\nabla \cdot \vec{u} + \nabla \cdot (D\nabla\chi) \quad .$$

If $\vec{u}$ is constant, the second term is zero, which implies incompressible flow. Taking D to be constant also, we have

$$\frac{\partial \chi}{\partial t} + \vec{u} \cdot \nabla \chi = D \nabla^2 \chi \tag{11}$$

which is the fundamental equation of diffusion commonly used in the case of a fluid w th laminar flow.

In a situation where D is a function of time only, $D = D(t)$, the problem can be handled by defining a new time scale τ by

$$d\tau = D\, dt \quad .$$

Then, by differentiation,

$$\frac{\partial \chi}{\partial t} = \frac{\partial \chi}{\partial \tau} \frac{d\tau}{dt} = \frac{\partial \chi}{\partial \tau} D$$

$$u_x = \frac{dx}{dt} = \frac{dx}{d\tau} \frac{d\tau}{dt} = v_x D \quad .$$

Similarly,

$$u_y = v_y D \quad , \quad u_z = v_z D$$

so that equation (11) becomes

$$\frac{\partial \chi}{\partial \tau} + \vec{v} \cdot \nabla \chi = \nabla^2 \chi \quad , \tag{12}$$

which is a form identical to equation (11) except that D does not enter the equation. It should be clear that $\vec{v}$ is the velocity in terms of the new time scale τ. For a known $\vec{u}$ and D(t), the value of $\vec{v}$ is given by

$$\vec{v} = \frac{\vec{u}}{D(t)} \quad .$$

C. Anisotropic Medium

In all of the equations developed thus far, the diffusion coefficient has been assumed to be the same in all directions. When this is not the case, the medium is said to be anisotropic. The equations for the flux as given by equation (10) in the general case of a moving medium must now be modified. It is convenient at this point to express the flux equations (10) and succeeding equations in rectangular coordinates. By a coordinate transformation the equations may then be cast in terms of any other system of coordinates.

The new equations for the flux are

$$F_x = u_x\chi - D_{11}\frac{\partial\chi}{\partial x} - D_{12}\frac{\partial\chi}{\partial y} - D_{13}\frac{\partial\chi}{\partial z}$$

$$F_y = u_y\chi - D_{21}\frac{\partial\chi}{\partial x} - D_{22}\frac{\partial\chi}{\partial y} - D_{23}\frac{\partial\chi}{\partial z}$$

$$F_z = u_z\chi - D_{31}\frac{\partial\chi}{\partial x} - D_{32}\frac{\partial\chi}{\partial y} - D_{33}\frac{\partial\chi}{\partial z} \quad ,$$

which can be written concisely in tensor notation as

$$F_i = u_i\chi - D_{ij}\frac{\partial\chi}{\partial x_j} \tag{13}$$

with summation implied on the repeated subscript i, and with the understanding that F_x, F_y, F_z are replaced with F_1, F_2, F_3, respectively, and x, y, z are replaced with x_1, x_2, x_3.

The quantity D_{ij} is the tensor diffusivity and consists of nine quantities, which can be written in the matrix form

$$D_{ij} = \begin{bmatrix} D_{11} & D_{12} & D_{13} \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{bmatrix} \quad . \tag{14}$$

It is evident from equation (13) that the diffusion in a particular direction depends not only on $\partial\chi/\partial x$ but also on $\partial\chi/\partial y$ and $\partial\chi/\partial z$.

Substituting equation (13) into equation (4),

$$\begin{aligned} \frac{\partial\chi}{\partial t} &= -\nabla \cdot \bar{F} \\ &= -\frac{\partial F_i}{\partial x_i} \\ &= -\frac{\partial}{\partial x_i}\left(u_i\chi - D_{ij}\frac{\partial\chi}{\partial x_j}\right) \\ &= -\frac{\partial u_i}{\partial x_i}\chi - u_i\frac{\partial\chi}{\partial x_i} + \frac{\partial D_{ij}}{\partial x_i}\frac{\partial\chi}{\partial x_j} + D_{ij}\frac{\partial^2\chi}{\partial x_i\partial x_j} \quad . \end{aligned} \tag{15}$$

Assuming u_i and D_{ij} are constant, equation (15) reduces to

$$\frac{\partial \chi}{\partial t} = - u_i \frac{\partial \chi}{\partial x_i} + D_{ij} \frac{\partial^2 \chi}{\partial x_i \partial x_j} \quad . \tag{16}$$

Because of the difficulty in finding solutions of the general equation (15), we shall restrict ourselves to the more useful particular form, equation (16). By transformation of coordinates to a new set of rectangular axes, ξ_1, ξ_2, ξ_3 (called principal axes), equation (16) can be simplified to

$$\frac{\partial \chi}{\partial t} = -u_i \frac{\partial \chi}{\partial \xi_i} + D_i \frac{\partial^2 \chi}{\partial \xi_i^2} \tag{17}$$

or, in expanded form,

$$\frac{\partial \chi}{\partial t} = -u_1 \frac{\partial \chi}{\partial \xi_1} - u_2 \frac{\partial \chi}{\partial \xi_2} - u_3 \frac{\partial \chi}{\partial \xi_3} + D_1 \frac{\partial^2 \chi}{\partial \xi_1^2} + D_2 \frac{\partial^2 \chi}{\partial \xi_2^2} + D_3 \frac{\partial^2 \chi}{\partial \xi_3^2} \quad . \tag{18}$$

Evidently, the transformation has eliminated the cross derivatives and reduced the diffusion tensor to a diagonal form:

$$D_{ij} = \begin{bmatrix} D_1 & 0 & 0 \\ 0 & D_2 & 0 \\ 0 & 0 & D_3 \end{bmatrix} \quad . \tag{19}$$

The values of the coefficients D_1, D_2, D_3 (known as principal diffusion coefficients) in general will depend on the former coefficients D_{ij} given in equation (14) and also on the coordinate transformation coefficients.

We might note at this point that the equations developed herein are linear differential equations if D (or the D_{ij} in the case of anisotropic media) are constants or functions only of the coordinates and time. The property of linearity is important because it implies the principle of superposition; i.e., if one or more solutions are found the sum of these solutions is also a solution. It is not at all evident that the boundary conditions associated with a given problem can be satisfied. In some cases a particular solution will be sufficient, but generally a sum, usually an infinite sum, of particular solutions will be necessary to satisfy boundary conditions.

In summary, we list here the equations most tractable to solution in a practical situation together with the conditions under which they are applicable:

Equation (8):

$$\frac{\partial \chi}{\partial t} = D\nabla^2\chi$$ Isotropic media, constant D

Equation (11):

$$\frac{\partial \chi}{\partial t} + \vec{u} \cdot \nabla\chi = D\nabla^2\chi$$ Isotropic media, constant D, laminar flow with constant u

Equation (17):

$$\frac{\partial \chi}{\partial t} + u_i \frac{\partial \chi}{\partial x_i} = D_i \frac{\partial^2 \chi}{\partial x_i^2}$$ Anisotropic media, constant D_i, laminar flow with constant $\bar{u}$

In this last equation we have reverted to the standard symbols x_1, x_2, x_3 to denote the coordinates, with the understanding that these are principal coordinates.

III. SOURCE SOLUTIONS

A. Instantaneous Sources

The diffusion equations (8), (11), and (17) can be solved by the standard method of separation of variables or by the Laplace transformation. The literature on this is quite extensive [1-3]. The purpose here is to consider some solutions which are relevant to the atmosphere and which form a guide for the statistical theory of turbulent diffusion. The simplest example is the one-dimensional problem of a medium at rest ($u = 0$). If the diffusion is along one direction only, this implies that the concentration is uniform in the other two directions, meaning that the concentration gradient everywhere along these two directions is zero.

Denoting the diffusion direction by x, one can easily verify by direct substitution that the following expression, which can be derived by use of the Laplace transformation, is a solution of equation (8):

$$\chi = \frac{A}{\sqrt{t}} e^{-\frac{x^2}{4\,Dt}} \tag{20}$$

where A is an arbitrary constant. If we integrate this from $-\infty$ to $+\infty$, we obtain the total amount Q of diffusing substance per unit cross-sectional area of a cylinder of infinite length and cross section:

$$Q = \int_{-\infty}^{\infty} \chi dx = \frac{A}{\sqrt{t}} \int_{-\infty}^{\infty} e^{-\frac{x^2}{4Dt}} dx = 2A\sqrt{\pi D} \quad .$$

From this it follows that

$$A = \frac{Q}{2\sqrt{\pi D}} \quad ;$$

therefore, equation (20) becomes

$$\chi = \frac{Q}{2\sqrt{\pi Dt}}\, e^{-\frac{x^2}{4Dt}} \quad . \tag{21}$$

This result describes the diffusion of a quantity of substance Q which was initially concentrated in the plane $x = 0$, known as an instantaneous plane source. The fact that this is an idealized source is evident by observing that $\chi \to \infty$ as $t \to 0$. Nevertheless, this solution, as we shall see, forms the basis for obtaining more realistic solutions.

Since the solution, equation (21), has the functional form of a Gaussian or normal curve, we may compute the second moment of χ, defined by the integral

$$\int_{-\infty}^{\infty} \chi x^2\, dx = \frac{Q}{2\sqrt{\pi Dt}} \int_{-\infty}^{\infty} x^2 e^{-\frac{x^2}{4Dt}}\, dx = 2QDt \quad .$$

This result characterizes the "spread" of the concentration χ about its maximum value, which occurs at the origin. If we take this result and divide it by the total amount of diffusing matter Q, we obtain a quantity σ defined by

$$\sigma^2 = 2Dt \quad . \tag{22}$$

The quantity σ has the dimensions of a length and defines a kind of root-mean-square distance to which the substance has diffused. To make this clear, a plot of equation (21) for several values of σ^2 is shown in Figure 2. It is evident that the spread increases as σ increases. This behavior justifies the use of σ as a parameter characterizing the spread of χ. In statistical work, σ serves as a convenient scale of the width of the distribution and is known as "standard deviation." Its square is called the variance. Note that σ is a function of the

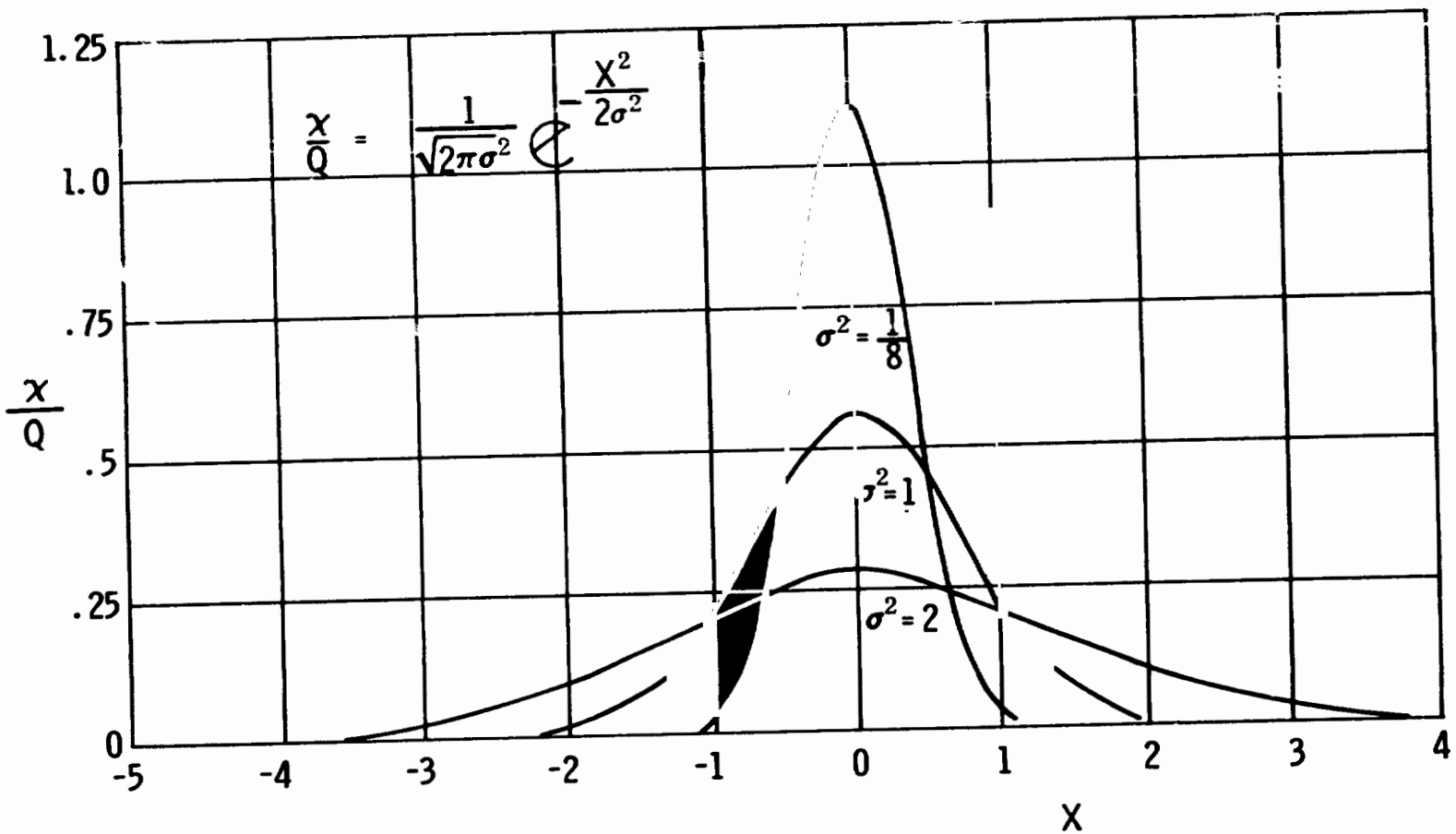

Figure 2. The solution for the instantaneous plane source for three values of σ^2, illustrating the spread of the distribution with increasing σ.

diffusivity and time. In terms of σ, equation (21) is

$$\chi = \frac{Q}{\sqrt{2\pi\sigma^2}} e^{-\frac{x^2}{2\sigma^2}} \quad . \tag{23}$$

As pointed out earlier, the instantaneous plane source is an idealized construct. A more realistic approach is to consider a source distributed over a finite region of x.

Such a formulation would be

$$\chi = \chi_0 \quad \text{for } -a < x < a \quad , \quad \text{and } t = 0$$

$$\chi = 0 \quad \text{elsewhere, } t = 0$$

where 2a is the thickness of the cloud. Uniformity along the y and z axes is again assumed. If we divide the interval $-a < x < a$ into an infinite number of infinitesimally thin sheets, each sheet can be considered an instantaneous plane source as defined previously. Then, because the diffusion equation is linear, the solution is obtained by summing up all the plane-source solutions arising from each sheet.

If x' denotes the coordinate of one of these thin sheets, the distance of a point x from the sheet is $x - x'$, where dx' is the differential thickness of the sheet. Thus, each sheet contributes an amount $d\chi$ to the total χ. That is,

$$d\chi = \frac{\chi_0}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-x')^2}{2\sigma^2}} dx' \quad .$$

Integrating from -a to +a, we obtain the solution

$$\chi = \frac{\chi_0}{\sqrt{2\pi\sigma^2}} \int_{-a}^{a} e^{-\frac{(x-x')^2}{2\sigma^2}} dx' \quad . \tag{24}$$

It is possible to write this integral in terms of the error function if we define a new variable by

$$s = \frac{x - x'}{\sqrt{2\sigma^2}} \quad , \quad ds = -\frac{dx'}{\sqrt{2\sigma^2}} \quad ;$$

and, denoting the new limits on the integral by p and q,

$$p = \frac{x + a}{\sqrt{2\sigma^2}} \quad , \quad q = \frac{x - a}{\sqrt{2\sigma^2}} \tag{25}$$

we can write

$$\chi = -\frac{\chi_0}{\sqrt{\pi}} \int_{p}^{q} e^{-s^2} ds$$

$$= -\frac{\chi_0}{\sqrt{\pi}} \left\{ \int_{0}^{q} e^{-s^2} ds - \int_{0}^{p} e^{-s^2} ds \right\}$$

$$= \frac{\chi_0}{\sqrt{\pi}} \left\{ \int_{0}^{p} e^{-s^2} ds - \int_{0}^{q} e^{-s^2} ds \right\}$$

$$= \frac{\chi_0}{2} \left\{ \frac{2}{\sqrt{\pi}} \int_0^p e^{-s^2} ds - \frac{2}{\sqrt{\pi}} \int_0^q e^{-s^2} ds \right\}$$

$$\equiv \frac{\chi_0}{2} \{\text{erf } p - \text{erf } q\}$$

or

$$\chi = \frac{\chi_0}{2} \left\{ \text{erf} \frac{x + a}{\sqrt{2\sigma^2}} - \text{erf} \frac{x - a}{\sqrt{2\sigma^2}} \right\} \tag{26}$$

where erf p and erf q represent the error functions of p and q as defined by the preceding integrals. Tables exist for evaluating the error function for a given value of its argument. Moreover, the error function possesses the following properties:

$$\text{erf}(-p) = -\text{erf } p \quad , \quad \text{erf}(0) = 0 \quad , \quad \text{erf}(\infty) = 1 \quad .$$

Figure 3 presents a plot of equation (26) for several values of the parameter Dt/a^2. At this point it might be well to remember that the time dependence of χ is contained in the quantity σ defined by equation (22).

The maximum value of χ at any given time occurs at $x = 0$, the center of the cloud. With $x = 0$ we have

$$p = \frac{a}{\sqrt{2\sigma^2}} \quad , \quad q = -p \quad ;$$

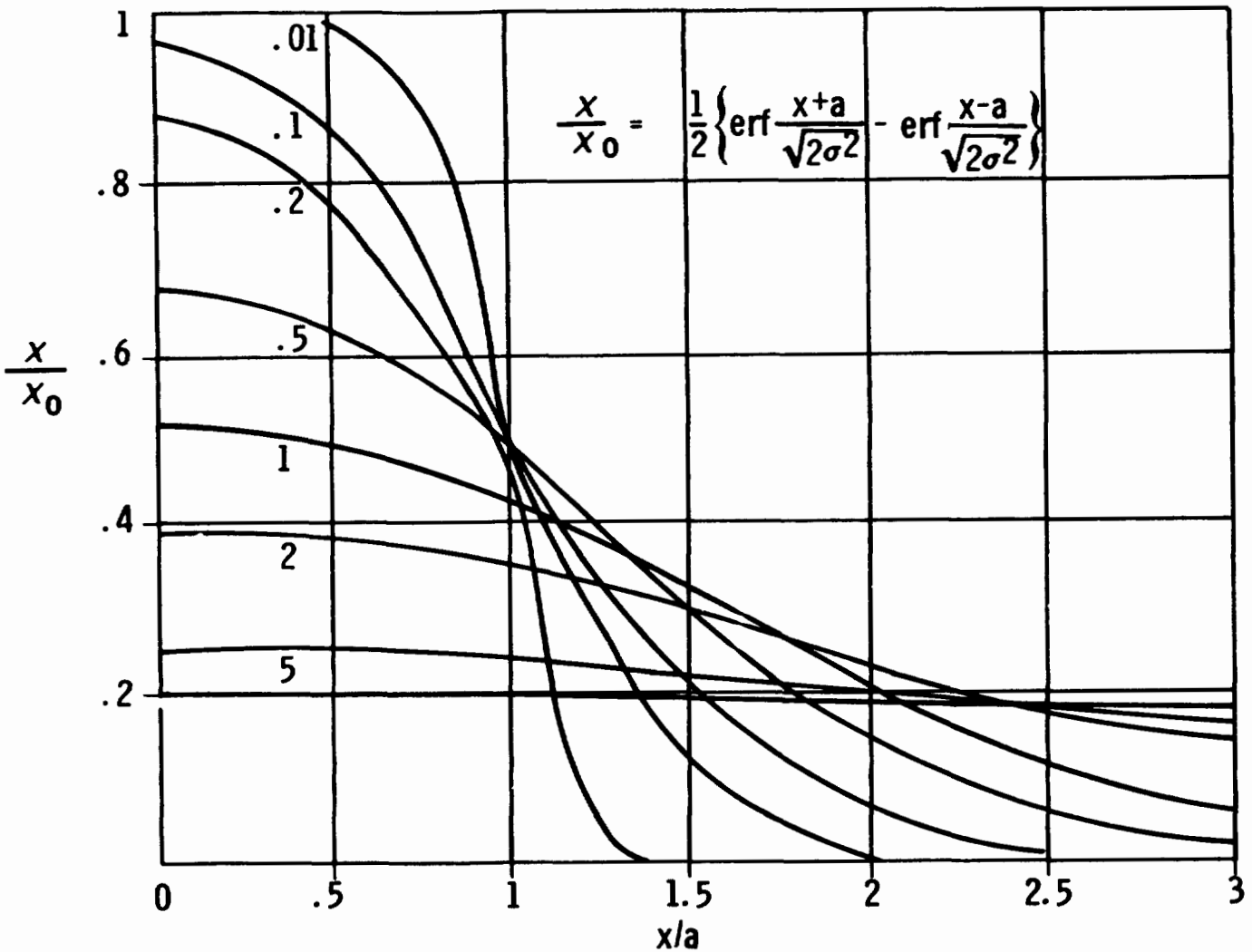

Figure 3. The solution for an instantaneous source of thickness 2a for several values of the dimensionless parameter $\sigma^2/2a^2$.

therefore, equation (26) yields

$$\chi_{max} = \chi_0 \operatorname{erf}\left(\frac{a}{\sqrt{2\sigma^2}}\right) \quad . \tag{27}$$

As an example of the use of the foregoing formulas, let the half-thickness a of the cloud, the diffusivity D, and the initial concentration χ_0 be given by

$$a = 1\text{m} \quad , \quad D = 0.66 \frac{\text{m}^2}{\text{sec}} \quad , \quad \chi_0 = 0.60 \frac{\text{kg}}{\text{m}^3}$$

and suppose we seek the concentration at a distance x = 60 m when t = 1800 sec (30 min). We first compute σ,

$$\sigma = \sqrt{2\,Dt} = \sqrt{2\left(0.66 \frac{\text{m}^2}{\text{sec}}\right)(1800 \text{ sec})} = 48.7 \text{ m} \quad ,$$

then p and q,

$$p = \frac{60 + 1}{\sqrt{2\,(48.7)}} = 0.89 \quad , \quad q = \frac{60 - 1}{\sqrt{2\,(48.7)}} = 0.86$$

and finally, with the aid of a table of the error function, equation (26) gives

$$\chi = \frac{0.60}{2} \frac{\text{kg}}{\text{m}^3} \{0.792 - 0.776\} = 0.0048 \frac{\text{kg}}{\text{m}^3} \quad .$$

In addition, one might compute also the maximum concentration of the distribution for this given time of 1800 sec. From equation (27) this is

$$\chi_{max} = 0.60 \frac{kg}{m^3} (0.017) = 0.010 \frac{kg}{m^3} \quad .$$

Note: Any consistent set of units may be used. For example, if length is measured in meters and time in seconds, D must be in m^2/sec. If length is measured in centimeters, then D should be in cm^2/sec. Similarly, the concentration may be in kg/m^3 or gm/cm^3. A larger unit for the time may be used provided D is expressed in this larger unit. For example, if $D = 0.2$ cm^2/sec, it would convert to $D = 0.2\ cm^2/sec \times 60\ sec/min$, or $D = 12\ cm^2/min$.

Thus far we have treated the problem of a source extended in a finite region in an infinite medium. For this problem, therefore, the solution tends to zero as x approaches infinity. If, however, the medium is not infinite, then we must assume the existence of a boundary at some distance $x = L$. At such a boundary, we can have either total reflection or total absorption of the diffusing matter or, more generally, some reflection and some absorption, all depending on the nature of the boundary. In the case of the atmosphere, this boundary may be the ground, a hillside, a building in the path of the diffusing matter, or it may even be another layer of the atmosphere which possesses different diffusion characteristics.

If at the boundary we have a prescribed flux, the mathematical statement of the flux should be a linear function of χ. If not, a solution can rarely, if ever, be found. An example of a linear flux condition is

$$-D \frac{\partial \chi}{\partial n} = H (\chi - \chi_0) \text{ at } x = L \quad ,$$

where the left member is the definition of flux (n specifies the normal direction at the boundary surface). The right side, where H is some constant, states that the flux is proportional to the difference in concentration between the surface

and the surrounding medium at constant concentration χ_0. In the case of heat flow, this condition is an expression of Newton's law of cooling, valid for small temperature differences.

If, however, the flux is totally reflected at the boundary surface, we have the condition of zero flux:

$$D \frac{\partial \chi}{\partial n} = 0 \text{ at } x = L \quad .$$

A solution with this boundary condition can be easily determined by the method of images. For example, we imagine that there is a source at $x = 2L$ which is a mirror image of the real source, i.e. identical in every respect. The two sources diffuse in identical fashion, and midway between at $x = L$ at the boundary surface, the flux from one exactly cancels the flux from the other, resulting in the prescribed zero flux. The geometry of this is depicted in Figure 4. Furthermore, since the diffusion equation is linear, the sum of the two solutions will yield the desired solution to our boundary-value problem with the impermeable boundary.

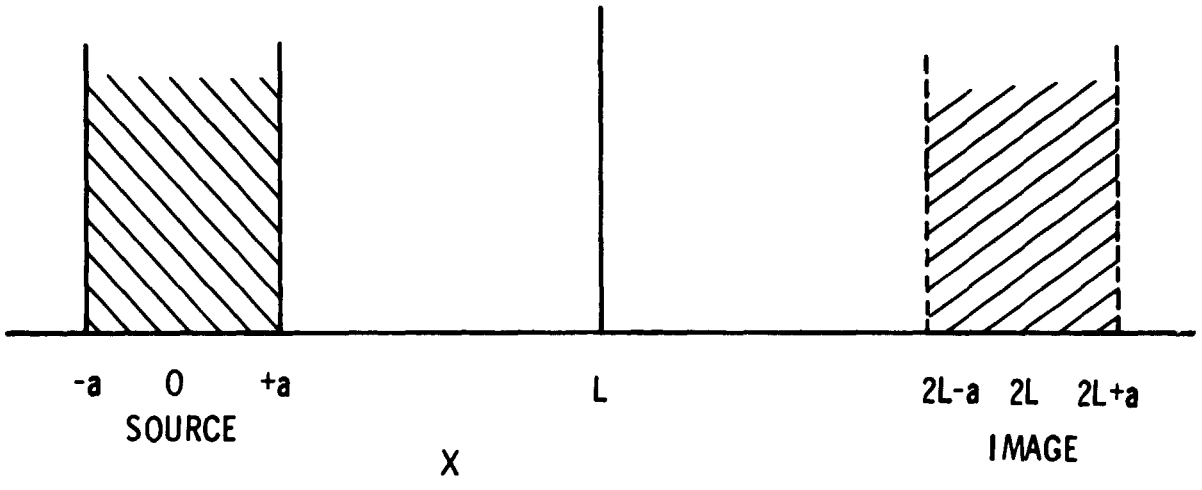

Figure 4. The real source and its image, where $\chi = L$ is an impermeable boundary and all quantities are measured relative to a coordinate x whose origin is at the center of the source.

The solution of the mirror-image source will be an integral similar to equation (24) for the actual source. That integral was obtained by placing the origin of the coordinate system at the center of the source. We do the same with the image source except now the new coordinate is denoted by $\tilde{x}$. Thus, this solution is

$$\tilde{\chi} = \frac{\chi_0}{\sqrt{2\pi\sigma^2}} \int_{\tilde{x}=-a}^{\tilde{x}=a} e^{-\frac{(\tilde{x}-\tilde{x}')^2}{2\sigma^2}} d\tilde{x}' \quad .$$

The coordinate transformation connecting $\tilde{x}$ and the original coordinate x is

$$\tilde{x} = x - 2L \quad .$$

With this relation, the integral can be written relative to the original coordinate. The relevant quantities transform as follows:

$$\tilde{x} - \tilde{x}' = (x - 2L) - (x' - 2L)$$

$$= x - x'$$

$$d\tilde{x}' = dx \quad ,$$

and the lower and upper limits become 2L - a and 2L + a. Thus, the mirror-image solution is

$$\chi = \frac{\chi_0}{\sqrt{2\pi\sigma^2}} \int_{2L-a}^{2L+a} e^{-\frac{(x-x')^2}{2\sigma^2}} dx' \quad .$$

This integral is identical to equation (24) except for the limits. Proceeding as before, we find

$$p' = \frac{x + a - 2L}{\sqrt{2\sigma^2}} \qquad q' = \frac{x - a - 2L}{\sqrt{2\sigma^2}}$$

and the solution is

$$\chi = \frac{\chi_0}{2} \{\text{erf } p' - \text{erf } q'\} \quad .$$

Finally, the complete solution is the sum of this and equation (24):

$$\chi = \frac{\chi_0}{2} \{\text{erf } p - \text{erf } q + \text{erf } p' - \text{erf } q'\}$$

or, in explicit form,

$$\chi = \frac{\chi_0}{2} \left\{ \text{erf} \frac{x + a}{\sqrt{2\sigma^2}} - \text{erf} \frac{x - a}{\sqrt{2\sigma^2}} + \text{erf} \frac{x + a - 2L}{\sqrt{2\sigma^2}} - \text{erf} \frac{x - a - 2L}{\sqrt{2\sigma^2}} \right\} . \quad (28)$$

At the boundary $x = L$,

$$\chi\ (x = L) = \chi_0 \left\{ \text{erf} \frac{a + L}{\sqrt{2\sigma^2}} + \text{erf} \frac{a - L}{\sqrt{2\sigma^2}} \right\} \quad . \quad (29)$$

We consider next two- and three-dimensional problems. It can be verified that a source solution of the two-dimensional diffusion equation,

$$\frac{\partial \chi}{\partial t} = D \left(\frac{\partial^2 \chi}{\partial x^2} + \frac{\partial^2 \chi}{\partial y^2} \right) \quad ,$$

where again we assume the flow velocity to be zero, is given by

$$\chi = Ae^{-\frac{x^2}{2\sigma^2} - \frac{y^2}{2\sigma^2}}$$

where A is an arbitrary constant. For the diffusion to be indeed two-dimensional everywhere, it must be presumed that there is uniformity of concentration in the z direction and that the source is uniformly distributed over the entire z axis. Therefore, the constant A can be determined by demanding that the total amount of diffusing matter, Q_T, in a cylinder of finite height concentric with the z axis, but of infinite radius, must be conserved. This Q_T is given by

$$Q_T = \int_{z_1}^{z_2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \chi \, dx \, dy \, dz$$

$$= A \int_{z_1}^{z_2} dz \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\sigma^2}} dx \int_{-\infty}^{\infty} e^{-\frac{y^2}{2\sigma^2}} dy$$

$$= A \, (z_2 - z_1) \, (\sqrt{2\pi\sigma^2} \sqrt{2\pi\sigma^2})$$

$$= 2\pi\sigma^2 A \, (z_2 - z_1)$$

or

$$\frac{Q_T}{z_2 - z_1} = 2\pi\sigma^2 A \quad .$$

Since $z_2 - z_1$ is the height of the cylinder, the quantity on the right is the total matter per unit length of cylinder which, to be conserved, must equal the initial line density Q on the z axis. Thus

$$Q = 2\pi\sigma^2 A$$

or

$$A = \frac{Q}{2\pi\sigma^2}$$

so that

$$\chi = \frac{Q}{2\pi\sigma^2} e^{-\frac{x^2}{2\sigma^2} - \frac{y^2}{2\sigma^2}} \quad . \tag{30}$$

Note the dimensions of Q: the amount of matter per unit length of line.

The solution, equation (30), governs the diffusion of an instantaneous and infinitesimally thin source located on the z axis; hence, the name "line source" is given to it. Converting to the polar coordinate ρ defined by

$$\rho^2 = x^2 + y^2 \quad ,$$

the solution can be written as

$$\chi = \frac{Q}{2\pi\sigma^2} e^{-\frac{\rho^2}{2\sigma^2}} \tag{31}$$

which, with the exception of the constant $Q/2\pi\sigma^2$ (constant with respect to the coordinates, since σ is still a function of time), has exactly the same form as the one-dimensional solution. The role of x is now played by ρ. Thus, at any given time the concentration at points equidistant from the origin is the same; i.e., the contours of constant χ are circles centered at the origin. Any plane parallel to the z axis and through the origin would show a concentration profile exactly as in the one-dimensional case.

The solution for a long cylindrical source of radius a cannot be obtained in terms of elementary functions. We merely quote the result which is

$$\chi = \frac{\chi_0}{\sigma^2} e^{-\frac{\rho^2}{2\sigma^2}} \int e^{-\frac{\rho'^2}{2\sigma^2}} I_0\left(\frac{\rho\rho'}{\sigma^2}\right) \rho' \, d\rho' \tag{32}$$

where ρ' represents the radial coordinate of a point in the cylinder (the integration variable over the region), ρ is the observation point, and I_0 is the modified Bessel function of the first kind of zero order. There is no way of evaluating this integral except numerically. An elementary solution, however, exists for points on the axis of the cylinder. At such points $\rho = 0$ and $I_0(0) = 1$. By elementary integration, we obtain

$$\chi = \chi_0 \left(1 - e^{-\frac{a^2}{2\sigma^2}}\right) \quad . \tag{33}$$

This simple formula is useful in determining the decay of the concentration on the axis, where the concentration is always above that of surrounding points.

In three dimensions the instantaneous point source solution is

$$\chi = Ae^{-\frac{x^2}{2\sigma^2} - \frac{y^2}{2\sigma^2} - \frac{z^2}{2\sigma^2}} .$$

In this case the integral over all space must equal the initial source strength, which we now denote by χ_0 instead of Q because it has the same dimensions as χ. Thus

$$\chi_0 = A \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\sigma^2} - \frac{y^2}{2\sigma^2} - \frac{z^2}{2\sigma^2}} \, dx \, dy \, dz$$

$$= A \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\sigma^2}} dx \int_{-\infty}^{\infty} e^{-\frac{y^2}{2\sigma^2}} dy \int_{-\infty}^{\infty} e^{-\frac{z^2}{2\sigma^2}} dz$$

$$= A\,(2\pi\sigma^2)^{3/2}$$

or

$$A = \frac{\chi_0}{(2\pi\sigma^2)^{3/2}} \quad ;$$

therefore,

$$\chi = \frac{\chi_0}{(2\pi\sigma^2)^{3/2}} e^{-\frac{x^2 + y^2 + z^2}{2\sigma^2}}$$

$$= \frac{\chi_0}{(2\pi\sigma^2)^{3/2}} e^{-\frac{r^2}{2\sigma^2}} \qquad (34)$$

where $r^2 = x^2 + y^2 + z^2$ is the radial coordinate. Again we see that the cloud grows along any diameter, as in the one-dimensional case.

The point source solution, equation (34), may be integrated to obtain the solution for a uniform spherical source of radius a. In spherical coordinates with axes at the center of the sphere, we let r be the radial coordinate to the point of observation, r' the coordinate of a volume element of the sphere, and R the distance to the observation point. Because the concentration is spherically symmetric, without loss of generality we choose the observation point on the z axis.

Referring to Figure 5, we see that

$$R^2 = r^2 + r'^2 - 2rr' \cos \theta \quad .$$

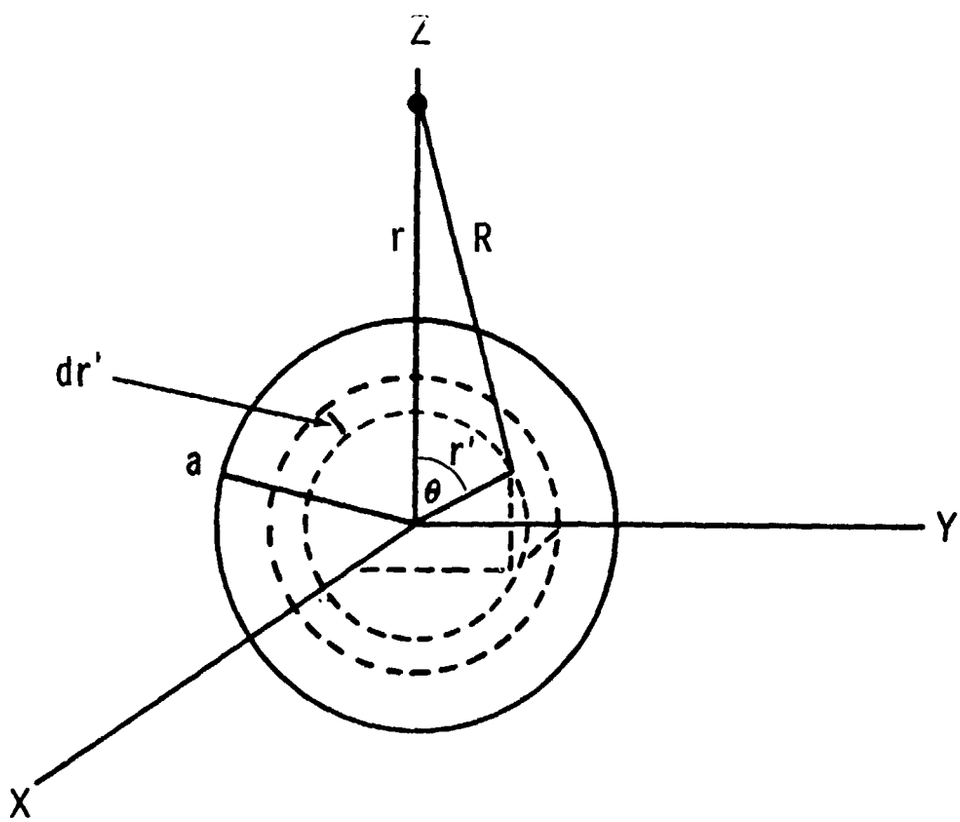

Figure 5. The geometry for the integration of the point source solution for a spherical source of radius a.

Therefore,

$$\chi = \frac{\chi_0}{(2\pi\sigma^2)^{3/2}} \int_0^{2\pi} \int_0^{\pi} \int_0^{a} e^{-\frac{r^2+r'^2-2rr'\cos\theta}{2\sigma^2}} r'^2 \sin\theta \, dr' \, d\theta \, d\phi$$

$$= \frac{\chi_0}{(2\pi\sigma^2)^{3/2}} \int_0^{2\pi} d\phi \int_0^{\pi} e^{+\frac{2rr'\cos\theta}{2\sigma^2}} \sin\theta \, d\theta \int_0^{a} r'^2 e^{-\frac{r^2+r'^2}{2\sigma^2}} dr' \quad .$$

$$= \frac{\chi_0}{(2\pi\sigma^2)^{3/2}} \frac{2\pi\sigma^2}{r} \int_0^{a} r' e^{-\frac{r^2+r'^2}{2\sigma^2}} \left[e^{\frac{2rr'}{2\sigma^2}} - e^{-\frac{2rr'}{2\sigma^2}} \right] dr'$$

$$= \frac{\chi_0}{\sqrt{2\pi}\sigma r} \left\{ \int_0^{a} r' e^{-\frac{(r-r')^2}{2\sigma^2}} dr' - \int_0^{a} r' e^{-\frac{(r+r')^2}{2\sigma^2}} dr' \right\} \quad .$$

We now make a change of variable to u in the first integral and to v in the second:

$$u = \frac{r - r'}{\sqrt{2}\,\sigma} \quad , \quad v = \frac{r + r'}{\sqrt{2}\,\sigma} \quad .$$

Writing also

$$p = \frac{r + a}{\sqrt{2}\,\sigma} \qquad q = \frac{r - a}{\sqrt{2}\,\sigma} \quad ,$$

we have

$$\chi = \frac{\chi_0}{\sqrt{\pi}\, r} \left\{ - \int_{\frac{r}{\sqrt{2}\sigma}}^{q} (r - \sqrt{2}\,\sigma u)\, e^{-u^2}\, du \right.$$

$$\left. + \int_{\frac{r}{\sqrt{2}\sigma}}^{p} (r - \sqrt{2}\,\sigma\, v)\, e^{-v^2}\, dv \right\} .$$

These integrands are identical, u and v being variables of integration. We can, therefore, interchange the limits on the first integral and then write the sum of the two integrals as a single integral, which is allowed by the fundamental property of definite integrals for continuous intervals. Thus

$$\chi = \frac{\chi_0}{\sqrt{\pi}\, r} \int_q^p (r - \sqrt{2}\,\sigma u)\, e^{-u^2}\, du$$

$$= \frac{\chi_0}{\sqrt{\pi}\, r} \left\{ r \int_q^p e^{-u^2}\, du - \sqrt{2}\,\sigma \int_q^p u e^{-u^2}\, du \right\} .$$

We now write the first integral as the difference of two integrals, one from 0 to p and the other from 0 to q. The second integral is integrated directly by elementary means. Thus

$$\chi = \frac{\chi_0}{\sqrt{\pi}\, r} \left\{ r \int_0^p e^{-u^2}\, du - r \int_0^q e^{-u^2}\, du + \frac{\sqrt{2}\,\sigma}{2} \left(e^{-p^2} - e^{-q^2} \right) \right\}$$

$$= \frac{\chi_0}{2} \left\{ \operatorname{erf} p - \operatorname{erf} q + \sqrt{\frac{2}{\pi}}\, \frac{\sigma}{r} \left(e^{-p^2} - e^{-q^2} \right) \right\} \tag{35}$$

which is the solution for a sphere of radius a.

B. Continuous Sources

We consider now the three fundamental sources, plane, line, and point, when they emit continuously for times $t > 0$ at the rate of $Q(t')$ units per unit time. In the time element from t' to $t' + dt'$, an amount $Q(t')\, dt'$ of material is emitted. Moreover, the standard deviation of the distribution will depend on the time t' in the following way:

$$\sigma^2 = 2D(t - t') \quad . \tag{36}$$

From equation (23) the contribution to χ due to an elemental plane source $Q\, dt'$ is

$$d\chi = \frac{Q\, dt'}{2\sqrt{\pi D}}\, \frac{e^{-\frac{x^2}{4D(t-t')}}}{(t - t')^{1/2}} \quad .$$

Integrating this over the time of emission, we have

$$\chi = \frac{1}{2\sqrt{\pi D}} \int_0^t Q(t')\, \frac{e^{-\frac{x^2}{4D(t-t')}}}{(t - t')^{1/2}}\, dt'$$

which is the general solution if the emission rate Q is some general function of time. For a constant emission rate, this becomes

$$\chi = \frac{Qx}{2D\sqrt{\pi}} \int_{\frac{x}{2\sqrt{Dt}}}^{\infty} \frac{e^{-s^2}}{s^2}\, ds$$

where we put

$$s = \frac{x}{2\sqrt{D(t - t')}} \quad .$$

Integrating by parts,

$$\chi = \frac{Qx}{2D\sqrt{\pi}} \left\{ -\frac{1}{s} e^{-s^2} \Bigg|_{\frac{x}{2\sqrt{Dt}}}^{\infty} -2 \int_{\frac{x}{2\sqrt{Dt}}}^{\infty} e^{-s^2}\, ds \right\}$$

$$= \sqrt{\frac{t}{\pi D}}\, Qe^{-\frac{x^2}{4Dt}} - \frac{Qx}{\sqrt{\pi D}} \int_{\frac{x}{2\sqrt{Dt}}}^{\infty} e^{-s^2}\, ds$$

$$= \sqrt{\frac{t}{\pi D}}\, Qe^{-\frac{x^2}{4Dt}} - \frac{Qx}{2D} \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}}\right) \tag{37}$$

where erfc α is the complementary error function defined by

$$\operatorname{erfc} \alpha = \frac{2}{\sqrt{\pi}} \int_{\alpha}^{\infty} e^{-s^2}\, ds$$

$$= \frac{2}{\sqrt{\pi}} \int_{0}^{\infty} e^{-s^2}\, ds - \frac{2}{\sqrt{\pi}} \int_{0}^{\alpha} e^{-s^2}\, ds$$

$$= 1 - \operatorname{erf} \alpha$$

since the first integral evaluates to unity and the second is the error function, by definition.

Similarly, employing equation (31), the solution for a continuous line source is

$$\chi = \frac{1}{4\pi D} \int_{0}^{t} Q(t') \frac{e^{-\frac{\rho^2}{4D(t-t')}}}{t - t'}\, dt'$$

which for constant Q is

$$\chi = \frac{Q}{4\pi D} \int_{\frac{\rho^2}{4Dt}}^{\infty} \frac{e^{-s}}{s}\, ds$$

where in this case we defined s by

$$s = \frac{\rho^2}{4D(t - t')} \quad .$$

The exponential integral involved in this solution cannot be evaluated in closed form. Its series expansion is

$$\int_{\alpha}^{\infty} \frac{e^{-s}}{s}\, ds = -\gamma - \ln \alpha - \sum_{n=1}^{\infty} \frac{(-1)^n \alpha^n}{nn!}$$

where $\gamma = 0\ 57721 \ldots$ is Euler's constant. Thus,

$$\chi = \frac{Q}{4\pi D} \left\{ \ln \frac{4Dt}{\rho^2} - \gamma - \sum_{n=1}^{\infty} \frac{(-1)^n}{nn!} \left(\frac{\rho^2}{4Dt}\right)^n \right\} \quad . \tag{38}$$

For large values of t the series term can be neglected, giving the approximate form

$$\chi \sim \frac{Q}{4\pi D} \left(\ln \frac{4Dt}{\rho^2} - \gamma \right) \quad . \tag{39}$$

Finally, in like fashion, we can write the solution for a continuous point source with the aid of equation (34):

$$\chi = \frac{1}{8(\pi D)^{3/2}} \int_0^t Q(t') \frac{e^{-\frac{r^2}{4D(t-t')}}}{(t-t')^{3/2}}\, dt' \quad .$$

Putting

$$s = \frac{r}{2\sqrt{D(t-t')}}$$

and for constant Q, we have

$$\chi = \frac{Q}{2\pi^{3/2}\,Dr} \int_{\frac{r}{2\sqrt{Dt}}}^{\infty} e^{-s^2}\,ds$$

$$= \frac{Q}{4\pi Dr}\,\mathrm{erfc}\left(\frac{r}{2\sqrt{Dt}}\right) \quad . \tag{40}$$

We might note for this solution that as $t \to \infty$ it reduces to $Q/4\pi Dr$ which is a steady state distribution.

C. Source Solutions in a Moving Medium

The extension of the source solutions to the case of a moving medium is rather simple. We note that the solutions obtained in the case of a stationary medium may be considered solutions as observed from a coordinate system moving with the medium. Then, by transforming coordinates to a stationary system, the corresponding solutions for a medium in motion relative to the system at rest are obtained immediately.

If u, v, w are the vector components, assumed constant, of the velocity of the medium, and x', y', z' are the coordinates of a point as observed in the stationary system, then the coordinates of the point relative to a moving system are given by

$$\begin{aligned} x &= x' - ut \\ y &= y' - vt \quad . \\ z &= z' - wt \end{aligned} \tag{41}$$

Substitution of these expressions into the equations for instantaneous sources for a stationary medium will yield the solutions for a moving medium. For example, the point-source solution, equation (34), would take the form

$$\chi = \frac{\chi_0}{(2\pi)^{3/2}\sigma^3} e^{-\frac{(x'-ut)^2}{2\sigma^2} - \frac{(y'-vt)^2}{2\sigma^2} - \frac{(z'-wt)^2}{2\sigma^2}} ,$$

with similar results for the plane and line sources. One can always choose a coordinate system such that one of the axes, e.g. the X axis, is parallel to the velocity. For the point source we would have the simpler result:

$$\chi = \frac{\chi_0}{(2\pi)^{3/2}\sigma^3} e^{-\frac{(x'-ut)^2}{2\sigma^2} - \frac{y^2}{2\sigma^2} - \frac{z^2}{2\sigma^2}} \tag{42}$$

where the prime on x may be dropped with the understanding that it is measured from a fixed system. The fact that these expressions satisfy the diffusion equation for a moving medium can be verified by direct substitution.

In general, if $\chi(x', y', z', t)$ is any instantaneous source solution of the diffusion equation for a stationary medium

$$\frac{\partial \chi}{\partial t} = D\nabla'^2 \chi ,$$

where the prime on the Laplacian indicates derivatives with respect to the primed coordinates, then $\chi(x, y, z, t)$ is a solution of the diffusion equation for a moving medium

$$\frac{\partial \chi}{\partial t} + \vec{V} \cdot \nabla\chi = D\nabla^2\chi$$

where x, y, z are given by the relations of equation (41) and $\vec{V} = (u, v, w)$.

From the solution of equation (42), the expression for a continuous point source in a wind can be determined. This would represent roughly a model of a chimney plume, because the plume may be considered as a continuous series of point source clouds or puffs. At time t' the source emits an elemental amount Qdt' of matter, while an element of air at the point (x, y, z) at time t will have been initially at x - u(t - t'), y, z because of the wind. Thus, the concentration $d\chi$ at (x, y, z) and at time t due to an instantaneous puff of amount Qdt' is

$$d\chi = \frac{Qdt'}{8[\pi D(t-t')]^{3/2}} e^{-\frac{[x-u(t-t')]^2+y^2+z^2}{4D(t-t')}} .$$

If the emission rate Q is constant, the total concentration will be

$$\chi = \frac{Q}{8(\pi D)^{3/2}} \int_0^t \frac{e^{-\frac{[x-u(t-t')]^2+y^2+z^2}{4D(t-t')}}}{(t-t')^{3/2}} dt' .$$

For a source maintained indefinitely, which is most important in practice, the limits on this integral would be from 0 to ∞. In this case the integral can be evaluated in closed form. Thus,

$$\chi = \frac{Qe^{\frac{ux}{2D}}}{2\pi^{3/2}Dr} \int_0^\infty e^{-\left(s^2+\frac{u^2r^2}{16D^2s^2}\right)} ds$$

$$= \frac{Q}{4\pi Dr} e^{-\frac{u}{2D}(r-x)} \qquad (43)$$

where $r^2 = x^2 + y^2 + z^2$ and

$$s = \frac{r}{2\sqrt{D(t - t')}} \quad .$$

We might note that equation (43) is independent of time, as expected for a source maintained indefinitely at a constant emission rate.

Furthermore, studies on smoke clouds have shown that the cloud has the form of a long, thin plume if the wind velocity is not too low. In this case one is usually interested in the concentration values near the axis of the plume, where $y = z = 0$. On the axis itself the above expression takes the very simple form

$$\chi = \frac{Q}{4\pi Dx} \quad .$$

For points near the axis relatively far downwind the quantity $(y^2 + z^2)/x^2$ is small. With the aid of the binomial expansion and neglecting powers of this quantity higher than the first,

$$r = x\left(1 + \frac{y^2 + z^2}{x^2}\right)^{1/2}$$

$$\simeq x\left(1 + \frac{y^2 + z^2}{2x^2}\right) \quad .$$

Putting this into the exponent of equation (43) gives the approximate form

$$\chi = \frac{Q}{4\pi Dr}\, e^{-\frac{u(y^2+z^2)}{4Dx}} \quad .$$

One can also, in practice, replace the r in the coefficient of the exponential factor by x because in most instances $r \simeq x$ for points near the axis.

Similarly, from the solution of equation (30) we determine the formula for a constant continuous line source in a wind:

$$\chi = \frac{Q}{4\pi D} \int_0^t \frac{e^{-\frac{[x-u(t-t')]^2+y^2}{4D(t-t')}}}{t-t'} dt' \quad .$$

Again, assuming the source is maintained indefinitely and making a change of variable to

$$s = \frac{1}{4D(t-t')} \quad ,$$

we have

$$\chi = \frac{Qe^{\frac{ux}{2D}}}{2\pi D} \int_0^\infty \frac{e^{-\left(\rho^2 s - \frac{u^2}{16D^2 s}\right)}}{s} ds$$

$$= \frac{Qe^{\frac{ux}{2D}}}{2\pi D} K_0\left(\frac{\rho u}{2D}\right) \tag{44}$$

where K_0 is the modified Bessel function of the second kind.

For sufficiently large values of the argument $\rho u/2D$, we may use the asymptotic expansion for K_0, i.e.,

$$K_0\left(\frac{\rho u}{2D}\right) \simeq \sqrt{\frac{2\pi D}{\rho u}}\, e^{-\frac{\rho u}{2D}}$$

so that equation (44) becomes approximately

$$\chi = \frac{Qe^{\frac{ux}{2D}}}{\sqrt{2\pi D\rho u}}\, e^{-\frac{\rho u}{2D}} \quad \text{for} \quad \frac{\rho u}{2D} >> 1 \quad .$$

If one is interested in the concentration relatively far downwind and near the x axis, which is usually the case, then a further simplification is possible. Expanding

$$\rho = (x^2 + y^2)^{1/2}$$

$$\simeq x\left(1 + \frac{y^2}{2x^2}\right) \quad \text{for} \quad \frac{x}{y} >> 1 \quad ,$$

the asymptotic solution becomes

$$\chi \simeq \frac{Q}{\sqrt{2\pi D\rho u}}\, e^{-\frac{uy^2}{4Dx}} \quad \text{for} \quad \frac{\rho u}{2D} >> 1 \quad \text{and} \quad \frac{x}{y} >> 1 \quad .$$

In this expression one may also replace ρ by x without serious error.

Thus far in treating continuous sources with or without wind, we have implied an atmosphere continuous in all directions, i.e., one with no boundaries. Often, however, the source of the diffusing cloud is on or near the Earth's surface, where reflection, absorption, or deposition of particulate matter under gravity can occur. Although in reality all three effects take place more or less,

in many problems it can be assumed without serious error that the surface acts as an impervious boundary, implying total reflection. Since the continuous point source in a wind at or near the ground is of considerable importance, we will obtain the solution to this problem in the presence of an impervious boundary (the ground).

The method of images will be employed, as was done for the extended instantaneous plane source. In obtaining the solution, equation (43), the origin of coordinates was placed at the source. For reasons of convenience and symmetry we now place the origin on the ground and the source on the Z axis at a height $z = H$; therefore, the image source is placed at $z = -H$ (Fig. 6). For the two sources, the solution is still given by equation (43) except now the distance to the observation point r from the actual source is given by

$$r^2 = x^2 + y^2 + (z - H)^2$$

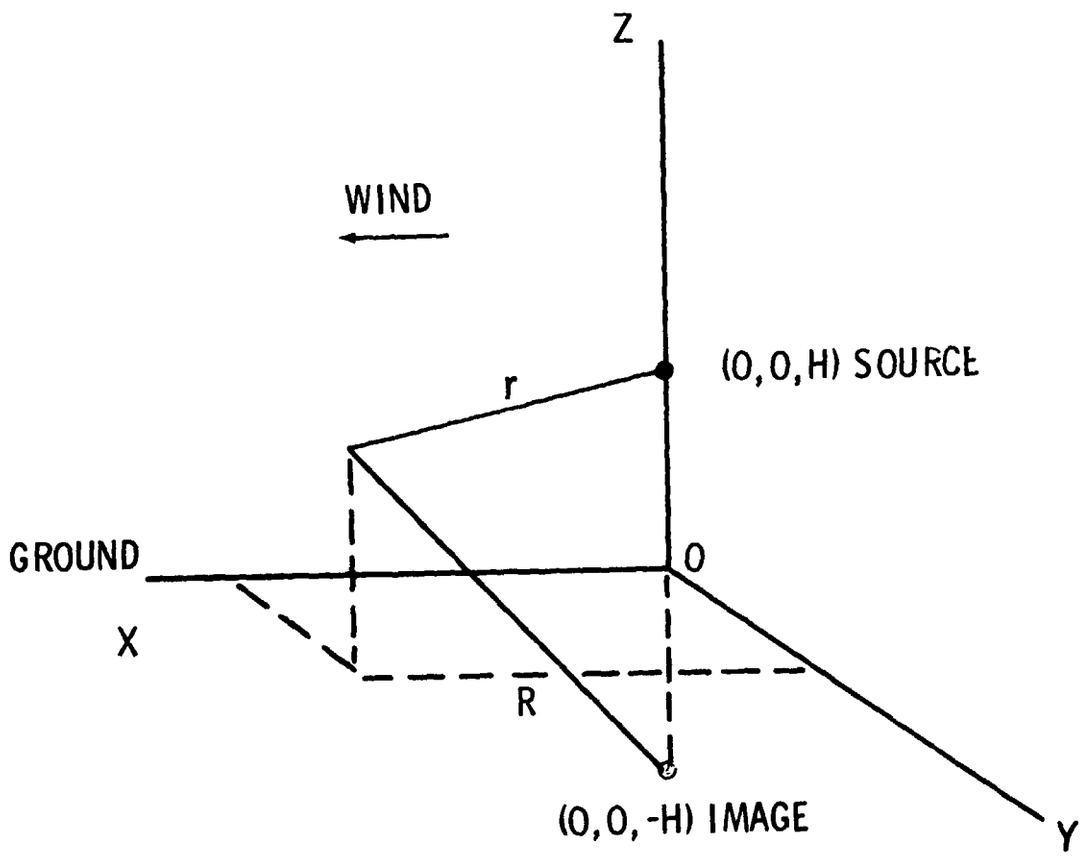

Figure 6. The continuous point source in a wind and its image.

and that of the image source is given by

$$R^2 = x^2 + y^2 + (z + H)^2 \quad .$$

Taking the sum of the two solutions, we have

$$\chi = \frac{Q}{4\pi D}\left\{\frac{1}{r}\, e^{-\frac{u(r-x)}{2D}} + \frac{1}{R}\, e^{-\frac{u(R-x)}{2D}}\right\}$$

which is the exact solution. Making the same approximation for points near the x axis as was done previously, we have

$$\chi = \frac{Qe^{-\frac{uy^2}{4Dx}}}{4\pi Dx}\left\{e^{-\frac{u(z-H)^2}{4Dx}} + e^{-\frac{u(z+H)^2}{4Dx}}\right\} \quad .$$

For a source on the ground, one puts $H = 0$ in these expressions. Along the centerline of the plume, $y = z = 0$, this equation reduces to

$$\chi = \frac{Q}{2\pi Dx}\, e^{-\frac{uH^2}{4Dx}} \quad .$$

D. Source Solutions in an Anisotropic Medium

For a nonisotropic and moving medium, the basic equation is equation (17). Assuming that the velocity of the medium is parallel to the X direction, the equation in expanded form is

$$\frac{\partial \chi}{\partial t} + u\,\frac{\partial \chi}{\partial x} = D_1\,\frac{\partial^2 \chi}{\partial x^2} + D_2\,\frac{\partial^2 \chi}{\partial y^2} + D_3\,\frac{\partial^2 \chi}{\partial z^2} \quad . \tag{45}$$

To obtain solutions of this equation appropriate to an infinite medium such as the atmosphere, we first make a change of coordinates defined by

$$x' = \frac{(D_1D_2D_3)^{1/6}}{D_1^{1/2}}\, x$$

$$y' = \frac{(D_1D_2D_3)^{1/6}}{D_2^{1/2}}\, y \qquad . \tag{46}$$

$$z' = \frac{(D_1D_2D_3)^{1/6}}{D_3^{1/2}}\, z$$

Then, by differentiation, the derivatives with respect to x transform as follows:

$$\frac{\partial\chi}{\partial x} = \frac{\partial\chi}{\partial x'}\,\frac{\partial x'}{\partial x} = \frac{\partial\chi}{\partial x'}\,\frac{(D_1D_2D_3)^{1/6}}{D_1^{1/2}}$$

$$\frac{\partial^2\chi}{\partial x^2} = \frac{\partial^2\chi}{\partial x'^2}\left(\frac{\partial x'}{\partial x}\right)^2 + \frac{\partial\chi}{\partial x'}\,\frac{\partial^2 x'}{\partial x}$$

$$= \frac{\partial^2\chi}{\partial x'^2}\,\frac{(D_1D_2D_3)^{1/3}}{D_1}$$

and similarly for the derivatives with respect to y and z

$$\frac{\partial\chi}{\partial y} = \frac{\partial\chi}{\partial y'}\,\frac{(D_1D_2D_3)^{1/6}}{D_2^{1/2}}$$

$$\frac{\partial^2\chi}{\partial y^2} = \frac{\partial^2\chi}{\partial y'^2}\,\frac{(D_1D_2D_3)^{1/3}}{D_2}$$

$$\frac{\partial \chi}{\partial z} = \frac{\partial \chi}{\partial z'} \frac{(D_1 D_2 D_3)^{1/6}}{D_3^{1/2}}$$

$$\frac{\partial^2 \chi}{\partial z^2} = \frac{\partial^2 \chi}{\partial z'^2} \frac{(D_1 D_2 D_3)^{1/3}}{D_3} \quad .$$

Also, the velocity along the new coordinate is found by differentiating x' with respect to time, resulting in

$$u' = \frac{(D_1 D_2 D_3)^{1/6}}{D_1^{1/2}} u \quad .$$

Thus, the diffusion equation takes the form

$$\frac{\partial \chi}{\partial t} + u' \frac{\partial \chi}{\partial x'} = (D_1 D_2 D_3)^{1/3} \left\{ \frac{\partial^2 \chi}{\partial x'^2} + \frac{\partial^2 \chi}{\partial y'^2} + \frac{\partial^2 \chi}{\partial z'^2} \right\} \tag{47}$$

which has the same mathematical structure as the equation for isotropic media with an effective diffusivity equal to $(D_1 D_2 D_3)^{1/3}$. Therefore, the appropriate solutions can be written by inspection in analogy to the solutions developed for isotropic media.

The procedure is as follows. Treating the instantaneous point source first, we see that the solution of equation (47) is given by equation (42):

$$\chi = \frac{\chi_0}{(2\pi)^{3/2} \sigma'^3} e^{-\left[\frac{(x' - u' t)^2}{2\sigma'^2} + \frac{y'^2}{2\sigma'^2} + \frac{z'^2}{2\sigma'^2}\right]} \tag{48}$$

where now the standard deviation σ', by analogy to equation (22), is defined by

$$\sigma'^2 = 2\,(D_1 D_2 D_3)^{1/3}\, t \quad .$$

We can write this in terms of the separate standard deviations for each coordinate direction, defined by the following quantities

$$\sigma_x^{\,2} = 2D_1 t$$

$$\sigma_y^{\,2} = 2D_2 t$$

$$\sigma_z^{\,2} = 2D_3 t \quad .$$

Eliminating D_1, D_2, D_3, we find

$$\sigma' = (\sigma_x \sigma_y \sigma_z)^{1/3} \quad . \tag{49}$$

Also, eliminating D_1, D_2, D_3 from x', y', z', and u', we have

$$x' = \frac{(\sigma_x \sigma_y \sigma_z)^{1/3}}{\sigma_x}\, x$$

$$y' = \frac{(\sigma_x \sigma_y \sigma_z)^{1/3}}{\sigma_y}\, y \tag{50}$$

$$z' = \frac{(\sigma_x \sigma_y \sigma_z)^{1/3}}{\sigma_z}\, z$$

$$u' = \frac{(\sigma_x \sigma_y \sigma_z)^{1/3}}{\sigma_x} u \quad . \tag{51}$$

Finally, substituting equations (51), (50), and (49) into equation (48), we find the instantaneous point source solution for a moving anisotropic medium in terms of the original coordinates x, y, and z:

$$\chi = \frac{\chi_0}{(2\pi)^{3/2}\sigma_x \sigma_y \sigma_z} e^{-\left[\frac{(x-ut)^2}{2\sigma_x^2} + \frac{y^2}{2\sigma_y^2} + \frac{z^2}{2\sigma_z^2}\right]} \quad .$$

Relative to an observer moving with the medium, u = 0; therefore,

$$\chi = \frac{\chi_0}{(2\pi)^{3/2}\sigma_x \sigma_y \sigma_z} e^{-\left(\frac{x}{2\sigma_x^2} + \frac{y^2}{2\sigma_y^2} + \frac{z^2}{2\sigma_z^2}\right)} \quad . \tag{52}$$

Similarly, for the instantaneous line source

$$\chi = \frac{Q}{2\pi\sigma'^2} e^{-\left[\frac{(x'-u't)^2}{2\sigma'^2} + \frac{y'^2}{2\sigma'^2}\right]}$$

$$= \frac{Q}{2\pi(\sigma_x \sigma_y \sigma_z)^{2/3}} e^{-\left[\frac{(x-ut)^2}{2\sigma_x^2} + \frac{y^2}{2\sigma_y^2}\right]} \quad .$$

Since these solutions exhibit Gaussian distributions in the flow directions, they are basic forms employed in turbulent diffusion, with additional assumptions on σ_x, σ_y, and σ_z whenever Gaussian dispersion can be assumed.

Many attempts have been made to solve the diffusion equation with variable diffusivities D_1, D_2, and D_3. These efforts have succeeded only for certain special functional forms for these coefficients. Details and references to the original investigations can be found in Reference 4.

IV. TURBULENT DIFFUSION

A. Taylor's Theorem

The basic solutions of the diffusion equation developed in the preceding sections are generally valid for molecular diffusion. In general, however, dispersion of matter can also occur by turbulent motion. For example, the dispersion of a pollutant in the atmosphere almost always occurs in a turbulent flow field in which molecular diffusion is negligible. Unlike molecular motion, turbulent flow occurs on a macroscopic scale. Turbulence in the atmosphere can arise from thermal and pressure gradients, variations in wind velocity, boundary reflections such as occur on the ground, and buoyancy forces which are related to vertical temperature variations. The complexity of turbulence is well known. Even with some simplifying assumptions, a theory of turbulent flow based on dynamical considerations leads to coupled differential equations which are virtually intractable to solution.

Inasmuch as turbulence plays a primary role in airborne dispersion, it can be said flatly that the Fickian diffusion equations (17) and (11), characterized by constant eddy diffusivities, fail completely in the atmosphere. The solutions of equation (17), the equation for a moving and anisotropic medium, have been employed as a basis to describe, with some success, the diffusion process in the real atmosphere. Even then, some modifications and some new assumptions are necessary for these solutions to conform adequately to empirical data. As we shall see later, a significant method of modification involves assumptions on the functional forms of σ_x, σ_y, and σ_z, and on the wind velocity. In summary, much of the empirical data can be absorbed in a theory that treats these parameters not as fixed constants but as subject to variation in time or constant over limited regions of space. A fair question is how the solutions obtained from the molecular diffusion equation on the assumption of constant diffusivities can be carried over to turbulent diffusion in which the diffusivities are not constant. Obviously, if these are point functions of the coordinates, this cannot be done. However, if they depend solely on time, then as we have seen in Section II, a time scale transformation leads to an equation of the same mathematical form and, therefore, with the same type of solutions.

A fairly successful theory of turbulence has been based on stochastic theory rather than on dynamical considerations. A statistical technique which originated with Taylor and which has found frequent application is based on a Lagrangian treatment of the flow field, i.e., one in which attention is focused on a single particle as it moves about the field. The theory involves the use of mean values of quantities characterizing the particle, such as its velocity and displacement, with fluctuations about the mean which are assumed to be stationary, homogeneous, isotropic, and Gaussian. By stationary it is meant that statistical properties do not vary with time. For example, a covariance computed from the data in a particular time interval is assumed to be the same for any other time interval. Homogeneity implies that these properties do not depend on the space coordinates; that is, a measurement taken at a particular point in the field will possess statistical characteristics identical to those taken at some neighboring point. Isotropy means that the fluctuations do not vary in direction about a fixed point.

With respect to the atmosphere, homogeneity in the horizontal direction is a reasonable assumption in regions under which the topography is similar over a large area. Such cannot be said for the vertical direction. Because of the presence of vertical forces of gravity, buoyancy, and the Earth's surface, the assumption of vertical homogeneity is unrealistic in most cases. The concept of isotropy suffers from similar limitations.

Once a random process is assumed, a distribution function has to be postulated. It has been determined from empirical data that many atmospheric conditions can be represented by a Gaussian distribution, which yields the normal probability curve. However, any other distribution may be assumed if it offers a better prediction of the variables under certain conditions.

It is not the purpose of this report to give detailed accounts of the statistical theories of turbulence. We limit ourselves to an elementary treatment of a significant statistical method founded on Taylor's theorem and from it derive expressions for σ_x, σ_y, and σ_z. This will be followed by two examples illustrating the use of these expressions in actual diffusion problems, one example from Brownian motion and the other from Sutton's early work. Although this particular aspect of Sutton's work has been superseded on theoretical grounds, it has produced several practical formulas with good predictive power under certain conditions. This section is concluded with a brief description of the Hay-Pasquill method of cloud spread prediction. The purpose here is to provide a background for further reading.

We imagine an ensemble of particles in random motion and fix our attention on a single particle. If the particle at time $t = 0$ is at the vector position $\vec{r}'$ and at time t at position $\vec{r}$, the displacement $\vec{r} - \vec{r}'$ will be a random function of time. If we now introduce a probability density function $P(\vec{r} - \vec{r}', t)$, i.e. a probability per unit volume, then the probability that the particle is in the volume element $d\vec{r}$ about $\vec{r}$ at time t is

$$P(\vec{r} - \vec{r}', t)\, d\vec{r} \quad .$$

The assumption of homogeneity implies that P is solely a function of the displacement $\vec{r} - \vec{r}'$ and not of the starting point, or release point, $\vec{r}'$. That is, every elementary region of the ensemble is represented by the same probability density. Physically, the meaning of P is that it approximates the fraction of particles in a given volume element. The term "approximates" is used because of the inherent statistical nature of P in particular and of the theory in general. If Q denotes the total mass released (which constitutes the ensemble) and χ some mean concentration, it follows that

$$\chi(\vec{r}', t) = QP(\vec{r} - \vec{r}', t) \quad . \tag{54}$$

If we place the observer in a frame of reference moving with the mean velocity of the ensemble, the mean velocity need not be considered. However, the mean of the square of the ensemble velocity is not necessarily zero, although it must be independent of time. Thus, if u denotes the x component of velocity and the bar over a quantity denotes its mean value, then

$$\overline{u(t)} = 0 \qquad \overline{u^2(t)} = \text{constant} \quad .$$

We have similar expressions for the y and z components. After a small time τ, the velocity will be $u(t + \tau)$. Therefore, the velocity covariance is, by definition,

$$\overline{u(t)\, u(t + \tau)} \quad .$$

Since the process is stationary, the covariance is a constant. This implies that the starting point t at which $u(t)$ and $u(t + \tau)$ are computed does not affect the mean value of their product. An important result of this is that the covariance is an even function of τ, meaning that it has the same value for τ as for $-\tau$. To understand this, let us take the starting time $t = 0$, so that the covariance is

$$\overline{u(0)\ u(\tau)} \quad .$$

Now let us take $t = -\tau$, giving

$$\overline{u(-\tau)\ u(0)} \quad .$$

Because of the assumption of stationarity these must be equal;

$$\overline{u(0)\ u(\tau)} = \overline{u(-\tau)\ u(0)}$$

which is clearly even.

The next step is to introduce a velocity correlation function $R(\tau)$ (sometimes called a Lagrangian correlation coefficient) defined by the ratio of the covariance to the mean of the squared velocity:

$$R(\tau) = \frac{\overline{u(t)\ u(t + \tau)}}{\overline{u^2}} \quad , \tag{55}$$

which is also independent of t because numerator and demonator are independent of t.

We now compute the mean time rate of change of the square of the displacement $x(t)$:

$$\overline{\frac{d}{dt}\ x^2(t)} = 2\ \overline{x\ \frac{dx}{dt}} \quad .$$

Since

$$\frac{dx}{dt} = u(t) \quad , \quad x(t) = \int_0^t u(t')\, dt' \quad ;$$

hence, the above becomes

$$\overline{\frac{d}{dt} x^2(t)} = 2 \int_0^t \overline{u(t)\, u(t')}\, dt' \quad ,$$

where we used the justifiable process of interchanging the order of integration and averaging. Making a change of variable defined by $t' = t + \tau$, we have

$$\overline{\frac{d}{dt} x^2(t)} = 2 \int_{-t}^{0} \overline{u(t)\, u(t+\tau)}\, d\tau$$

$$= 2 \int_0^t \overline{u(t)\, u(t+\tau)}\, d\tau$$

where in this last step we replaced the integration from -t to 0 by 0 to t because, as noted previously, the integrand is an even function. Finally, substituting from equation (55), we obtain

$$\overline{\frac{d}{dt} x^2(t)} = 2\overline{u^2} \int_0^t R(\tau)\, d\tau$$

which upon integration over the interval t results in

$$\overline{x^2(t)} = 2\overline{u^2} \int_0^t \int_0^{t'} R(\tau)\, d\tau\, dt' \tag{56}$$

$$= 2\overline{u^2} \int_0^t (t - \tau)\, R(\tau)\, d\tau \quad .$$

This result is known as Taylor's theorem and is of fundamental importance in turbulence. It relates the mean squared displacement of a particle in time t to its mean squared eddy velocity and velocity correlation function.

We now seek a connection between the autocorrelation function $R(\tau)$ and the standard deviations σ_x, σ_y, and σ_z which quantities, as we have noted, characterize the spread of the dispersion along the three coordinate directions. We recall that in one dimension σ_x was defined by

$$\sigma_x^{\,2} = \frac{1}{Q} \int_{-\infty}^{\infty} x^2 \chi(x, t)\, dx \quad .$$

Extending this definition to three dimensions, we have

$$\sigma_x^{\,2} = \frac{1}{Q} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x^2 \chi(x, y, z, t)\, dx\, dy\, dz$$

with similar expressions for $\sigma_y^{\,2}$ and $\sigma_z^{\,2}$. Substituting from equation (54), we get

$$\sigma_x^{\,2} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x^2 P(x, y, z, t)\, dx\, dy\, dz \quad ,$$

but from statistical theory this integral is just the mean or expected value of x^2. Thus

$$\sigma_x^{\,2} = \overline{x^2}$$

$$= 2\,\overline{u^2} \int_0^t (t - \tau)\, R(\tau)\, d\tau \tag{57}$$

from Taylor's theorem. This is the relation sought. In general, for all three dimensions, we have

$$\sigma_y^{\,2} = 2\,\overline{u^2} \int_0^t (t - \tau)\, R_y(\tau)\, d\tau$$

$$\sigma_z^{\,2} = 2\,\overline{w^2} \int_0^t (t - \tau)\, R_z(\tau)\, d\tau$$

where v and w are the velocity components in the y and z directions, and R_y and R_z are their respective correlation functions. Thus, in this theory the problem of turbulence is reduced to that of determining the velocity correlation function. The difficulty, however, is that there is no satisfactory theory from which this function can be predicted. The function can be predicted if it can be assumed that the velocity history is a Markov process. A Markov process is one in which the value of a random variable at times greater than some t depends on the value it has at t but not on any previous value. There are some theoretical inconsistencies in the assumption of a Markov process for the velocity fluctuations, however. These will be discussed in a later paragraph.

Some general properties of $R(\tau)$ are worth noting. We have already seen that it is independent of t and an even function of τ. Also, at $t = 0$, $R(0) = 1$, and as $\tau \to 0$, $R(\tau) \to 0$. In general it can be shown that for all τ,

$$-1 \leq R(\tau) \leq 1 \quad .$$

B. Example from Brownian Motion

It is an enlightening exercise to apply Taylor's theorem to Brownian motion, which is the agent by which molecular diffusion occurs, and to show that it gives the same result for σ as does the phenomenologically based diffusion equation. The exercise is expressive of the significance and power of the statistical approach. When small particles of colloidal size suspended in a fluid are observed under a microscope, the particles are seen to move about with apparently random motion. This motion was observed by the botanist Robert Brown in 1826. Not until 1905, when Einstein published his classic paper, was the phenomenon completely understood. He showed that the motion is the result of collisions with the molecules of the surrounding fluid, which eventually leads to the dispersal of the particles.

We apply Newton's second law of motion to a single particle of mass m and velocity u moving in one dimension. The assumed forces acting on the particle are viscous drag and collision forces taken as a group of random impulses. The drag force is assumed proportional to the first power of the velocity, with K denoting the proportionality constant and f(t) denoting the random force component along X. The equation of motion is

$$m \frac{du}{dt} = -Ku + f(t) \quad .$$

Writing $\beta = K/m$, we have

$$\frac{du}{dt} + \beta u = \frac{f(t)}{m} \quad .$$

This first-order, linear differential equation can be integrated with the aid of the integration factor $e^{\beta t}$. Multiplying by this factor and rearranging gives

$$\frac{d}{dt} \left(ue^{\beta t}\right) = \frac{f(t)}{m} e^{\beta t} \quad ,$$

so that

$$ue^{\beta t} = u_0 + \frac{1}{m} \int_0^t f(t') \, e^{\beta t'} \, dt'$$

where u_0 is the initial velocity. Solving for u,

$$u = u_0 e^{-\beta t} + \frac{e^{-\beta t}}{m} \int_0^t f(t') \, e^{\beta t'} \, dt' \quad . \tag{58}$$

This result shows that the particle's velocity depends on the initial velocity and on the random acceleration f/m. For times $t \gg 1/\beta$, the first term decays to zero, making u independent of its initial velocity. It may be stated that after a sufficiently long time the particle "forgets" its initial velocity and is thereafter "pushed" around by the random forces. Thus, after a long time the process becomes a Markov process. It might also be noted that in spite of the presence of the decay factor $e^{-\beta t}$ in the second term, this term does not necessarily decay, at least at the same rate, as the first term because the integral is not constant but some function of t.

If we now take the ensemble average of equation (58) (the average of a large number of randomly moving particles), the contribution to u from the second term vanishes; therefore,

$$\bar{u} = u_0 \, \overline{e^{-\beta t}} \quad . \tag{59}$$

Moreover, from the principle of equi-partition of energy founded on the statistical theory of gases, we have

$$\frac{1}{2} m \, \overline{u^2} = \frac{1}{2} kT$$

where the left side is the mean kinetic energy of the particle, k is the Boltzmann constant, and T is the absolute temperature. This simple result shows that $\overline{u^2}$ is independent of time, indicating that Brownian motion involves a stationary process.

We are now able to determine the velocity correlation function for Brownian motion. Because the process is stationary, we can take t = 0. Thus, with the aid of equation (55), we find

$$R(\tau) = \frac{\overline{u(t)\ u(t+\tau)}}{\overline{u^2}}$$

$$= \frac{\overline{u(0)\ u(\tau)}}{\overline{u^2}}$$

$$= e^{-\beta\tau} \quad .$$

Substituting this correlation function into Taylor's theorem, we have

$$\sigma_x^{\ 2} = 2\,\overline{u^2} \int_0^t (t-\tau)\, R(\tau)\, d\tau$$

$$= 2\,\overline{u^2} \left\{ \int_0^t te^{-\beta\tau}\, d\tau - \int_0^t \tau e^{-\beta\tau}\, d\tau \right\}$$

$$= 2\,\overline{u^2} \left\{ \left[-\frac{t}{\beta}\, e^{-\beta\tau} \right]_0^t - \left[-\frac{\tau}{\beta}\, e^{-\beta\tau} - \frac{1}{\beta^2}\, e^{-\beta\tau} \right]_0^t \right\}$$

$$= 2\,\overline{u^2} \left\{ \frac{t}{\beta} - \frac{1}{\beta^2} (1 - e^{-\beta t}) \right\} \quad . \tag{60}$$

To interpret this result and relate it to the expression obtained from the phenomenological theory, we need some insight as to the magnitude and significance of the quantity β. Its reciprocal has the dimensions of time. It is the time for the velocity to decay to $1/e$ of its initial value, or the "relaxation time" of the viscous effects. Its magnitude may be computed from Stokes' law:

$$\beta = \frac{6\pi a \mu}{m}$$

where a is the radius of the particle and μ is the viscosity of the fluid. For a particle of mass $m \simeq 10^{-12}$ g in air, $\mu = 1.6 \times 10^{-1}$ g-sec^{-1}-cm^{-1}, and $a \simeq 10^{-4}$ cm, we have

$$\beta^{-1} \simeq 1.4 \times 10^{-8} \text{ sec}$$

which is much smaller than the time scale of normal diffusion. Thus, for $t \gg 1/\beta$ we neglect the second term in equation (60), giving

$$\sigma_x^{\,2} \simeq \frac{2\,\overline{u^2}}{\beta}\, t \quad .$$

Comparing with $\sigma_x^{\,2} = 2Dt$, we see that both expressions are in accord in that each depends linearly on t. Also, it follows that

$$D = \frac{\overline{u^2}}{\beta}$$

$$= \frac{kT}{6\pi a \mu} \quad .$$

This relation has been repeatedly verified by experiment and is a well established result of the theory.

We have seen that for Brownian motion the velocity correlation function has the form of an exponential decay and, therefore, the motion is of the Markov type. If we assume that eddy motion is also of this type, then

$$R(\tau) \sim e^{-\tau/\theta} \tag{61}$$

where θ would be some appropriate time scale for the process. For Brownian motion, θ is determined by viscous effects which was found to be $\theta = 1/\beta$. It would seem, therefore, that θ in general is determined by some characteristic length related to the size of an eddy and some characteristic velocity. On this basis, θ would be expected to be proportional to the ratio of the characteristic length to the characteristic velocity. All this appears quite reasonable; however, an obvious difficulty arises from the assumed functional form of $R(\tau)$ if we recall that it should be even. Replacing τ with its absolute value in equation (61) makes it an even function; however, it has a discontinuity at $\tau = 0$. Physically, this implies an infinite acceleration of the particle (or eddy) or a vanishing inertia. Thus, the type of function being considered is not acceptable on theoretical grounds. However, for large values of τ the particle is no longer influenced by its initial velocity; therefore, a Markov process should be an acceptable model for such times. In the limit of large τ, the dispersion σ^2 is proportional to the time, which is characteristic of molecular diffusion but not generally valid in turbulence. The obvious inference is that the Markov process is applicable only when the turbulent medium has reached a quiescent state dominated by molecular diffusion, at which time the problem may no longer be of interest.

As indicated by Sutton [5], the difficulty with an exponential decay correlation function is that it implies eddies all having the same size, analogous to the molecules of a simple gas, which is definitely not in accord with the facts of turbulence. The conclusion is that this type of function cannot form the basis of any general theory.

Other theories, including the "mixing length," have been proposed. In these theories one introduces a characteristic length, akin to the mean free path of a molecule whose magnitude depends on the intensity of turbulence. The idea is that a randomly moving fluid element transfers its momentum to the mean flow in a distance of the order of the mixing length. This implies that the elements behave independently of the mean motion for brief periods during which

they transfer their momentum, much like independent, colliding molecules. No model of the structure of an eddy is necessary. The velocity fluctuation therefore becomes a function of the mixing length. Unlike the mean free path, the mixing length may be a function of position, mean velocity, and other variables. In practice, the mixing length is a convenient parameter lacking any solid physical foundation. A result of the theory is an expression for a virtual coefficient of diffusion equal to the product of the mixing length and the square root of the mean of the squared velocity fluctuation. The details of the derivation can be found on page 72 of Reference 5.

C. Sutton's Formulas for the Dispersion

In Sutton's analysis, it is assumed that the correlation between fluctuating velocities near a smooth surface depends on the mean eddy energy $\rho\,\overline{u^2}$, the fluid viscosity μ, and the time t. The only dimensionless number that can be formed with these quantities is $\mu/\rho\,\overline{u^2}\,\tau$, which, with $\nu \equiv \mu/\rho$, can be written $\nu/\overline{u^2}\,\tau$. The quantity ν is the kinematical viscosity. Considering the limiting properties of $R(\tau)$ for small and large τ, the simplest function with these properties is the power law

$$R(\tau) = \left(\frac{\nu}{\nu + \overline{u^2}\,\tau}\right)^n ,$$

where n is a positive number. Thus, in nonisotropic diffusion, e.g., diffusion near the ground, one can assume

$$R_x(\tau) = \left(\frac{\nu}{\nu + \overline{u^2}\,\tau}\right)^n$$

$$R_y(\tau) = \left(\frac{\nu}{\nu + \overline{v^2}\,\tau}\right)^n$$

$$R_z(\tau) = \left(\frac{\nu}{\nu + \overline{w^2}\,\tau}\right)^n$$

where u, v, and w are the velocity fluctuation components. Furthermore, Sutton suggests that for rough surfaces ν in these expressions be replaced by the "macroviscosity," a quantity without precise definition except that it is, for the most part, empirically determined and several orders of magnitude greater than ν. Its magnitude, from Sutton's computations, ranges from 0.016 for ice and mud flats to 560 for thick grass up to 50 cm high.

From equation (57), we calculate

$$\sigma_x^2 = 2\,\overline{u^2} \int_0^t (t - \tau) \left(\frac{\nu}{\nu + \overline{u^2}\,\tau} \right)^n d\tau$$

$$= 2\,\overline{u^2} \left\{ t\nu^n \int_0^t \frac{d\tau}{(\nu + \overline{u^2}\,\tau)^n} - \nu^n \int_0^t \frac{\tau\, d\tau}{(\nu + \overline{u^2}\,\tau)^n} \right\}$$

$$= \frac{2\nu^n (\nu + \overline{u^2}\,t)^{2-n}}{(1-n)(2-n)\,\overline{u^2}} - \frac{2\nu^2}{(1-n)(2-n)\,\overline{u^2}} - \frac{2\nu t}{1-n} \quad .$$

Neglecting terms of order ν compared to $\overline{u^2}\,t$, we have

$$\sigma_x^2 = \frac{2\nu^n (\overline{u^2}\,t)^{2-n}}{(1-n)(2-n)\,\overline{u^2}} \quad .$$

Similarly, we find

$$\sigma_y^2 = \frac{2\nu^n (\overline{v^2}\,t)^{2-n}}{(1-n)(2-n)\,\overline{v^2}}$$

$$\sigma_z^2 = \frac{2\nu^n (\overline{w^2}\,t)^{2-n}}{(1-n)(2-n)\,\overline{w^2}} \quad .$$

Defining "generalized diffusion coefficients" C_x, C_y, C_z by

$$C_x = \frac{4\nu^n}{(1-n)(2-n)\,\overline{u^2}} \left(\frac{\overline{u^2}}{U^2}\right)^{1-n}$$

$$C_y = \frac{4\nu^n}{(1-n)(2-n)\,\overline{v^2}} \left(\frac{\overline{v^2}}{U^2}\right)^{1-n}$$

$$C_z = \frac{4\nu^n}{(1-n)(2-n)\,\overline{w^2}} \left(\frac{\overline{w^2}}{U^2}\right)^{1-n}$$

where U is the mean (constant) cloud velocity, one can write

$$\sigma_x^{\,2} = \frac{1}{2} C_x^{\,2} (Ut)^{2-n}$$

$$\sigma_y^{\,2} = \frac{1}{2} C_y^{\,2} (Ut)^{2-n}$$

$$\sigma_z^{\,2} = \frac{1}{2} C_z^{\,2} (Ut)^{2-n} \quad . \tag{62}$$

For $n = 1$, one finds that σ^2 is proportional to t, a behavior characteristic of molecular or Brownian diffusion. For $n = 1/4$, σ^2 is proportional to $t^{7/4}$ which, according to Sutton, gives a reasonably accurate description of diffusion in the atmosphere from a few meters to hundreds of kilometers.

We can arrive at Sutton's formula for the instantaneous point source in a reference frame moving with the cloud by formally substituting the relations of equation (62) into equation (52):

$$\chi = \frac{Q}{\pi^{3/2} C_x C_y C_z (Ut)^{3/2(2-n)}} e^{(Ut)^{n-2}\left(\frac{x^2}{C_x^2} + \frac{y^2}{C_y^2} + \frac{z^2}{C_y^2}\right)} . \quad (63)$$

From this basic solution Sutton obtains, by integration, the formula for the continuous point source near the ground (the ground reflection is taken into account):

$$\chi = \frac{2Q}{\pi C_y C_z U x^{2-n}} e^{-x^{n-2}\left(\frac{y^2}{C_y^2} + \frac{z^2}{C_z^2}\right)} ,$$

where x = Ut. Expressions for line sources are also given (see page 288 of Reference 5).

A first criticism of Sutton's development is that the constants C_x, C_y, C_z do not have fixed dimensions but depend on the value of n. Furthermore, the correlation function varies as τ^{-n}, which yields divergent diffusion time scales and infinite spectral density at zero frequency under Fourier analysis. In spite of these theoretical inconsistencies, Sutton's basic formula, equation (63), is found to be identical to that derived by some other theoretical methods, e.g., by treating turbulent diffusion as a random walk process. Csanady [6] suggests that the theoretical discrepancies may be due to the nonuniformity of the turbulent field near the ground as the cloud rises and the eddies grow in size. Since the field is no longer stationary, the concept of a velocity correlation function is undermined. We might reverse the reasoning as follows. Starting with the presumably correct power law formulas, equation (62), a velocity correlation function deduced from them would be invalid.

For a continuous elevated point source in the presence of a constant mean wind along x and total reflection at the ground, Sutton assumes the expression

$$\chi = \frac{Qe^{-\frac{y^2}{2\sigma_y^2}}}{2\pi U\sigma_y\sigma_z}\left\{e^{-\frac{(z-H)^2}{2\sigma_z^2}} + e^{-\frac{(z+H)^2}{2\sigma_z^2}}\right\}$$

where H is the source height measured from an origin on the ground beneath the source. In this formula we have replaced Sutton's C_y and C_z with σ_y and σ_z defined by equation (62). This general form for the concentration allows different assumptions on the values of σ_y and σ_z and has been widely employed by others to predict cloud concentration at ground level from smoke stacks. At ground level $(z = 0)$, the formula becomes

$$\chi = \frac{Q}{\pi U\sigma_y\sigma_z}\, e^{-\left(\frac{y^2}{2\sigma_y^2} + \frac{H^2}{2\sigma_z^2}\right)} ,$$

and along the axis of the plume $(y = 0)$, it becomes

$$\chi = \frac{Q}{\pi U\sigma_y\sigma_z}\, e^{-\frac{H^2}{2\sigma_z^2}} .$$

It is easily seen that the maximum concentration along the plume axis occurs at the point downwind where the relation $\sigma_z = H/\sqrt{2}$ satisfied; the concentration there is

$$\chi_{max} = \frac{2Q}{\pi UeH^2}\left(\frac{\sigma_z}{\sigma_y}\right) .$$

D. Hay-Pasquill Method for Determining the Dispersion

In deriving Taylor's theorem it was explicitly assumed that the velocities were Lagrangian velocities, i.e., the mean velocity and fluctuating components of a particle as it moves about from one point to another. In contrast to this Lagrangian description, the Euler description deals with velocities at a fixed point of the fluid. Since in the determination of experimental data on diffusion velocities samples are often taken with instruments fixed at a point in the flow, it would be useful to determine the relationship, if any, between Lagrangian and Euler velocities. The difference is, primarily, that the velocity fluctuations at a fixed point occur in a shorter time than those of a drifting particle. The Hay-Pasquill method is based on the realization of this time difference.

In this method one introduces a shortened time interval T, or simulation time, related to t by $t = \beta T$, where β is some empirically determined constant. With this new time scale and by the same arguments used to derive Taylor's theorem, one now obtains

$$\overline{x^2} = 2\,\overline{u_E^{\,2}}\,\beta^2 \int_0^T \int_0^{t'} R_E(\tau)\, d\tau\, dt'$$

for the simulated mean-square displacement, where U_E is the Eulerian velocity and $R_E(\tau)$ is the Eulerian velocity correlation function. One then assumes that the Langrangian velocity fluctuations are equal to the Eulerian fluctuations but that they occur on a time scale longer by a factor of β. That is, $\overline{U_E^{\,2}} = \overline{U^2}$, where $\overline{U^2}$ is the corresponding Lagrangian quantity. Employing this equality in equation (56) and then equating equation (56) to the above expression for $\overline{x^2}$, it follows that

$$R_E(\tau) = R(\beta\tau)$$

where the right member is the Lagrangian correlation function. This result implies that the Eulerian and Lagrangian correlation functions have the same

shape but that the Lagrangian one falls more slowly. Although it has been definitely determined that the two correlation functions do not, in reality, have the same shape, the standard deviations obtained by this method give good predictions of cloud concentration [4, 6].

V. NASA/MSFC MULTILAYER DIFFUSION MODEL

A. Point Source Solutions in a Layer with Impervious Boundaries

The real atmosphere quite often possesses a stratified structure, primarily as a result of temperature and wind shear. The turbulent mixing of a cloud with ambient air (entrainment) tends to decrease the buoyancy and vertical momentum of the cloud. As a result the region in which turbulent mixing is occurring will be bounded by a stable layer which acts as a lid, preventing complete admixture of the air across the boundary. This would be the case when buoyancy forces are stabilized by gravity. Given that the ground also acts as a similar boundary, the task is to determine solutions in a vertical layer of atmosphere. The simplest diffusion model which accounts for such boundaries is one which assumes total reflection at the boundaries. The solutions for the instantaneous and continuous point sources will now be derived, followed by a summary of the multilayer model developed by the Cramer Company for NASA.

A layer, by definition, consists of two distinct boundaries. Mathematically, the problem can be treated by the method of images. The flux reflected at the first boundary is reflected at the second boundary which, in turn, is reflected at the first boundary, etc. The general solution can be constructed by assuming multiple images, one for each reflection. Each image upon reflection at the opposite boundary creates a second image which, in turn, creates a third, etc. The essential steps will be given in the following paragraphs.

The origin of coordinates is placed on the ground, $z = 0$, the source at $z = H$ above ground, and the top of the mixing layer at $z = h$, with $h > H$. Total reflection is assumed at both boundaries, the ground and the top of the mixing layer. For the instantaneous and continuous point sources we assume the basic Gaussian form

$$\chi = Ae^{-\frac{(z-H)^2}{2\sigma_z^2}}$$

where we let

$$A = \frac{Q}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} e^{-\frac{(x-Ut)^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2}}$$

for the instantaneous source, and

$$A = \frac{Q}{2\pi U\sigma_y\sigma_z} e^{-\frac{y^2}{2\sigma_y^2}}$$

for the continuous source.

Consider first the reflection of the real source at the boundary $z = 0$. For this reflection an image source is placed at $z = -H$. The solution due to this image is

$$Ae^{-\frac{(z+H)^2}{2\sigma_z^2}} .$$

The flux from this image is also reflected at the boundary $z = h$. Therefore, we place a second image at $z = 2h + H$ (at the same distance from the boundary $z = h$ as the first image). The solution due to this second image is

$$Ae^{-\frac{[z-(2h+H)]^2}{2\sigma_z^2}} .$$

The flux from this secondary image is itself reflected at the boundary $z = 0$; therefore, a third image is placed at $z = -(2h + H)$, giving rise to the solution

$$Ae^{-\frac{[z+(2h+H)]^2}{2\sigma_z^2}} .$$

The flux from this tertiary image is reflected at $z = h$; therefore, a fourth image is placed at $z = 4h + H$, giving the solution

$$Ae^{-\frac{[z-(4h+H)]^2}{2\sigma_z^2}} .$$

A fifth image at $z = -(4h + H)$ yields

$$Ae^{-\frac{[z+(4h+H)]^2}{2\sigma_z^2}} .$$

Generalizing the results and taking the sum of the solutions, we have the expression

$$A\left\{\sum_{i=0}^{\infty} e^{-\frac{(z-H-2ih)^2}{2\sigma_z^2}} + \sum_{i=0}^{\infty} e^{-\frac{(z+H+2ih)^2}{2\sigma_z^2}}\right\}$$

or

$$A\sum_{i=0}^{\infty}\left\{e^{-\frac{(z-H-2ih)^2}{2\sigma_z^2}} + e^{-\frac{(z+H+2ih)^2}{2\sigma_z^2}}\right\} . \qquad (64)$$

To this expression we now have to add the sum of the solutions arising from reflection of the real source with the boundary $z = h$. In this case we first place an image source at $z = 2h - H$, yielding the solution

$$Ae^{-\frac{[z-(2h-H)]^2}{2\sigma_z^2}} .$$

For reflection of this image at $z = 0$, we place a second image at $z = -(2h - H)$, yielding the solution

$$Ae^{-\frac{[z+(2h-H)]^2}{2\sigma_z^2}} .$$

For the next two reflections at $z = h$ and $z = 0$, we have, respectively,

$$Ae^{-\frac{[z-(4h-H)]^2}{2\sigma_z^2}}$$

$$Ae^{-\frac{[z+(4h-H)]^2}{2\sigma_z^2}}$$

etc. The sum of these solutions is

$$A\left\{\sum_{i=1}^{\infty} e^{-\frac{(z+H-2ih)^2}{2\sigma_z^2}} + \sum_{i=1}^{\infty} e^{-\frac{(z-H+2ih)^2}{2\sigma_z^2}}\right\}$$

or

$$A \sum_{i=1}^{\infty} \left\{ e^{-\frac{(z+H-2ih)^2}{2\sigma_z^2}} + e^{-\frac{(z-H+2ih)^2}{2\sigma_z^2}} \right\} . \tag{65}$$

The term $i = 0$ is not included here because it has been included in the preceding partial sum, equation (64).

Thus, the general solution is the sum of the two partial sums, equations (64) and (65):

$$\chi = A \left\{ \sum_{i=0}^{\infty} \left[e^{-\frac{(z-H-2ih)^2}{2\sigma_z^2}} + e^{-\frac{(z+H+2ih)^2}{2\sigma_z^2}} \right] + \sum_{i=1}^{\infty} \left[e^{-\frac{(z+H-2ih)^2}{2\sigma_z^2}} + e^{-\frac{(z-H+2ih)^2}{2\sigma_z^2}} \right] \right\} . \tag{66}$$

In the literature on diffusion these sums are written in several equivalent forms. The form used by the Cramer Company in its reports [7, 8] is obtained by writing the terms for $i = 0$ explicitly and combining the two sums into one as follows:

$$\chi = A \left\{ e^{-\frac{(z-H)^2}{2\sigma_z^2}} + e^{-\frac{(z+H)^2}{2\sigma_z^2}} + \sum_{i=1}^{\infty} \left[e^{-\frac{(z-H-2ih)^2}{2\sigma_z^2}} + e^{-\frac{(z+H+2ih)^2}{2\sigma_z^2}} + e^{-\frac{(z+H-2ih)^2}{2\sigma_z^2}} + e^{-\frac{(z-H+2ih)^2}{2\sigma_z^2}} \right] \right\} . \tag{67}$$

Except for minor differences, such as the use of the equivalent $(2ih + H - z)^2$ for $(z - H - 2ih)^2$, and the use of H_m for our h, the expression in braces is identical to the "vertical term" of the Cramer group.

Another equivalent form of equation (66), and the most concise, is obtained by replacing the summation range in the second sum by $i = -1$ to $-\infty$ and accommodating this change by an appropriate sign change in the affected terms. One can easily verify the result

$$\chi = A \sum_{i=-\infty}^{\infty} \left\{ e^{-\frac{(z+H+2ih)^2}{2\sigma_z^2}} + e^{-\frac{(z-H+2ih)^2}{2\sigma_z^2}} \right\} . \tag{68}$$

The ground-level concentration along the axis of the plume is of interest. With $z = 0$ and $y = 0$, we obtain in the case of the continuous source:

$$\chi = \frac{Q}{\pi U \sigma_y \sigma_z} \sum_{i=-\infty}^{\infty} e^{-\frac{(H+2ih)^2}{2\sigma_z^2}} . \tag{69}$$

We recall that σ_z characterizes the spread of the concentration in the vertical direction and, therefore, increases with time; for example, as $t \to \infty$, $\sigma_z \to \infty$, and χ approaches some asymptotic value independent of z. Since the total amount of diffusing matter must be conserved, the integration of equation (68) over all space must equal the total mass released. The integration results in the asymptotic form

$$\chi_\infty = \frac{Q}{2\pi U \sigma_y \sigma_z} e^{-\frac{y^2}{2\sigma_y^2}} \left(\frac{\sqrt{2\pi}\, \sigma_z}{h} \right) . \tag{70}$$

Thus, the summation factor in equation (68), which expresses the vertical distribution, approaches the distribution $\sqrt{2\pi}\,\sigma_z/h$ asymptotically. That is, the Gaussian distribution eventually becomes rectangular.

B. Summary of the NASA/MSFC Model

The NASA/MSFC Multilayer Diffusion Model developed by the Cramer Company is employed in the prediction of fuel hazards resulting from NASA activities. In particular, this model was designed to permit concentration and dosage calculations downwind of toxic clouds from rocket vehicles. The basic concepts of this model are summarized here in the context of the stated purpose of this report. The specific details of the method and associated computer program can be found in References 4 and 6.

The stratification of the atmosphere into regions of significantly different meteorological parameters, such as wind velocity and temperature, is the basis for assuming a multilayer model. Each layer is assumed homogeneous and the boundaries impervious to the turbulent flux. However, the formulation does permit taking into account flux of matter across the boundaries due to gravitational settling and precipitation scavenging. The diffusion process is repeated from layer to layer, each layer assigned a new set of source and meteorological data.

The model takes into account the loss of matter from the cloud resulting from decay processes, precipitation scavenging, and gravitational settling. All these effects combine to deplete the matter that forms the cloud. The expression for the concentration, therefore, consists of the product of two terms: a diffusion term and a depletion term. If a Gaussian distribution is assumed, the diffusion term is that developed here, equation (67), for the instantaneous or continuous point source, depending on the function A as already defined. The standard deviations σ_x, σ_y, and σ_z are now generalized entities significantly, but not conceptually, different from the relatively simple meaning we have attached to them. They are defined by certain rather awkward semi-empirical relationships involving quantities that vary during the time required for the cloud to stabilize with respect to ambient air. In the main, therefore, these quantities are functions of one or more of the following: (1) the standard deviations of azimuth and elevation angles of the wind; (2) the distances over which vertical and crosswind expansion of the cloud occurs; (3) the standard

deviations of the vertical, crosswind, and alongwind distributions at the time of cloud stabilization; (4) vertical and lateral diffusion coefficients; and (5) the time for the cloud to reach equilibrium with ambient conditions. Much of the input data required to calculate these σ' s must be empirically determined.

If gravitational settling is neglected, the depletion term consists of the product of two exponential decay factors of the form e^{-bt}, one for decay processes and one for precipitation scavenging, where b is some appropriate constant for the particular process.

If gravitational settling is not neglected, then the sum (but not A) in the diffusion term, equation (68), is replaced with the expression

$$e^{-\frac{\left(z-H+\frac{Vx}{U}\right)^2}{2\sigma_z^2}} + e^{-\frac{\left(z+H-2h-\frac{Vx}{U}\right)^2}{2\sigma_z^2}} \tag{71}$$

where V is the settling velocity. This replacement is made because the ground can no longer be considered a reflecting boundary, reflection now occurring only at the upper boundary z = h. Equation (71) is, therefore, really a diffusion term. Neglecting for the moment the term Vx/U, equation (71) can be written as

$$e^{-\frac{(z-H)^2}{2\sigma_z^2}} + e^{-\frac{[z-(2h-H)]^2}{2\sigma_z^2}} \tag{72}$$

which, aside from the factor A, we recognize as the solution for the point source with source at z = H and a single reflecting boundary at z = h.

The inclusion of the term Vx/U is based on Schmidt' s studies on sedimentation as modified by Csanady [6]. In equation (72) the source height H is replaced by H - Vx/U, resulting in equation (71).

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APPROVAL

SOME BASIC MATHEMATICAL METHODS OF DIFFUSION THEORY

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The information in this report has been reviewed for security classification. Review of any information concerning Department of Defense or nuclear energy programs or activities has been made by the MSFC Security Classification Officer. This report, in its entirety, has been determined to be unclassified.

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