

CHAPTER 6

Chapter 6 contains

- *an introduction to the formal description of fluid particle dispersion (in both inertial and non-inertial frames) via stochastic and deterministic Green's functions,*
- *a discussion of the modified A.D.E. in relation to other dispersion models,*
- *a review of time-domain methods for determining relative dispersion parameters (including similarity analysis, Langevin equation methods and conditioned motion methods),*
- *a discussion of spectral methods for determining relative dispersion parameters and presentation of an iterative filtering algorithm that utilizes observed atmospheric spectra for this objective.*

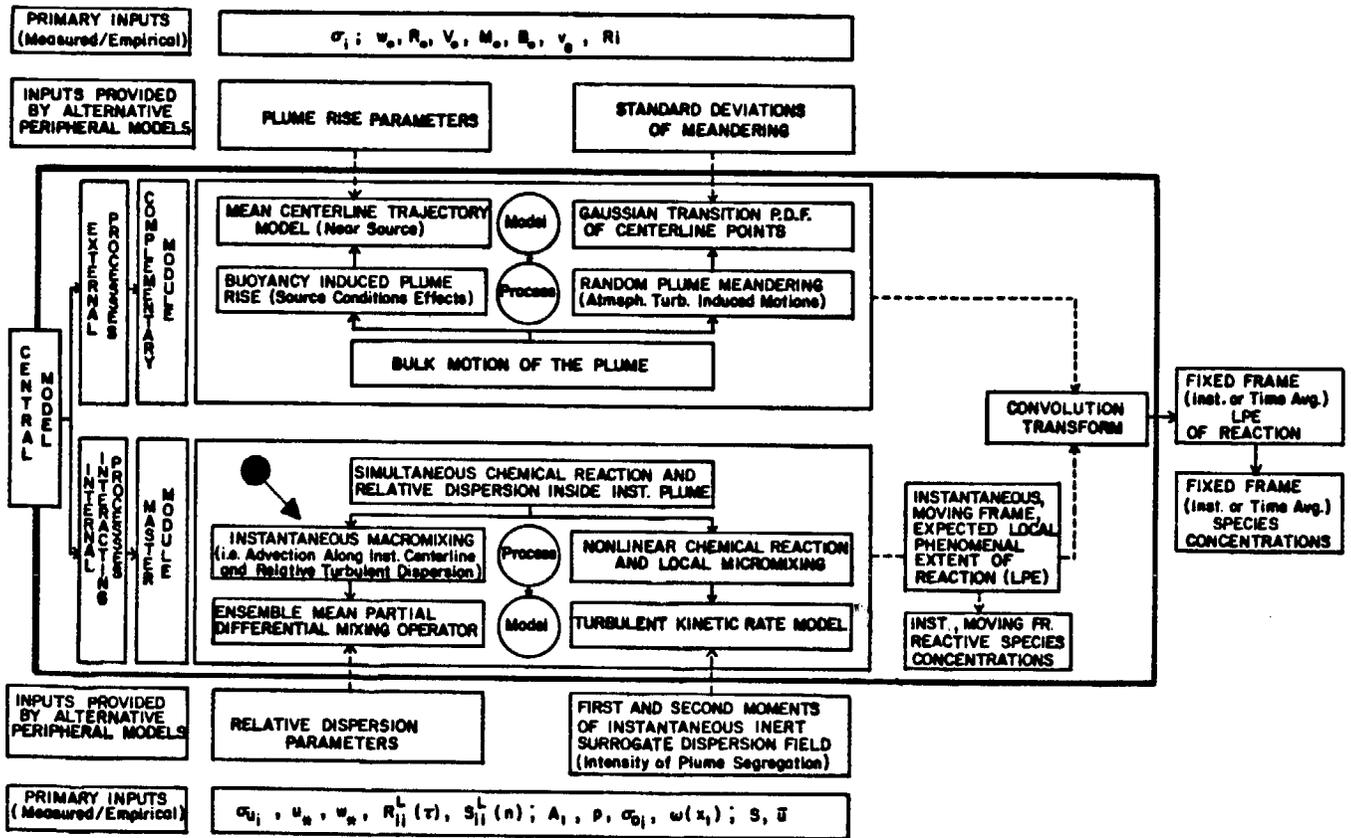


Figure 2-1c
TRPM Components Discussed in Chapter 6

CHAPTER 6

PARAMETERIZATION OF RELATIVE DISPERSION

6.1 INTRODUCTION

This chapter discusses some aspects, both formal and practical, of the multi-scale turbulent dispersion problem, as it appears in the overall reactive plume phenomenon. The treatment of dispersion adopted in the TRPM formulation is explained here in more detail than this was done in Chapter 2.

The present chapter is intended as a tutorial introduction to the subjects of absolute and relative diffusion (in particular atmospheric), and a brief review of the various modeling approaches in the area, which cover an enormous range, from simple dimensional and similarity analyses, to sophisticated formulations involving complex numerical schemes and methods of functional analysis. (*) What we intend to do here is, in parallel to presenting and discussing the formulations of the particular schemes proposed for use with the TRPM, to bring together and summarize various concepts

* Among many excellent general introductions to the subject of turbulent transport we mention Tennekes and Lumley (1972, Chapters 7 and 8), Csanady (1973), Monin and Yaglom (1971, Section 10) and Hinze (1975, Chapter 5). Some of the more advanced methods of analysis are discussed in Leslie (1973, Chapters 8 and 12) and Monin and Yaglom (1975, Section 24). The work of Monin and Yaglom focuses in particular on atmospheric dispersion; for other specialized analyses of this topic see Seinfeld (1975, Chapter 6; 1983), Hanna et al. (1982), Pasquill and Smith (1983) and Tchen (1984ab). Further information directly related to the atmospheric dispersion problem can be found in Panchev (1971), Haugen (1973, 1975), Berlyand (1975), Vinnichenko et al. (1980), Nieuwstadt and von Dop (1982), Plate (1982), Randerson (1984) and Panofsky and Dutton (1984).

that are useful for a better understanding of these formulations, the conditions for their validity, and their relation to other approaches. Thus this chapter should be seen not only as an elaboration on a particular component of the TRPM but also as a guide to the relative dispersion literature, linking ideas and methods that can be found scattered in a variety of sources.

Formally, description of dispersion in the TRPM was based on the linear stochastic Eulerian Mixing Operator \mathcal{L}^M , as given by equation (1.3-4), whose "ensemble mean action" (equation (1.3-7)) was approximated by the action of the "modified K-theory operator" $\mathcal{L}_K^M(\cdot)$ (also linear), given by equation (2.3-2), on the mean concentration field $\langle c \rangle$.

These operators were assumed capable of describing dispersion in a frame of reference following the meandering motion of the plume centerline. Some further discussion is needed on this point, which may be a source of confusion. *Our approach is Lagrangian*, in the sense this term has been used to describe a certain class of air pollution models (trajectory models) but *at a scale smaller* than relevant to those models. To make this more clear we must emphasize the fact that the term "Lagrangian description" is in general used in a very loose manner in air pollution modeling. In fact, in the trajectory models mentioned above the "Lagrangian description" concept applies only to the process of advection by the mean wind and *not* to random movements caused by the smaller scales of atmospheric motion. Turbulent transport processes inside the large scale (macroscopic) control volume (between the different computational cells) that follows the trajectory are most often described in Eulerian terms in these models, typically through conventional K theory (see, e.g., Appendix A1.2) with all the subsequent limitations (see, e.g., Corrsin, 1974). Thus these models are essentially hybrid formulations. (The governing equations in the moving frame are Eulerian equations with transformed coordinates.) A "fully" Lagrangian description of an advection-dispersion field would be formulated in terms of fluid particles (see also Chapter 4) and would necessarily be statistical in nature. (This kind of approach would perhaps conform better to the essence of Lagrangian

methodology of continuum mechanics, which focuses on the kinematics and dynamics of material points rather than on finite control volumes and their infinitesimal limiting approximations to describe processes in continua). However, the whole problem is essentially one of terminology and semantics and as long as the concepts and assumptions involved are clearly identified there should not be confusion in using the term "Lagrangian methodology" either to refer to the description in terms of fluid particles, which are subject to the entire spectrum of motions existing in the field under observation, or to the formulation of transport-balance equations in a frame of reference that moves along some, appropriately defined "mean flow." We could call these two descriptions "micro-Lagrangian" and "macro-Lagrangian" respectively, understanding that the latter might be a hybrid approach; then the dispersion scheme of the TRPM could be called a "meso-Lagrangian" hybrid description (not to be confused, of course, with meso-scale air pollution models) in the following sense: the moving frame of reference follows not only the "mean" flow but is also affected by an additional portion of the velocity spectrum (of higher frequency than what is included in the estimation of mean velocities), i.e., the portion that "causes plume meandering." The effects of this portion of the spectrum can only be estimated in a probabilistic fashion. In this frame one can form Eulerian type equations accounting for transport due to the rest ("unused") portion of the motion spectrum. Nevertheless, we will not adopt any further use of the macro-, meso- and micro- prefixes neologism to discriminate between different Lagrangian methodologies, hoping that the concept of the advected-meandering frame (with the axes always parallel to fixed directions) has been sufficiently clarified.

A final question (that has already been addressed in earlier chapters) in under what conditions does the fixed frame form of the mixing operator (in either its stochastic original version or in any approximate form that results from closure) remain a valid representation in the advected-meandering frame. A similar question appears in Lagrangian Trajectory model formulation (see Liu and Seinfeld, 1975) where the ADE is assumed valid, in its fixed frame form, in the transformed coordinates. There

the answer is obtained by examining the equations resulting from a straightforward Galilean transformation of coordinates. The requirement is that the local curvature of the plume centerline is locally small. This limitation exists also in our approach as far as the *mean* centerline trajectory, determined mainly by buoyancy effects, is concerned; however one should expect the above requirement not to be violated except in extreme cases.

Hence the main question here is: what is the effect of the random meandering motions of the moving reference frame? This question is discussed in Section 6.3 where we justify the assumption that, at least for homogeneous and stationary turbulence, these motions should not affect the form of the mixing operator (although of course they alter its parameters).

In the following we proceed in a more detailed analysis of the relative dispersion and meandering concepts and of the modified ADE model.

6.2 BASIC LAGRANGIAN CONCEPTS AND FLUID PARTICLE DISPERSION

6.2.1 Lagrangian Methods

Proceeding from the stochastic representation of the mixing operator (1.3-5) to the 1st order (non-local) closure scheme given by equation (2.3-2), involving coefficients that depend on dispersion time, cannot be justified on a strictly Eulerian basis (via, e.g., a conventional mixing length-gradient transport hypothesis). This would result to a local, dispersion-time independent, scheme, i.e. a differential equation model with eddy diffusivities that are properties of the flow field and not of the particular dispersion process. Furthermore, the associated practical problem of estimating the appropriate values of the plume dispersion parameters and the related diffusivities in terms of statistical characteristics of the velocity field represents another essential aspect of the modeling scheme for dispersion.

Having set the a priori requirement that the operational form of the dispersion model adopted by the TRPM should be at the level of the complexity of the ADE, in combination with the necessity to account for the non-local character of dispersion, leads us to consideration of Lagrangian schemes. Indeed, the Lagrangian description of dispersion (the term to be exclusively associated in the following with the representation of flow in terms of fluid particles) inherently offers a more general perspective in a first order description of the phenomenon than a straightforward Eulerian formulation.

The statistical fluid particle description of turbulent dispersion, originated by Taylor (1921), has been pursued via three major approaches.

(a) In the direct kinematic approach, that follows the original analysis by Taylor, the moments of the displacement of a fluid particle are related kinematically to the Lagrangian velocity correlation functions. Since typically Eulerian and not Lagrangian

correlations are more conveniently measured and are available, the basic fundamental problem encountered in this approach is the derivation of the Lagrangian velocity correlation from the respective Eulerian function. Although the original exact analysis was limited to the case of homogeneous stationary turbulence, the kinematic approach has been extended over the years to approximate various more realistic situations (see, e.g., Pasquill and Smith, 1983; Hunt, 1985). A point that needs to be mentioned here (and on which we will further elaborate in Section 6.5) is that applying the direct approach in the frequency (or wavenumber) rather than in the time domain, and the consequent use of spectra instead of correlations, offers some advantages, both conceptual and computational, that can facilitate relative dispersion parameters estimation.

(b) In the second approach, originated by Batchelor (1949, 1952), one tries to determine the transition probability densities of the fluid particles positions, to be briefly referred to as *transition functions* in the following. Originally this was done on the basis of dimensional and similarity analysis, and it was thus limited to idealized flow fields. From the perspective of current research the essence of this approach is to construct a "master" equation that gives the evolution of the transition function in space and time. From a practical standpoint what is necessary is to reduce the master equation into a tractable form on the basis of reasonable assumptions and, finally, express it in terms of Eulerian velocity correlation functions. A derivation of the form of the master equation that most closely resembles the A.D.E., namely the Fokker-Planck equation, can be found in Seinfeld (1975, Section 6.2.4), the analysis there being in terms of an appropriate ensemble mean concentration (instead of the equivalent transition function). One should mention here that according to the *independence approximation* (Corrsin, 1959), to be discussed in the following, the Lagrangian-Eulerian transformation requires the determination of a weighting function, which is equivalent to the transition function.

(c) The third approach conceptually lies between the two others mentioned above. It is based on the use of Langevin equations for the fluid particles velocities and

although it is more narrow in perspective than the general transition function methods (*) it seems able to provide more directly simple results relevant to both absolute and relative dispersion providing at the same time conceptually simple models for these processes. This approach was originated by Obukhov (1949) and currently receives revived interest, in particular in connection with relative dispersion models (see Sections 6.4.2, 6.4.3).

In the presentation that follows we will first briefly review some fundamental concepts related to the approaches outlined in the preceding paragraphs and also introduce the problem of relative dispersion. In the following sections we will use this information, first to examine the transition function approach in order to explain where the modified ADE adopted in the TRPM formulation (essentially of course a Fokker-Planck equation) stands conceptually in this general Lagrangian framework, and what assumptions are involved in its construction, and then to treat the practical aspect of relative dispersion parameters estimation.

6.2.2 Fundamental Concepts and Definitions

Let $\mathbf{x} = (x_1, x_2, x_3)$, $\mathbf{u} = (u_1, u_2, u_3)$ be the Eulerian coordinates and velocities in the flow field under consideration and $\mathbf{y} = (y_1, y_2, y_3)$, $\mathbf{v} = (v_1, v_2, v_3)$ the corresponding Lagrangian (fluid particle) quantities. An elegant method of defining \mathbf{u} and \mathbf{v} fields is to consider them as special cases of a generalized or Kraichnian velocity field \mathbf{w} (see Leslie, 1973). The Kraichnian velocity $\mathbf{w}(t|\mathbf{x}, t^*)$ is defined as the velocity at time t of fluid particle that was at \mathbf{x} at time t^* (t is called the *measuring time* and t^* the *labelling time*). Then the Eulerian velocity is identified with \mathbf{w} for $t = t^*$:

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{w}(t|\mathbf{x}, t) \quad (6.2 - 1)$$

* In fact this approach, in its most common form, is equivalent to a Fokker-Planck equation governing the transition function of the derivatives of the fluid particles positions (i.e. the Lagrangian velocities). For a brief but very informative discussion of the relationship between the Fokker-Planck and Langevin equations methods of description of random processes see van Kampen (1981, Chapter VIII)

and the Lagrangian velocity is identified with \mathbf{w} for $t > t^*$ with $t^* = t_0$ (and $\mathbf{x} = \mathbf{x}_0$):

$$\mathbf{v}(\mathbf{x}_0, t) = \mathbf{w}(t|\mathbf{x}_0, t_0) \quad (6.2 - 2)$$

The assumptions regarding the nature and properties of the fluid particles in a general Lagrangian analysis may vary widely. In the present study we consider for simplicity "ideal volume fluid particles" (see also Chapter 4) and ignore any transformations on the identity of these particles that may be due to molecular level processes. If we assume that the differential volume element $d\mathbf{x}^3$ "surrounding" the position coordinates \mathbf{x} can be "occupied" by one particle only at a time, we can view these particles "marked" (or uniquely identified) by their position in Eulerian coordinates at some fixed labelling time instant t_0 . However this would be inconsistent with the concept of the ideal instantaneous point source. To avoid further elaboration of this point here (and of the associated need to properly define continuity requirements) we proceed as follows:

Suppose that during the total period of observation (say from time 0 to t) a total number of N marked particles each carrying mass m of some given species, has been introduced (and remains) into the continuum field under consideration and each one is assigned an abstract "identity number" $k = 1, 2, \dots, N$ (which remains unchanged through the entire "life" of the fluid particle). If the particle with "identity number k " was at \mathbf{x}_0 at time t_0 (*), then its Lagrangian position vector will be denoted by the equivalent notation

$$\mathbf{y}(\mathbf{x}_0, t) \equiv \mathbf{y}(t|\mathbf{x}_0, t_0) \equiv \mathbf{y}^{(k)}(t)$$

Two points are worthy of mentioning here:

(a) Different initial sets of assumptions regarding the fluid particle concept may be more useful in specific situations. Thus for example one may want to apply the

* A more precise expression of this statement would be: "in the differential volume element surrounding the coordinate vector," but in the following we will avoid these rather tedious clarifications assuming that the meaning of statements like this are obvious.

Lagrangian analysis to the case where an arbitrary number of fluid particles can simultaneously occupy the same position coordinates, a condition that may be convenient when one wants to model interactions between the fluid particles, or one may consider volume particles (see Chapter 4) that after any finite time interval since their introduction in the flow field they obey conventional volume and mass continuity constraints.

(b) The principles of the analysis to be presented here are valid if other properties of the fluid particle - such as e.g. chemical composition, temperature etc. - besides its spatial-temporal coordinates are taken into account. These properties can be viewed as additional coordinates in which case the Lagrangian position vector \mathbf{y} will follow the evolution path of the particle in an *extended configuration space* that incorporates these properties as extra dimensions. The only such property that we are going to use in the present analysis is the *age* of the fluid particle, i.e. the time elapsed since its introduction in the flow field. Identifying the subset of all particles with the same age is useful not only in dealing with instantaneous releases but also with respect to continuous releases where advection dominates turbulent diffusion in the downstream direction.

Now, having the possibility of the aforementioned generalization of the present analysis in mind, we return to the more standard version of the problem.

The stepping stone for

- (i) a formal development of the transition function approach and,
- (ii) establishing and understanding the relationship between Eulerian and Lagrangian methodologies,

is the introduction of the quantity

$$\psi(\mathbf{x}, t | \mathbf{x}_0, t_0) \equiv \psi^{(k)}(\mathbf{x}, t) \equiv \delta[\mathbf{x} - \mathbf{y}(\mathbf{x}_0, t)] \quad (6.2 - 3)$$

subject to the initial condition

$$\psi(\mathbf{x}, t | \mathbf{x}_0, t_0) = \delta(\mathbf{x} - \mathbf{x}_0) \quad (6.2 - 3a)$$

which can be identified with

- the fundamental “*conservative characteristic*” of Monin and Yaglom (1971, p. 534),
- the “*Lagrangian position function*” of Leslie (1973) (see also Batchelor, 1952),
- the “*microdistribution*” or “*instantaneous transition function*” of Jiang (1985),
- the “*stochastic Green’s function*” of Adomian (1963, 1983) employed by Seinfeld (1983) in the description of turbulent dispersion,

and is also conceptually identical to

- the “*fine grained density function*” of quantum statistical mechanics that has also been employed in studies of turbulent fluid mechanical phenomena (Lundgren, 1967; O’Brien, 1980)

(There are other terms that are also appropriate for ψ – e.g., stochastic Euclidean propagator, stochastic resolvent kernel, etc.).

Some comments are necessary at this point regarding the nature of $\psi(\mathbf{x}, t | \mathbf{x}_0, t_0)$. This quantity is a *function* of the position variable \mathbf{x} and a *functional* of the random field $\mathbf{y}(\mathbf{x}_0, t)$, depending on the structure of the *entire ensemble* of values \mathbf{y} can assume. Consider a fixed value of \mathbf{x} , say \mathbf{x}_F and fix (\mathbf{x}_0, t) . Then $\psi(\mathbf{x}_F, t | \mathbf{x}_0, t_0)$ is zero if $\mathbf{y}(\mathbf{x}_0, t) \neq \mathbf{x}_F$ in any one realization of the random field \mathbf{y} and infinite if $\mathbf{y}(\mathbf{x}_0, t) = \mathbf{x}_F$. For a given realization ψ has all the properties of a pdf, including normalization since

$$\int \psi(\mathbf{x}, t | \mathbf{x}_0, t_0) d\mathbf{x} = 1$$

by the definition of the delta function.

Also the n -th moment of \mathbf{x} is by direct calculation equal to $\psi^n(\mathbf{x}_0, t)$ for all n . In other words, the fine grained density or microdistribution is a device through which each and every realization of the random field can be expressed in a pdf-like manner. However it must be realized that it is a *generalized* and not an ordinary function.

Now, appropriate averaging of $\psi(\mathbf{x}, t | \mathbf{x}_0, t_0)$ leads to the rational construction of various quantities employed in the analysis of turbulent dispersion:

(I) Averaging $\psi(\mathbf{x}, t | \mathbf{x}_0, t_0)$ over all possible starting positions (\mathbf{x}_0, t_0) (i.e. averaging over all particles k) for arbitrary but fixed (\mathbf{x}, t) produces a *random function* of (\mathbf{x}, t) , $\bar{\psi}(\mathbf{x}, t)$

$$\bar{\psi}(\mathbf{x}, t) = \frac{\int \int \psi(\mathbf{x}, t | \mathbf{x}_0, t_0) d\mathbf{x}_0 dt_0}{\int \int d\mathbf{x}_0 dt_0} \quad (6.2 - 4a)$$

or

$$\bar{\psi}(\mathbf{x}, t) = \frac{1}{N} \sum_{k=1}^N \psi^{(k)}(\mathbf{x}, t) \quad (6.2 - 4b)$$

that can be identified with the random fluid particle concentration (and within an appropriate factor that accounts for the dimensions involved in the definition of concentration used) with mass or molar concentration. Thus, in the idealized case under consideration, the random instantaneous mass concentration at (\mathbf{x}, t) will be

$$c(\mathbf{x}, t) = Nm\bar{\psi}(\mathbf{x}, t)$$

When the particular random realization corresponding to a random value of (\mathbf{x}, t) (i.e. for a given random choice of (\mathbf{x}, t)) is to be specified, say through an index α , we will use the left subscript notation

$$\bar{\psi}(\mathbf{x}, t) = {}_{\alpha}\bar{\psi}(\mathbf{x}, t)$$

Nevertheless, it must be clear that (even when this notation is not employed) $\bar{\psi}(\mathbf{x}, t)$ is different for every realization of the turbulent field.

(II) Ensemble averaging $\bar{\psi}(\mathbf{x}, t)$ over all possible realizations of the dispersion field (essentially over the ensembles of \mathbf{y} -trajectories corresponding to all initial (\mathbf{x}_0, t_0)) produces the probability density function that a fluid particle (i.e. *any* fluid particle) will be at \mathbf{x} at time t , which is equivalent to the ensemble mean (number) concentration of fluid particles at (\mathbf{x}, t) . The corresponding mean mass concentration will be

$$\langle c(\mathbf{x}, t) \rangle = Nm \langle \bar{\psi}(\mathbf{x}, t) \rangle$$

(III) Ensemble averaging $\psi(\mathbf{x}, t | \mathbf{x}_0, t_0)$ for fixed (\mathbf{x}_0, t_0) produces the *deterministic transition probability function* G , giving the probability that a fluid particle, starting from \mathbf{x}_0 at time t_0 will be at \mathbf{x} at time t :

$$G(\mathbf{x}, t | \mathbf{x}_0, t_0) = \langle \psi(\mathbf{x}, t | \mathbf{x}_0, t_0) \rangle \quad (6.2 - 5)$$

G is of course the (conventional) Green's function for the *forward* diffusion of the *mean* concentration field. Similarly, ensemble averaging $\psi(\mathbf{x}, t | \mathbf{x}_0, t_0)$ for fixed (\mathbf{x}, t) (i.e. over all trajectories passing from \mathbf{x} at time t) produces the Green's function for *backward* or *reversed* diffusion, $G(\mathbf{x}_0, t_0 | \mathbf{x}, t)$.

Thus, when we have adequate information about ψ we can (in principle) solve the one particle dispersion problem completely. The dynamics of $\psi(\mathbf{x}, t | \mathbf{x}_0, t_0)$ are governed by the generalized conservation (Liouville) equation (*)

$$\left\{ \frac{\partial}{\partial t^*} + w_j(t | \mathbf{x}, t^*) \frac{\partial}{\partial x_j} \right\} \psi(\mathbf{x}, t | \mathbf{x}_0, t^*) = 0 \quad (6.2 - 6)$$

which has the following Eulerian ($t = t^*$) form

$$\left\{ \frac{\partial}{\partial t} + u_j(\mathbf{x}, t) \frac{\partial}{\partial x_j} \right\} \psi(\mathbf{x}, t | \mathbf{x}, t) = 0 \quad (6.2 - 6a)$$

and the following Lagrangian form ($t^* = t_0 = \text{const}$)

$$v_j(\mathbf{x}_0, t) \frac{\partial}{\partial x_j} \psi(\mathbf{x}, t | \mathbf{x}_0, t_0) = 0 \quad (6.2 - 6b)$$

Thus the essence of "approach (b)" of Section 6.2.1 is to introduce appropriate closure approximations in (6.2-6a) in order to finally derive a solvable master equation for G (see Section 6.3.2).

Knowledge of G allows direct calculation of the mean concentration field $\langle c \rangle$ at (\mathbf{x}, t) , given its spatial distribution at t' , as long as this is affected solely by linear processes, through the "fundamental Lagrangian theorem"

$$\langle c(\mathbf{x}, t) \rangle = \int G(\mathbf{x}, t | \mathbf{x}', t') \langle c(\mathbf{x}', t') \rangle \exp \left[- \int_{t'}^t k(t'') dt'' \right] d\mathbf{x}' +$$

* We note here that in more complicated Lagrangian models, that incorporate interactions between the fluid particles, the dynamics of the instantaneous transition function will be governed by appropriate extensions of the Liouville equation, analogous to the Janossy equations described in Srinivasan (1969).

$$+ \int \int_{t'}^t G(\mathbf{x}, t | \mathbf{x}', t'') S(\mathbf{x}', t'') \exp \left[- \int_{t''}^t k(t''') dt''' \right] dt'' d\mathbf{x}' \quad (6.2-7)$$

where S represents the spatial-temporal distribution of sources and k the rate of linear removal of the species with mean concentration $\langle c \rangle$.

At this point a digression is needed in order to clarify that, formally, the above equation must be written in terms of the Green's function for backward diffusion, i.e. with the point (\mathbf{x}, t) determining the constraint of the conditional density, as realized by Corrsin (1952) – see also Tennekes and Lumley, (1972, p.236). Nevertheless, for homogeneous-stationary turbulence, i.e. for the case to which most of the theoretical knowledge on turbulent dispersion is typically confined (and the starting approximation for more realistic descriptions),

$$G(\mathbf{x}, t | \mathbf{x}_0, t_0) = G(\mathbf{x}_0, t_0 | \mathbf{x}, t)$$

as it was formally proved by Corrsin (1972) twenty years later. Thus the above requirement becomes a matter of notation rather than of substance; the same however is not true with regard to many-particle transition functions and the estimation of higher concentration moments (see relevant discussion later in the present subsection).

Another important point is that G also provides the connection between the Lagrangian methodology and the approaches (typically Eulerian) that result directly in some governing equation for $\langle c \rangle$. Indeed if G and $\langle c \rangle$ are related through (6.2-7), and G is governed by

$$\frac{\partial G}{\partial t} + \mathcal{L}G = 0 \quad (6.2-7a)$$

where \mathcal{L} is an *arbitrary* linear operator, then $\langle c \rangle$ must obey the equation

$$\frac{\partial \langle c \rangle}{\partial t} + \mathcal{L} \langle c \rangle + k(t) \langle c \rangle = S(\mathbf{x}, t) \quad (6.2-7b)$$

At this point it is useful to introduce the Eulerian space-time and the Lagrangian temporal velocity correlation functions (tensors), whose elements for stationary and homogeneous turbulence are

$$R_{ij}^E(\mathbf{x} - \mathbf{x}_0, t - t_0) = \langle u_i(\mathbf{x}, t) u_j(\mathbf{x}_0, t) \rangle$$

$$R_{ij}^L(t-t_0|\mathbf{x}_0) = R_{ij}^L(t-t_0) = R_{ij}^L(\tau) = \langle v_i(\mathbf{x}_0, t) v_j(\mathbf{x}_0, t_0) \rangle$$

(Typically the turbulent velocity fluctuations about the corresponding ensemble mean values are used in these definitions.) Now, the formal relation between R_{ij}^E and R_{ij}^L can be obtained by writing R_{ij}^L as

$$\begin{aligned} R_{ij}^L(t-t_0) &= \langle u_i(\mathbf{x} = \mathbf{y}(\mathbf{x}_0, t), t) u_j(\mathbf{x}_0, t_0) \rangle = \\ &= \int \langle u_i(\mathbf{x}, t) u_j(\mathbf{x}_0, t) \delta[\mathbf{x} - \mathbf{y}(\mathbf{x}_0, t)] \rangle d\mathbf{x} \\ &= \int \langle u_i(\mathbf{x}, t) u_j(\mathbf{x}_0, t) \psi(\mathbf{x}, t|\mathbf{x}_0, t_0) \rangle d\mathbf{x} \end{aligned} \quad (6.2-8)$$

The above equation reduces to an "applicable" form through a hypothesis introduced by Corrsin (1959, p.162), and known as "*Corrsin's conjecture*" or "*independence hypothesis*," which, in the present framework of analysis, can essentially be stated as

$$\langle u_i(\mathbf{x}, t) u_j(\mathbf{x}_0, t) \psi(\mathbf{x}, t|\mathbf{x}_0, t_0) \rangle = \langle u_i(\mathbf{x}, t) u_j(\mathbf{x}_0, t) \rangle \langle \psi(\mathbf{x}, t|\mathbf{x}_0, t_0) \rangle \quad (6.2-9)$$

The conditions under which this hypothesis should be valid, as well as corrections for other conditions, have been studied and discussed by Weinstock (1976).

Introducing (6.2-9) in (6.2-8) one has

$$R_{ij}^L(t-t_0) = \int R_{ij}^E(\mathbf{x} - \mathbf{x}_0, t-t_0) G(\mathbf{x} - \mathbf{x}_0, t-t_0) d\mathbf{x} \quad (6.2-10)$$

From a practical viewpoint the applicability of (6.2-10) is limited by our lack of knowledge about G ; in fact the most straightforward methods available for theoretically predicting G are based on an a priori knowledge of R_{ij}^L .

Finally, to complete this summary of basic concepts, we mention that two-particle (and many-particle) stochastic (and deterministic) Green's functions are similarly defined:

$$\begin{aligned} &\psi(\mathbf{x}^{(1)}, t_1; \mathbf{x}^{(2)}, t_2 | \mathbf{x}_0^{(1)}, t_{01}; \mathbf{x}_0^{(2)}, t_{02}) = \\ &= \delta[\mathbf{x}^{(1)} - \mathbf{y}(t|\mathbf{x}_0^{(1)}, t_{01}); \mathbf{x}^{(2)} - \mathbf{y}(t|\mathbf{x}_0^{(2)}, t_{02})] \end{aligned}$$

$$G\left(\mathbf{x}^{(1)}, t_1; \mathbf{x}^{(2)}, t_2 | \mathbf{x}_0^{(1)}, t_{01}; \mathbf{x}_0^{(2)}, t_{02}\right) = \left\langle \psi\left(\mathbf{x}^{(1)}, t_1; \mathbf{x}^{(2)}, t_2 | \mathbf{x}_0^{(1)}, t_{01}; \mathbf{x}_0^{(2)}, t_{02}\right) \right\rangle$$

However the use of many-particle Green's functions (e.g., for the calculation of two-point covariances of concentration through equations similar to (6.2-7)) is associated with some subtle problems, relevant to the concept of backward diffusion, that have often been neglected in atmospheric dispersion modeling (see Sawford, 1983b, for a relevant discussion). Indeed, contrary to what holds for single-particle transition functions, for the corresponding two-particle functions one has

$$G\left(\mathbf{x}^{(1)}, t_1; \mathbf{x}^{(2)}, t_2 | \mathbf{x}_0^{(1)}, t_{01}; \mathbf{x}_0^{(2)}, t_{02}\right) \neq G\left(\mathbf{x}_0^{(1)}, t_{01}; \mathbf{x}_0^{(2)}, t_{02} | \mathbf{x}^{(1)}, t_1; \mathbf{x}^{(2)}, t_2\right)$$

even for homogeneous-stationary turbulence. However, in connection to relative dispersion, that can be directly seen as a two-particle problem, these subtleties are more relevant to modeling higher order moments, whereas mean concentrations require only appropriate "distance-neighbour" functions – to be discussed later – that are obtained through integration of the two-particle transition functions. Thus, by examining dispersion relative to the meandering center of mass, we essentially use always single-particle Green's functions.

6.2.3 Fixed and Meandering Frame Representations:

Position Moments and Relative Dispersion

We now proceed to define and discuss some quantities that are essential in the description of relative or two-particle turbulent dispersion (equivalently dispersion with respect to the center of mass of dispersion or with respect to a meandering frame). Use of the stochastic and deterministic functions defined in the previous section allows a formal construction of these definitions. For simplicity we confine attention to instantaneous releases(*), or, equivalently, to subsets of particles that

* A continuous release will be viewed as a sequence of instantaneous releases. For a (slender) atmospheric plume in particular, where dispersion is negligible compared to advection in the direction of the mean wind, every cross-section of the plume perpendicular to its centerline (of differential thickness) can be seen as the result of such an instantaneous release.

have the same age. Without any loss of generality we set $\mathbf{x}_0 = 0$, $t_0 = 0$ (and assume this implicitly included in the definitions that follow).

(I) The position of the center of mass of the marked fluid particles in any instantaneous (say the α -th) realization of the dispersion field will be

$$\alpha \bar{\mathbf{y}}(t) = \int \alpha \bar{\psi}(\mathbf{x}, t) \mathbf{x} d\mathbf{x} \quad (6.2 - 11)$$

Clearly this quantity is a random function of time. An alternative interpretation of $\alpha \bar{\mathbf{y}}(t)$ is that of the random spatial average position of any single fluid particle in the α -th realization.

(II) The ensemble average position of the center of mass of all fluid particles at time t (i.e. averaged over all possible positions of all fluid particles) will be

$$\langle \bar{\mathbf{y}}(t) \rangle = \int \mathbf{x} \langle \bar{\psi}(\mathbf{x}, t) \rangle d\mathbf{x} \quad (6.2 - 12a)$$

i.e.

$$\langle \bar{\mathbf{y}}(t) \rangle = \int \mathbf{x} G(\mathbf{x}, t) d\mathbf{x} \quad (6.2 - 12b)$$

When there is no mean flow (or if we consider an *inertial* coordinate system that follows the mean flow) $\langle \bar{\mathbf{y}}(t) \rangle \equiv 0$.

At this point we introduce the following definitions:

- *Absolute Diffusion* is diffusion with respect to $\langle \bar{\mathbf{y}}(t) \rangle$, i.e. with respect to a frame of reference with axes that remain parallel to fixed directions and origin that follows $\langle \bar{\mathbf{y}}(t) \rangle$. Since, for steady mean flow, motion in this frame is given by a straightforward Galilean transformation of the corresponding motion with respect to a frame fixed to the ground, we may use the term "*fixed frame representation*" for the description of turbulent dispersion in this frame. A more exact term is "*deterministic inertial frame representation*." Here the term "deterministic" has been used to discriminate from the representation with respect to ensembles of inertial frames, each frame moving with constant velocity randomly

selected from an appropriate set. This description constitutes a conceptually subtle but very important approach that will be discussed later, in Section 6.4.2.

- *Relative Diffusion* is diffusion with respect to the (random) ${}_{\alpha}\bar{\mathbf{y}}(t)$, i.e. with respect to a frame of reference with axes that remain parallel to fixed directions and origin that follows the random motion of ${}_{\alpha}\bar{\mathbf{y}}(t)$. This is a “meandering” or “non-inertial” frame (undergoing random accelerations). (In the following we will further discuss the terms “two-particle dispersion”, “puff” or “cluster” dispersion and “conditioned dispersion”.)

(III) The “extent of dispersion” of the systems of fluid particles, in the non-inertial and inertial frames of reference, will be described by:

(IIIa) a *dyadic* (2nd order tensor) of instantaneous weighted deviations from the (instantaneous) center of mass (of course these deviations will be stochastic variables)

$${}_{\alpha} \left[\tilde{\Sigma}_{ij}^{(R)} \right] = \int (\mathbf{x} - {}_{\alpha}\bar{\mathbf{y}}(t)) (\mathbf{x} - {}_{\alpha}\bar{\mathbf{y}}(t)) {}_{\alpha}\bar{\psi}(\mathbf{x}, t) d\mathbf{x} \quad (6.2 - 13a)$$

(Note the use of the indefinite or dyadic product of the deviation vectors in the above definition).

Now, let

$$\mathbf{r} = \mathbf{x} - {}_{\alpha}\bar{\mathbf{y}}(t)$$

and let $\mathbf{y}^{(R)}$ be defined exactly as \mathbf{y} but in the system of \mathbf{r} -coordinates (i.e. $\mathbf{y}^{(R)}$ is the position vector of the fluid particle in the meandering frame of reference). Then

$$\begin{aligned} \left\langle \left[\tilde{\Sigma}_{ij}^{(R)} \right] \right\rangle &= \int \mathbf{r}\mathbf{r} \langle \bar{\psi}(\mathbf{x}, t) \rangle d\mathbf{x} = \\ &= \int \mathbf{r}\mathbf{r} \left\langle \bar{\psi} \left(\mathbf{r} + \int \bar{\psi}(\mathbf{x}, t) \mathbf{x} d\mathbf{x}, t \right) \right\rangle d\mathbf{r} \end{aligned}$$

We define

$$G^{(R)}(\mathbf{r}, t) = \left\langle \bar{\psi} \left(\mathbf{r} + \int \bar{\psi}(\mathbf{x}, t) \mathbf{x} d\mathbf{x}, t \right) \right\rangle \quad (6.2 - 13b)$$

(compare Monin and Yaglom, 1975, eq.24.56), to be discussed in the following sections, and

$$\left[\Sigma_{ij}^{(R)} \right] \equiv \left\langle \left[\tilde{\Sigma}_{ij}^{(R)} \right] \right\rangle = \left\langle \mathbf{y}^{(R)} \mathbf{y}^{(R)} \right\rangle \quad (6.2 - 13c)$$

(IIIb) a dyadic of standard deviations from the ensemble average center of mass (a deterministic tensor)

$$[\Sigma_{ij}] = \int (\mathbf{x} - \langle \bar{\mathbf{y}}(t) \rangle) (\mathbf{x} - \langle \bar{\mathbf{y}}(t) \rangle) \langle \bar{\psi}(\mathbf{x}, t) \rangle d\mathbf{x} =$$

$$[\Sigma_{ij}] = \int (\mathbf{x} - \langle \bar{\mathbf{y}}(t) \rangle) (\mathbf{x} - \langle \bar{\mathbf{y}}(t) \rangle) G(\mathbf{x}, t) d\mathbf{x} \quad (6.2-14a)$$

Thus, when the reference frame is chosen so that $\langle \bar{\mathbf{y}}(t) \rangle = 0$, as is typically done for the definition of Σ_{ij} ,

$$[\Sigma_{ij}] = \langle \mathbf{y}\mathbf{y} \rangle \quad (6.2-14b)$$

From definition (6.2-13a) now follows that

$$\alpha [\tilde{\Sigma}_{ij}^{(R)}] = \int \alpha \bar{\psi}(\mathbf{x}, t) \times$$

$$\times [(\mathbf{x} - \langle \bar{\mathbf{y}}(t) \rangle) (\mathbf{x} - \langle \bar{\mathbf{y}}(t) \rangle) - (\alpha \bar{\mathbf{y}}(t) - \langle \bar{\mathbf{y}}(t) \rangle) (\alpha \bar{\mathbf{y}}(t) - \langle \bar{\mathbf{y}}(t) \rangle)] d\mathbf{x}$$

and, after ensemble averaging,

$$[\Sigma_{ij}^{(R)}] = [\Sigma_{ij}] - \langle (\alpha \bar{\mathbf{y}}(t) - \langle \bar{\mathbf{y}}(t) \rangle) (\alpha \bar{\mathbf{y}}(t) - \langle \bar{\mathbf{y}}(t) \rangle) \rangle$$

or

$$[\Sigma_{ij}] = [\Sigma_{ij}^{(R)}] + [\Sigma_{ij}^{(M)}] \quad (6.2-15)$$

where

$$[\Sigma_{ij}^{(M)}] = \langle (\alpha \bar{\mathbf{y}}(t) - \langle \bar{\mathbf{y}}(t) \rangle) (\alpha \bar{\mathbf{y}}(t) - \langle \bar{\mathbf{y}}(t) \rangle) \rangle \quad (6.2-16a)$$

or, for $\langle \bar{\mathbf{y}}(t) \rangle = 0$

$$[\Sigma_{ij}^{(M)}] = \langle \alpha \bar{\mathbf{y}}(t) \alpha \bar{\mathbf{y}}(t) \rangle \quad (6.2-16b)$$

In other words expression (6.2-15) states that each element of the variance tensor of the ensemble of positions of all the fluid particles is equal to the ensemble average of the corresponding element of the tensor of instantaneous spatial variances from the instantaneous center of mass plus an ensemble mean square deviation of the individual centers of mass of possible realizations from the ensemble average center of

mass. More simply, the above states that total (i.e. absolute) dispersion is the “sum” of relative dispersion and meandering.* The situation discussed in the preceding paragraphs is also depicted schematically in Figure 6-1.

Typically, in atmospheric modeling, the off-diagonal elements of the above tensors, Σ_{ij} etc., are assumed negligible (see also Seinfeld, 1975, for the relevant discussion concerning K-theory applications). In the present work we have also adopted this assumption (nevertheless, it should be noted that the analysis of the following sections is not in general restricted by this approximation). Discussion of its validity is beyond the scope of this presentation; however, the interested reader is referred to Tavoularis and Corrsin (1985) for a relevant study.

The diagonal elements of Σ_{ij} etc. will be denoted as

$$\Sigma_{ii} = \sigma_i^2 \quad (6.2 - 17a)$$

$$\Sigma_{ii}^{(R)} = \sigma_{Ri}^2 \quad (6.2 - 17b)$$

$$\Sigma_{ii}^{(M)} = \sigma_{Mi}^2 \quad (6.2 - 17c)$$

and are recognized as the absolute dispersion relative dispersion, and meandering parameters respectively.

*Two-Particle Dispersion Concepts
and Distance-Neighbour Functions
(or Special Transition Functions)*

In the preceding paragraphs relative dispersion was identified as dispersion with respect to the instantaneous center of mass of the system of fluid particles. Another description of the same process is formulated in terms of the separation of two arbitrary fluid particles in the instantaneous release (or two particles of the same age

* This is true for homogeneous-stationary turbulence. In general one can also identify components of the total observed dispersion due to other effects, such as buoyancy and shear (see, e.g., Pasquill, 1975; McRae et al., 1982). For an introduction to the dispersive action of these effects one may consult Csanady (1973) or Fischer et al. (1979) – see also the discussion of the kinematic analysis of dispersion in Section 6.3 for further relevant references.

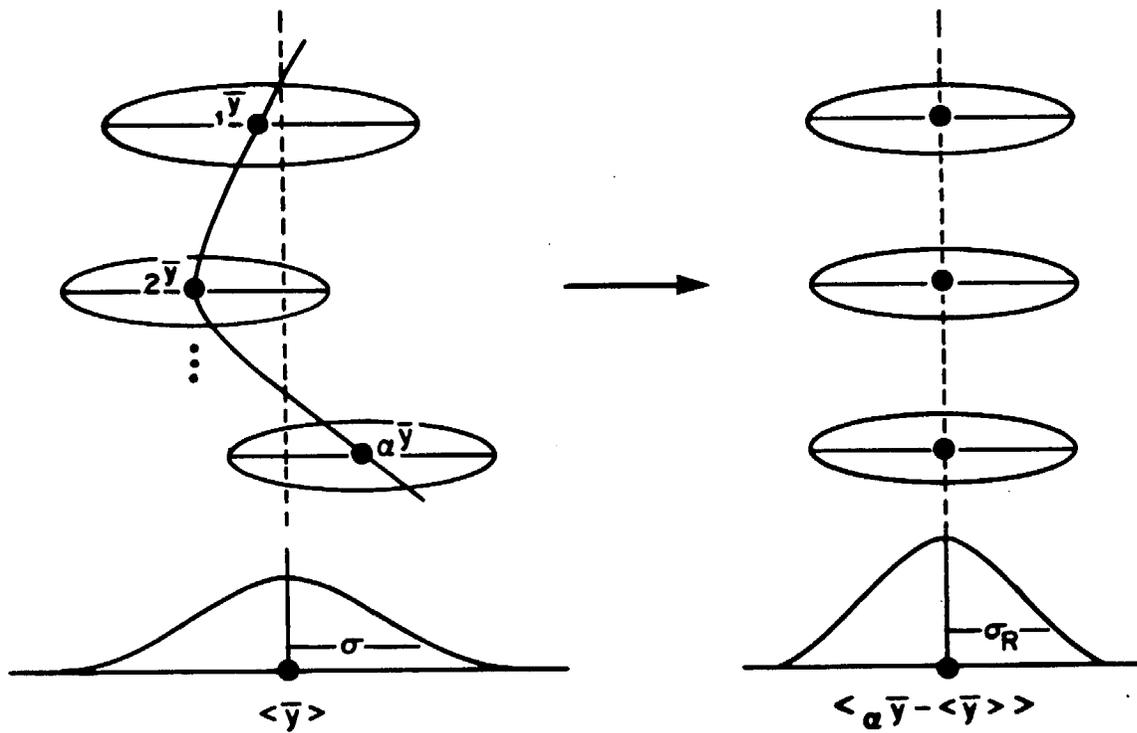


Figure 6-1
 Schematic Representation of
 Relative and Absolute (Relative plus Meandering) Dispersion

in a continuous release). Indeed, it was first perceived by Richardson (1926), and exploited theoretically by Batchelor (1952), that relative diffusion is closely linked to the rate at which two individual fluid particles separate. The first analyses of instantaneous dispersion were actually in terms of the probability densities of two-particle separations.

The equivalence between two-particle dispersion and dispersion with respect to the center of mass in an instantaneous release is implicitly or explicitly assumed in almost all standard references of the subject of turbulence and turbulent dispersion. However, there are various subtle points in formally relating the statistics of the motion of a single pair of particles to the "observable" statistics of puffs and plumes that are typically attributed to relative dispersion. Many authors simply do not address this problem; however one can find an informative discussion of relevant concepts in Monin and Yaglom (1975, pp.536-584 – see in particular pp.551-555, 577). What needs to be stressed here is that the equivalence between single pair motion and relative dispersion is strictly valid only for homogeneous turbulence and after the fluid particles have "forgotten" their initial separation (see also Fischer et al. 1979, p.75).

Studying the separation of a pair of fluid particles is of course, always equivalent to studying the random motion of a single particle (labelled, say, #1), with "fixed" frame position vector $\mathbf{y}^{(1)}$, in a (noninertial) reference frame O_s that follows the random motion of another arbitrary particle (#2) with "fixed" frame position vector $\mathbf{y}^{(2)}$, (in the same way the meandering frame that was introduced earlier follows the motion of the instantaneous center of mass). The first step towards defining the equivalent of the inertial frame transition function G in the O_s frame (which of course gives the expected concentration in the random non-inertial frame O_s), to be called $G^{(S)}$, is to integrate the joint (two-particle) deterministic Green's function $G(\mathbf{x}^{(1)}, t_1; \mathbf{x}^{(2)}, t_2 | \mathbf{x}_0^{(1)}, t_{01}; \mathbf{x}_0^{(2)}, t_{02})$ with respect to $\mathbf{x}^{(2)}$ (see also Leslie, 1973,

p.179). In fact, setting $\mathbf{x}_0^{(2)} = \mathbf{x}_0$, $\mathbf{x}_0^{(1)} = \mathbf{x}_0 + \mathbf{s}_0$, $\mathbf{x}^{(2)} = \mathbf{x}$, $\mathbf{x}^{(1)} = \mathbf{x} + \mathbf{s}$, we define

$$\begin{aligned} G^{(2P)}(\mathbf{s}, t_1, t_2 | \mathbf{x}_0, \mathbf{s}_0, t_{01}, t_{02}) &= \\ &= \int G(\mathbf{x} + \mathbf{s}, t_1; \mathbf{x}, t_2 | \mathbf{x}_0 + \mathbf{s}_0, t_{01}; \mathbf{x}_0, t_{02}) d\mathbf{x}_0 \end{aligned} \quad (6.2 - 18)$$

Thus $G^{(2P)}$ is the transition probability density of the two-particle separation vector, conditioned on the initial separation. In the special case of homogeneous-stationary turbulence and fluid particles of the same age ($t_{01} = t_{02} = 0, t_1 = t_2 = t$) we have

$$G^{(2P)} = G^{(2P)}(\mathbf{s}, t | \mathbf{s}_0)$$

If $q(\mathbf{s}_0)$ is the probability density of the initial separation vector, then $G^{(S)}$ is defined as

$$G^{(S)}(\mathbf{s}, t) = \int G^{(2P)}(\mathbf{s}, t | \mathbf{s}_0) q(\mathbf{s}_0) d\mathbf{s}_0 \quad (6.2 - 19)$$

After sufficient time from the release (when initial separations are forgotten)

$$G^{(2P)}(\mathbf{s}, t) = G^{(S)}(\mathbf{s}, t)$$

The dispersion process described by $G^{(S)}$ is typically what is called “puff” or “cluster” diffusion in the literature; for Monin and Yaglom (1975) this is defined to be the “relative dispersion process”.

Another common approximation is that the information carried by $G^{(S)}(\mathbf{s}, t)$ is equivalent to the information carried by $G^{(R)}(\mathbf{r}, t)$, as this was defined through (6.2-13b). Of course $G^{(S)}$ is the transition probability of the position of any fluid particle as seen in the frame of another (arbitrary but fixed) fluid particle; this transition function is essentially equivalent to the *distance-neighbour function* introduced (in a less formal manner) by Richardson (1926), although this term is often attributed to $G^{(2P)}$ rather than to $G^{(S)}$ (e.g. Leslie, 1973). $G^{(R)}$ is the transition probability of fluid particle positions in the meandering center of mass frame. We will refer to $G^{(2P)}$, $G^{(S)}$ and $G^{(R)}$ as “special” (non-inertial frame) transition functions and focus

on $G^{(R)}$ which has been the basis for the description of instantaneous dispersion in the TRPM model.

The single most important direct relationship between the 0r and 0s descriptions concerns the second order dispersion tensors in these frames. Letting $\mathbf{y}^{(S)}$ be the position vector of *any* fluid particle in the 0s frame one can define the second moments of $G^{(S)}$ with respect to the separation vector. The corresponding dyadic is

$$\left[\Sigma_{ij}^{(S)} \right] = \int (\mathbf{s} - \mathbf{y}^{(2)}) (\mathbf{s} - \mathbf{y}^{(2)}) G^{(S)}(\mathbf{s}, t) d\mathbf{s} \quad (6.2 - 20a)$$

or

$$\left[\Sigma_{ij}^{(S)} \right] = \left\langle \mathbf{y}^{(S)} \mathbf{y}^{(S)} \right\rangle \quad (6.2 - 20b)$$

Straightforward calculations (Brier, 1950; Batchelor, 1952 – see also Monin and Yaglom, 1975, p.555) then show that

$$\left[\Sigma_{ij}^{(S)} \right] = 2 \left(\left[\Sigma_{ij} \right] - \left[\Sigma_{ij}^{(M)} \right] \right) = 2 \left[\Sigma_{ij}^{(R)} \right] \quad (6.2 - 21)$$

Thus, the ensemble mean-square separation in all the pairs of diffusing particles, in an instantaneous release, is just twice their mean square distance from the center of mass of this release.

A final point to note is that in (6.2-20) $\Sigma_{ij}^{(S)}$ is defined in terms of $G^{(S)}(\mathbf{s}, t)$, which incorporates a full statistical description of the initial distribution of fluid particles. An alternative approach is to define a dispersion tensor $\Sigma_{ij}^{(2P)}$ that is conditioned on the value of the initial separation by using $G^{(2P)}$ (see Monin and Yaglom, 1975, where this approach is employed). Then

$$\Sigma_{ij}^{(S)}(\mathbf{s}, t) = \int \Sigma_{ij}^{(2P)}(\mathbf{s}, t | \mathbf{s}_0) q(\mathbf{s}_0) d\mathbf{s}_0 \quad (6.2 - 22)$$

6.3 THE MODIFIED ADE: DISCUSSION AND JUSTIFICATION

The objectives of the present section are

(i) to discuss the character of the special transition function $G^{(R)}$ in relation to that of the inertial frame G , (equivalently: the nature of the expected concentration profile in the random meandering frame), and

(ii) to explain the nature of the assumptions leading to a representation of G and $G^{(R)}$, (or of the corresponding expected concentration fields) and of the differential evolution equations that govern these quantities, in terms of diffusivities that depend on diffusion time, showing also the connection of these representations to various common dispersion models.

6.3.1 Fixed and Meandering Frame Representations: Point Releases and Green's Functions

As it has often been repeated in this work, a fundamental assumption in the formulation of both the master and peripheral components of the TRPM is that the expected concentration fields in both a fixed and a meandering frame of reference are governed by (parabolic partial differential) equations of identical structure (differing only in the values of the diffusivities employed). In other (but equivalent) words it is assumed that G and $G^{(R)}$ are identical in form, with different parameters. We will discuss this assumption here, focusing first on our knowledge regarding the aforementioned Green's functions for ideal situations; the general structure of the governing equations is discussed in the next subsections.

Let us consider in particular a "point" release of inert material in homogeneous stationary turbulence. Confining attention to the common case of slender plumes, where downwind advection dominates turbulent dispersion in the same direction, we can equivalently consider the instantaneous puff problem: a cross section of the plume

(of differential thickness) will essentially contain all the fluid particles released from the source in a given differential time interval. Thus the terms Green's function and expected concentration (for both the fixed frame and the puff or meandering frame cases) can be used interchangeably.

In the special case of homogeneous and stationary turbulence with random velocity components that obey Gaussian densities the inertial frame Green's functions G are of course Gaussian (the boundary conditions imposing appropriate finite or infinite combinations of Gaussian functions). This exact theoretical fact is indeed the first step towards the Gaussian plume approximation of actual field dispersion. However, even in the idealized case where G is exactly Gaussian for all times t , the corresponding $G^{(R)}$ is not always unambiguously known. Without delving into fine details (for which the reader is referred to Monin and Yaglom, 1975, secs.24.2, 24.3) we note that the relative motion of fluid particles undergoes a sequence of stages. Very schematically these stages are: (i) first, a "*source conditioned motion*," dependent on the initial distribution of separations among the fluid particles, (ii) second, a so called "*quasi-asymptotic motion*" (Batchelor, 1952), where the effect of the initial conditions has become negligible, but the motions of any two particles are still correlated, (iii) third, an "*asymptotic motion*," where the motions of different fluid particles are practically independent, and, finally, (iv) a "*large scale motion*," where the average separation between two particles becomes very large compared with the integral scale of turbulence and relative diffusion becomes identical to absolute diffusion (and of course $G = G^{(R)}$). The common A.D.E. is relevant to this final stage. Here our interest is mainly in stages (ii) and (iii), since, on one hand, we consider "point" sources and thus in general wish to avoid introducing source parameters other than the emissions rate in our models (*), and, on the other hand, available observations show that this stage in the atmosphere lasts for only a few seconds (see, e.g., Hanna et al. 1982, p.42).

* One must also take into account that identifying an effective initial distribution of separations for an actual source is far from being a trivial matter.

Let us consider first the stage of asymptotic motion where the trajectories of different fluid particles in the puff (i.e. of same age in the plume) are statistically independent. Then, if the number N of these fluid particles is large enough ($N \rightarrow \infty$), the random trajectory of the center of mass of any $N - 1$ particles is practically identical to that of the center of mass of all N particles, and, further, this trajectory and that of the N -th particle are statistically independent. In other words \mathbf{r} and $\bar{\mathbf{y}}(t)$ are independent random variables whose sum $\mathbf{x} = \mathbf{r} + \bar{\mathbf{y}}(t)$ has a Gaussian probability density G . This however directly implies that, according to an important theorem due to Cramér (see Papoulis, 1965, p.222), the probability densities of $\bar{\mathbf{y}}(t)$ and \mathbf{r} (the latter being exactly $G^{(R)}$) are also Gaussian. The Gaussian character of $G^{(R)}$ for the asymptotic stage, which plays a key role in the formulation of the TRPM, was demonstrated here in a very straightforward manner (that—to our knowledge—has not appeared formally in the literature before) strictly for point releases in homogeneous stationary turbulence, but it can be considered a plausible approximation in more general cases where homogeneity and stationarity of the turbulent velocity field are not strongly violated (the mean concentration field is of course inhomogeneous).

In the stage of quasi-asymptotic motion the shape of $G^{(R)}$ (more commonly referred to as the expected concentration distribution relative to the center of gravity of a cloud) has been a subject of continuing controversy. Typically it is assumed that for a substantial fraction of the duration of the stage of quasi-asymptotic motion the instantaneous dimensions of the dispersing cloud “most probably” do not exceed the maximum scales of the inertial subrange. Inertial subrange scaling and similarity analysis for locally isotropic turbulence allow for various modeling schemes that lead to different forms of $G^{(R)}$. (see also Monin and Yaglom, 1975, p.577, and Pasquill and Smith, 1983, p.153). Among the possible admissible models (on similarity grounds) the three most widely considered and discussed are essentially equivalent to semiempirical parabolic partial differential equations for $G^{(R)}(\mathbf{r}, t)$, with eddy diffusivities that depend on either the dispersion time t or the distance from the center of mass $r = |\mathbf{r}|$, or both. These are

- the Batchelor-Obukhov equation (see, e.g., Monin and Yaglom, 1975, secs. 24.2, 24.3), with

$$K \sim \epsilon t^2$$

producing a Gaussian solution (that decreases at infinity as $\exp(-br^2)$, b being an appropriate constant),

- the Richardson (1926) equation with

$$K \sim \epsilon^{1/3} r^{4/3}$$

producing a solution that is more steeply peaked than the Gaussian (and decreases at infinity as $\exp(-br^{2/3})$), and

- the Okubo (1962) equation with

$$K \sim \epsilon^{2/3} r^{2/3} t$$

producing a solution that decreases at infinity as $\exp(-br^{2/3})$.

(Note that the average value ϵ of the actually fluctuating energy dissipation rate is used in the above equations).

Thus, in the Batchelor-Obukhov formulation – the one leading to a *linear* equation for $G^{(R)}(\mathbf{r}, t)$ – only statistics of the fluid particle positions in the meandering frame (or the two-particles separation), i.e. their variances, affect the parameters of the governing equations for relative dispersion, whereas in the nonlinear models these parameters are functions of the actual position in this frame.

Available observations have not allowed for a definite conclusion on the superiority of the above schemes. Although some sets of data show excellent agreement with the Gaussian model (e.g. Csanady, 1966; Sullivan, 1971 – see also Figure 5-1 of the previous chapter) in certain cases some researchers have found a slightly better agreement with nonlinear models (e.g. Okubo, 1962). In view of the analytical advantages of the linear model, its proven validity for times beyond those of the quasi-asymptotic stage, and supportive observational evidence, it seems very reasonable to accept it

as the universal model for all dispersion times. This is in agreement with the recommendations of Monin and Yaglom (1975, pp. 562 and 578), and with practically all applied studies of instantaneous plume properties, such as Gifford's (1959) fluctuating plume model and Csanady's (1973) relative dispersion and fluctuations models.

What comes as an overall conclusion of the above discussion is that (at least in the ideal case of homogeneous stationary turbulence examined here) assuming $G(\mathbf{x}, t)$ and $G^{(R)}(\mathbf{r}, t)$ to have similar forms, and be governed by equations of similar structure, is a reasonable assumption. We will adopt this assumption as a first approximation for studying dispersion processes in more complicated turbulent fields. In the following we overview the most common equations that have been used to model G (most of which are also assumed appropriate for modeling $G^{(R)}$).

6.3.2 Master Equations and Practical Models

Obtaining the analytical form of the transition function $G(\mathbf{x}, t | \mathbf{x}_0, t_0)$ or, more generally, deriving a governing equation (a "master equation") for this probability, that, under certain simplifying assumptions, can be reduced to solvable form (analytically or numerically), constitutes the fundamental problem of the transition function Lagrangian approach. (*)

In the special case where the turbulent Lagrangian velocity field is unbounded and, beyond being homogeneous and stationary, is also Markovian and Gaussian with independent components (i.e. every component of the velocity vector is Gaussian and has an exponential autocorrelation: an Ornstein-Uhlenbeck process), and, furthermore, the fluid particle trajectories are independent, it can be directly shown, through kinematic considerations and the definition $G = \langle \psi \rangle$, that $G(\mathbf{x} - \mathbf{x}_0, t - t_0)$ is Gaussian. The details of the proof can be found in Seinfeld (1983, pp. 218-222).

Under the conditions where the common ADE is valid (briefly when the fluid

* The alternative to this theoretical determination of the transition function is of course to use laboratory (e.g. Willis and Deardorff, 1978, 1981) or numerical (e.g. Deardorff, 1974; Lamb, 1978) simulations of turbulent flow fields.

particles motion can be seen as a discrete random walk that is a 1st order Markovian process with effective step lengths in space and time that are comparable to the Lagrangian space-time scales) G will correspond to the *fundamental solution* (i.e. the response to an impulse forcing term) of any linear form of the ADE (which is local in space and time).

On smaller scales, however, the equation governing G must reflect the persistence of correlation over finite space and time. Batchelor and Townsend (1956, p. 360) first suggested that this non-localness may be best expressed by an integrodifferential equation. Such an equation was first derived by Bourret (1960) who generalized a property of a simple model of turbulent diffusion due to Taylor that assumed a finite Lagrangian time, i.e., a persistence of velocity correlation over the fluid particles trajectory. Bourret's equation uses the Lagrangian velocity autocorrelation

$$R_{ij}^L(t - t_0) = \langle v'_i(t) v'_j(t_0) \rangle$$

and holds for homogeneous-stationary turbulence:

$$\frac{\partial G(\mathbf{x}, t)}{\partial t} = \frac{\partial^2}{\partial x_i \partial x_j} \int_0^t R_{ij}^L(t - t') G(\mathbf{x}, t') dt'$$

Other general integrodifferential master equations, for both one- and two-particle transition functions, utilizing Eulerian velocity autocorrelations, were subsequently derived by Roberts (1961) who employed Kraichnan's Direct Interaction Approximation to obtain closure for equation (6.2-6a).(*) Since then many interesting results of similar nature have been obtained, e.g., by Deissler (1961), Bourret (1962, 1965) Kraichnan (1966), Saffmann (1969), Knobloch (1977), Lundgren (1981), and Jiang (1984, 1985). In general the evolution of G is found to be described by nonlinear integrodifferential equations, closely resembling that of Roberts, which are closed by a truncation of a series of correlations. Recently developed methods are reviewed by Jiang (1985) who, for the dispersion of a single particle, derived an equation for G

* The monograph of Leslie (1973) provides a comprehensive review of Kraichnan's methods and discusses extensively the equation of Roberts.

that, at the zeroth order, reduces to that of Roberts (while there are some differences regarding the behavior of the two-particle transition function dynamics).

From the perspective of the present discussion Roberts' equation (1961) provides a general framework of analysis that is more than adequate for practical purposes. Indeed, practically all first order operational models of (absolute and relative) turbulent dispersion, including the common ADE as well as the modified ADE adopted by the TRPM, can be derived as special cases of this equation when appropriate approximations are introduced. This procedure provides a most useful insight into the relative capabilities, limitations and relationships among the various "usable" models. So, in the following we will examine briefly the reduction of a general integrodifferential master equation into practical expressions.

The most general form of Roberts' (1961) equation (for the fixed frame G) is

$$\frac{\partial}{\partial t} G(\mathbf{x}, t | \mathbf{x}_0, t_0) = \int_{t_0}^{t'} dt' \int d\mathbf{x} R_{ij}^E(\mathbf{x}, t; \mathbf{x}', t') \frac{\partial}{\partial x_i} G(\mathbf{x}, t | \mathbf{x}', t') \frac{\partial}{\partial x_j} G(\mathbf{x}', t' | \mathbf{x}_0, t_0)$$

For homogeneous-stationary turbulence this equation becomes

$$\frac{\partial}{\partial t} G(\mathbf{x}, t) = \frac{\partial^2}{\partial x_i \partial x_j} \int_0^t dt' \int d\mathbf{x}' R_{ij}^E(\mathbf{x}', t') G(\mathbf{x}', t') G(\mathbf{x} - \mathbf{x}', t - t') \quad (6.3 - 3a)$$

Roberts (1961, p.266) replaced the product $R_{ij}^E(\mathbf{x}, t) G(\mathbf{x}, t)$ with a general correlation $Q_{ij}(\mathbf{x}, t)$. Hence, if Corrsin's conjecture holds, Q_{ij} is formally related to R_{ij}^L , and Roberts' equation is now written as

$$\frac{\partial}{\partial t} G(\mathbf{x}, t) = \frac{\partial^2}{\partial x_i \partial x_j} \int_0^t dt' \int d\mathbf{x}' Q_{ij}(\mathbf{x}', t') G(\mathbf{x} - \mathbf{x}', t - t')$$

or, equivalently (for \mathbf{x}' ranging from $-\infty$ to ∞),

$$\frac{\partial}{\partial t} G(\mathbf{x}, t) = \frac{\partial^2}{\partial x_i \partial x_j} \int_0^t dt' \int d\mathbf{x}' Q_{ij}(\mathbf{x} - \mathbf{x}', t - t') G(\mathbf{x}', t') \quad (6.3 - 3b)$$

a result that is found to resemble strongly the equation of Bourret (see also following paragraphs).

Evolution equations for the special non-inertial transition functions have also been formally derived (in particular for $G^{(2P)}$). The reader is referred to Leslie (1973) and Jiang (1985) for detailed analyses. As a representative example we mention that on the basis of the analysis of Roberts (and the equivalence of $G^{(S)}$ and $G^{(R)}$ after very small times) the analog of (6.3-3a) for $G^{(R)}(\mathbf{r}, t)$ becomes approximately

$$\begin{aligned} \frac{\partial}{\partial t} G^{(R)}(\mathbf{r}, t) &= \frac{\partial^2}{\partial r_i \partial r_j} \int_0^t dt' \int d\mathbf{r}' [R_{ij}^E(\mathbf{r}', t') - R_{ij}^E(\mathbf{r} - \mathbf{r}', t')] \times \\ &\quad \times G(\mathbf{x}', t') G^{(R)}(\mathbf{r} - \mathbf{r}', t - t') \end{aligned}$$

One should notice the dependence of the term replacing the Eulerian velocity correlation of (6.3-3a) on both $\mathbf{r} - \mathbf{r}'$ and \mathbf{r}' . For the purposes of the present work it seems reasonable to assume that the last equation can be represented in general by an equation identical to (6.3-3b) but with Q_{ij} depending on t as well as on $t - t'$ to reflect the nonstationarity present in the Lagrangian velocity correlations in the non-inertial frame (to be also discussed in the next section).

*Dispersion Parameters
(through the G-formalism)*

Equations (6.3-3ab) – or the corresponding equations for $G^{(R)}(\mathbf{r}, t)$ – can be combined directly with the definitions of the dispersion parameters Σ_{ij} etc. in order to express the latter directly in terms of the general correlation Q_{ij} . Defining the *turbulent diffusivities*

$$K_{ij} = \frac{1}{2} \frac{d}{dt} \Sigma_{ij}$$

and using definition (6.2-14a) one has

$$\begin{aligned} K_{ij} &= \frac{1}{2} \int x_i x_j d\mathbf{x} \frac{\partial^2}{\partial x_m \partial x_n} \int_0^t dt' \int d\mathbf{x}' Q_{mn}(\mathbf{x} - \mathbf{x}', t - t') G(\mathbf{x}', t') = \\ &= \int_0^t dt' \int d\mathbf{x} d\mathbf{x}' Q_{ij}(\mathbf{x} - \mathbf{x}', t - t') G(\mathbf{x}', t') \end{aligned}$$

and, since $\int G(\mathbf{x}, t) d\mathbf{x} = 1$,

$$K_{ij} = \int_0^t dt' \int d\mathbf{x} Q_{ij}(\mathbf{x} - \mathbf{x}', t - t') \quad (6.3-4)$$

A similar general expression will hold for the relative turbulent diffusivities $K_{ij}^{(R)}$.

Applicable Models of Dispersion

Let us now examine the applicable models that are obtained for various choices of Q_{ij} in (6.3-3b). Without loss of generality we consider an one-dimensional situation with $Q_{ij} = Q$.

• *A.D.E.: The Classic K-Model*

If

$$Q = K \delta(x - x') \delta(t - t') \quad (6.3 - 5a)$$

(with possibly $K = K(x, t)$) (6.3-3) reduces to the conventional K-model

$$\frac{\partial G(\mathbf{x}, t)}{\partial t} = K \frac{\partial^2 G(\mathbf{x}, t)}{\partial x^2} \quad (6.3 - 5b)$$

Notice that condition (6.5-4a) implies that the velocity of a fluid particle is delta-correlated (i.e. "immediately forgets" its earlier values) in both space and time. This of course can be true only when the "time instants" are actually longer than the Lagrangian time scale of the flow (and the adverb "immediately" is interpreted analogously). Thus the severe limitations in the description of turbulent dispersion through the ADE, already discussed in Chapter 1, are obvious.

• *The Equation of Bourret*

If correlation is assumed only in time, i.e.

$$Q = \delta(x - x') R^L(t - t') \quad (6.3 - 6a)$$

one obtains the (one-dimensional) form of Bourret's (1960) equation

$$\frac{\partial G(\mathbf{x}, t)}{\partial t} = \frac{\partial^2}{\partial x^2} \int_0^t R^L(t - t') G(\mathbf{x}, t') dt' \quad (6.3 - 6b)$$

• *The Hyperbolic Telegrapher's Equation*

Assuming correlation only in time (as before) that is specifically of exponential form

$$Q = \delta(x - x') R^L(t - t') = \delta(x - x') \sigma_v^2 \exp\left(-\frac{t - t'}{T^L}\right) \quad (6.3 - 7a)$$

where T^L is the Lagrangian time scale, one obtains the well known telegrapher's equation (see, e.g., Goldstein, 1951).

$$\frac{\partial^2 G}{\partial t^2} = -\frac{1}{T^L} \frac{\partial G}{\partial t} + \sigma_v^2 \frac{\partial^2}{\partial x^2} \quad (6.3 - 7b)$$

• *The Modified (Non-Local) A.D.E.*

The modified ADE is obtained through the same choice of Q as for the equation of Bourret (i.e. autocorrelation of fluid particle velocities only in time)

$$Q(x - x', t - t') = \delta(x - x') R^L(t - t') \quad (6.3 - 8a)$$

or

$$Q(r - r', t - t', t) = \delta(r - r') R^L(t, t - t') \quad (6.3 - 7b)$$

under the additional assumption that the positions of the fluid particles constitute Markovian processes (with arbitrary step). Then, the Chapman-Kolmogorov equation for G gives (for arbitrary (x^*, t^*))

$$G(x - x_0, t - t_0) = \int \int G(x - x^*, t - t^*) G(x^* - x_0, t^* - t_0) dx^* dt^*$$

Introducing this property to the master equation one obtains

$$\frac{\partial G(x - x_0, t - t_0)}{\partial t} = \int_{t_0}^t dt' R^L(t - t') \frac{\partial^2 G(x - x_0, t - t_0)}{\partial x^2}$$

which corresponds directly to a linear (non-local) differential dispersion equation with eddy diffusivities that depend on the travel time:

$$\frac{\partial G(x - x_0, t - t_0)}{\partial t} = K(t - t_0) \frac{\partial^2 G(x - x_0, t - t_0)}{\partial x^2} \quad (6.3 - 8c)$$

where (for $t_0 = 0$)

$$K(t) = \int_0^t dt' R^L(t-t') \quad (6.3-8d)$$

and similarly for $G^{(R)}(r, t)$ with

$$K^{(R)}(t) = \int_0^t dt' R^L(t, t-t')$$

• *The "Spectral Diffusivity" Model*

If one assumes correlation only in space, i.e.

$$Q = R^\#(x-x') \delta(t-t') \quad (6.3-9a)$$

where $R^\#$ is an appropriate space correlation function, equation (6.3-3) reduces to

$$\frac{\partial G(x, t)}{\partial t} = \frac{\partial^2}{\partial x^2} \int dx' R^\#(x-x') G(x', t)$$

The r.h.s. of this equation can be written as

$$-\frac{\partial}{\partial x} \int dx' R^\#(x'-x) G(x', t)$$

Integrating by parts this expression allows us to write

$$\frac{\partial G(x, t)}{\partial t} = \frac{\partial}{\partial x} \int R^\#(x-x') \frac{\partial G(x', t)}{\partial x'} dx' \quad (6.3-9b)$$

This equation is essentially equivalent to the pseudo-spectral model of Berkowicz and Prahm (1979ab, 1980).

Thus now, after clarifying how the modified ADE is related to other turbulent dispersion models, we proceed to examine methods for the estimation of the (relative) dispersion parameters appearing in this equation.

6.4 RELATIVE DISPERSION ANALYSIS:

I. TIME DOMAIN METHODS

6.4.1 The Direct Kinematic Approach:

General Relations and Asymptotic Results

In this section we briefly review the fundamentals of the direct kinematic approach for estimating dispersion parameters. The general kinematic relations that describe the statistics of the fluid particle motions provide some direct information regarding these parameters in the form of asymptotic expressions; however in the case of relative dispersion this information is more limited than in the case of absolute dispersion. Further results can be obtained through dimensional/similarity analysis and on the basis of assumptions regarding the turbulent velocities correlation tensors; these results are also reviewed in the next sub-sections.

In the following exposition the turbulence is assumed (locally) homogeneous and stationary (unless it is specified otherwise). Furthermore, for simplicity (and without any loss of generality) the analysis of the present section assumes that there is no mean flow (or equivalently the equations are formulated in an inertial frame following the mean flow), i.e.

$$\langle \mathbf{u} \rangle = 0, \quad \langle \mathbf{v} \rangle = 0$$

and

$$\mathbf{u}' = \mathbf{u}, \quad \mathbf{v}' = \mathbf{v}$$

and therefore

$$\langle \bar{\mathbf{y}}(t) \rangle = 0, \quad \mathbf{y}'(t) = \mathbf{y}(t) = \mathbf{y}(0, t)$$

We further set $\mathbf{x}_0 = 0, \mathbf{y}(0, 0) = 0$.

• *Review of Absolute Dispersion I*
General Relations and Definitions

Under the assumptions stated above

$$\begin{aligned}\Sigma_{ij}(t) &= \langle y_i(t) y_j(t) \rangle = \left\langle \int_0^t v_i(t') dt' \int_0^t v_j(t'') dt'' \right\rangle = \\ &= \int_0^t \int_0^t \langle v_i(t') v_j(t'') \rangle dt' dt''\end{aligned}$$

or

$$\begin{aligned}\Sigma_{ij}(t) &= \int_0^t \int_0^t R_{ij}^L(t' - t'') dt' dt'' = \\ &= \int_0^t \int_0^{t-t'} R_{ij}^L(\tau) d\tau dt' \quad (6.4 - 1a)\end{aligned}$$

Equation (6.4-1a) and its differential counterpart

$$\frac{d}{dt} \langle y_i(t) y_j(t) \rangle = 2 \int_0^t R_{ij}^L(t - t') dt' \quad (6.4 - 1b)$$

are the well known *Taylor's relations* and constitute the basis of the direct kinematic approach (Taylor, 1921). Now, by definition $R_{ij}^L(\tau) = R_{ji}^L(-\tau)$. Hence

$$\Sigma_{ij}(t) = \int_0^t (t - \tau) [R_{ij}^L(\tau) + R_{ji}^L(\tau)] d\tau \quad (6.4 - 2)$$

This relation was first obtained (in a slightly different form) by Kampé de Fériet (1939).(*)

* At this point it seems worthy of mentioning that relations analogous to (6.4-1ab) and (6.4-2) can also be directly formulated for the case of dispersion in uniform shear flow ("second order homogeneous" turbulence); the corresponding exact expressions were first obtained by Corrsin (1953). Various (approximate) extensions of the fundamental (homogeneous-stationary turbulence) kinematic Lagrangian analysis to more realistic situations, involving wind-shear and convective motions, are also possible, but discussing them is beyond the scope of this presentation. An excellent introduction to the problems of dispersion in flows with shear and density differences can be found in Csanady (1973, Chapters V and VI); for more recent relevant reviews of kinematic methods for describing fluid particle dispersion in complex (nonhomogeneous-nonstationary) flows one should consult Pasquill and Smith (1983) and Hunt (1985).

The (modified) eddy diffusivities K_{ij}^L are defined again as

$$K_{ij}^L(t) \equiv \frac{1}{2} \frac{\partial}{\partial t} \langle y_i(t) y_j(t) \rangle \quad (6.4 - 3a)$$

where the superscript L is used to note that they are derived from a Lagrangian analysis. Hence, in general

$$K_{ij}^L(t) = \frac{1}{2} \int_0^t [R_{ij}^L(\tau) + R_{ji}^L(\tau)] \delta\tau \quad (6.4 - 3b)$$

The elements of the Lagrangian time scale tensor are defined as

$$T_{ij}^L = \frac{1}{(\langle v_i^2 \rangle \langle v_j^2 \rangle)^{1/2}} \int_0^\infty [R_{ij}^L(\tau) + R_{ji}^L(\tau)] d\tau \quad (6.4 - 4)$$

• *Review of Absolute Dispersion II*

Asymptotic Results

The general relations (6.4-1ab) allow us to conclude directly that at very small and very large dispersion times the elements of $[\Sigma_{ij}]$ are independent of the particular form of the Lagrangian velocity correlation. Thus, for $t \rightarrow 0$

$$\Sigma_{ij}(t) = \langle v_i(0,0) v_j(0,0) \rangle t^2 \quad (6.4 - 5a)$$

or

$$K_{ij}^L(t) = \langle v_i(0,0) v_j(0,0) \rangle t \quad (6.4 - 5b)$$

whereas for $t \rightarrow \infty$

$$\Sigma_{ij}(t) = (\langle v_i^2 \rangle \langle v_j^2 \rangle)^{1/2} (T_{ij}^L + T_{ji}^L) t \quad (6.4 - 6a)$$

or

$$K_{ij}^L(\infty) = \frac{1}{2} (\langle v_i^2 \rangle \langle v_j^2 \rangle)^{1/2} (T_{ij}^L + T_{ji}^L) \quad (6.4 - 6b)$$

In particular for $i = j$ one has

$$(\text{for } t \rightarrow 0) \quad \sigma_i^2 = \sigma_{v_i}^2 t^2, \quad K_i^L = \sigma_{v_i}^2 t \quad (6.4 - 5c)$$

$$\text{(for } t \rightarrow \infty \text{) } \sigma_i^2 = 2\sigma_{v_i}^2 T_i^L t, \quad K_i^L = \sigma_{v_i}^2 T_i^L \quad (6.4 - 6c)$$

Of course for homogeneous-stationary turbulence

$$\sigma_{v_i}^2 = \sigma_{u_i}^2$$

• *Review of Absolute Dispersion III*

Extensions

As it was stated earlier, the above results were obtained for arbitrary Lagrangian velocity correlations; however, in order to calculate dispersion parameters for any (intermediate) dispersion time the shape of the above correlations has to be specified. The functional forms and properties of various permissible correlations are presented and discussed, e.g., in Monin and Yaglom (1975) and Pasquill and Smith (1983). For historical reasons the correlation of Sutton (1953), that was most extensively used for atmospheric applications, especially in the 1950's and early 1960's until it was replaced by the introduction of the Pasquill-Gifford curves, should be mentioned. Among the other possible correlations the simple exponential

$$R_{ii}^L = \sigma_{v_i}^2 \exp\left(-\frac{\tau}{T_i^L}\right)$$

has often proved to be a very useful approximation, and, as it has been pointed out by Tennekes (1977, 1979) provides also a connection between single and two-particle dispersion, that is of particular interest from the perspective of the present work (and for this it is worth mentioning). Integrating (6.4-2) (for $i = j$) for an exponential autocorrelation gives

$$\sigma_i^2(t) = 2\sigma_{v_i}^2 T_i^{L^2} \left[\frac{t}{T_i^L} - 1 + \exp\left(-\frac{t}{T_i^L}\right) \right]$$

which reduces to the asymptotic forms (6.4-5c) and (6.4-6c) for small and large times respectively. (It is interesting to note that the lines corresponding to these asymptotic limits meet roughly at $t = 2T_i^L$). Tennekes (1979) noted that by expanding the above relation in a Taylor series near $t = 0$

$$\sigma_i^2(t) = \sigma_{v_i}^2 t^2 - \frac{1}{3} \sigma_{v_i}^2 \frac{t^3}{T_i^L} + \dots$$

(valid for $t/T_i^L \ll 1$, i.e. for the inertial subrange of turbulence), one can associate the first, linear, term, that actually describes random advection with persistent velocities, with the process of turbulent diffusion very close to the source, and the second term with the gradual loss of correlation of Lagrangian velocities as dispersion time increases. This process of "decorrelation" allows the separation of neighbouring particles to increase and is therefore directly related to relative dispersion in the inertial subrange.

We next proceed to discuss the kinematic analysis of relative dispersion without considering the various approximate and semiempirical or empirical methods that aim at extending and applying the preceding analysis of absolute dispersion to actual atmospheric situations, and, finally, in providing "optimal" estimates for the parameters of Gaussian plume models (as well as for other atmospheric dispersion schemes). Among the many available references that review and summarize such practical methods we specifically mention Hanna et al. (1982), Seinfeld (1983), and Pasquill and Smith (1983) (see also Irwin, 1983); a collection of relevant review papers that cover some more recent information can be found in the November 1985 issue of the *Journal of Climate and Applied Meteorology*, whereas, at a more fundamental level, current reviews on methods for treating non-ideal turbulent environmental dispersion can be found in the 1985 issue of *Annual Reviews of Fluid Mechanics*. A final note that is appropriate at this point of our discussion should concern the effect of sampling time that is implicit in the values of the (semiempirical) dispersion parameters reviewed in the above references. As it will be further discussed in Section 6.5, the distinction between relative and absolute dispersion, for given dispersion time, can be essentially associated with the choice of the proper sampling period (or equivalently the turbulent frequency band relevant to each process). On the other hand empirical expressions relating dispersion parameters for different sampling times are sometimes available. For example Gifford (1975) suggests the following formula for the horizontal

crosswind dispersion parameter σ_y corresponding to sampling times $T_s^{(1)}$ and $T_s^{(2)}$:

$$\frac{\sigma_y^{(1)}}{\sigma_y^{(2)}} = \left(\frac{T_s^{(1)}}{T_s^{(2)}} \right)^q$$

where q is in the range 0.25 to 0.3 for $1 \text{ hr} < T_s^{(1)} < 100 \text{ hr}$ and equals approximately 0.2 for $3 \text{ min} < T_s^{(1)} < 1 \text{ hr}$. Thus, if one can identify approximately the value of the sampling time that will produce an estimate of relative dispersion parameters (and this value is in the range of validity of the above or a similar expression), one would have a crude model for these parameters. An approach following roughly the same lines, but based on general theoretical rather than empirical relations, is pursued in detail in Section 6.5.

• *Relative Dispersion I*

General Relations

The kinematic analysis of single particle motions was extended to relative dispersion in the early 1950's by Batchelor, Brier, Obukhov, and others (see, e.g., Monin and Yaglom, 1975, for detailed references), who initially considered the statistical properties of two-particle separations and relative velocities. Here we adhere to the (almost) equivalent but more practical concept of dispersion relative to the instantaneous center of mass and examine elements of the tensor $[\Sigma_{ij}^{(R)}]$ rather than $[\Sigma_{ij}^{(2P)}]$ or $[\Sigma_{ij}^{(S)}]$, where always

$$\Sigma_{ij}^{(S)} = 2\Sigma_{ij}^{(R)}$$

Now, the fluid particle velocity in the meandering frame is

$$\mathbf{v}^{(R)} = \mathbf{v} - \bar{\mathbf{v}}$$

where

$$\bar{\mathbf{v}}(t) = \frac{d\bar{\mathbf{y}}(t)}{dt}$$

For an inertial frame that follows the mean flow $\langle \mathbf{v} \rangle = 0$, $\langle \bar{\mathbf{v}} \rangle = 0$ and therefore

$$\langle \mathbf{v}^{(R)} \rangle = 0, \quad (\mathbf{v}^{(R)})' = \mathbf{v}^{(R)}$$

The relative displacement and velocity vectors of a diffusing particle are related by

$$\mathbf{y}^{(R)} = \int_0^t \mathbf{v}^{(R)} dt$$

and hence

$$\Sigma_{ij}^{(R)} = \langle y_i^{(R)}(t) y_j^{(R)}(t) \rangle = 2 \int_0^t \int_0^t \langle v_i^{(R)}(t') v_j^{(R)}(t'') \rangle dt' dt'' \quad (6.4 - 7a)$$

$$\frac{d}{dt} \langle y_i^{(R)}(t) y_j^{(R)}(t) \rangle = 2 \int_0^t \langle v_i^{(R)}(t) v_j^{(R)}(t') \rangle dt dt' \quad (6.4 - 7b)$$

However, even in homogeneous-stationary turbulence, the relative velocity components $v_i^{(R)}(t)$ do not constitute stationary processes. As the cloud of diffusing fluid particles grows increasingly larger eddies contribute to $\mathbf{v}^{(R)}(t)$ and the relative velocity correlation $\langle v_i^{(R)}(t) v_j^{(R)}(t') \rangle$ is a function of the dispersion time t as well as of the lag time $\tau = t' - t$

$$R_{ij}^{(R)}(t, \tau) = \langle v_i^{(R)}(t) v_j^{(R)}(t + \tau) \rangle \quad (6.4 - 8)$$

(Notice that we omit the superscript L when we refer to relative diffusion properties since it is obvious that we use a Lagrangian approach for their description).

Relating the general $R_{ij}^{(R)}(t, \tau)$ to absolute velocities statistics is a rather complicated task since this will involve the Lagrangian correlation for a single particle, the Eulerian correlation referring to two particles at a given instant, and a mixed correlation referring to two particles at different instants (see, e.g., Pasquill and Smith, 1983, pp.154-155). Expressing the latter correlation in terms of more manageable quantities is a major problem that has been pursued on the basis of different assumptions; Sawford (1982a) provides a rather detailed discussion and comparison of such assumptions and the reader is referred to this work for further details. Here we limit ourselves to the examination of the relative velocity variance in the i -th direction, defined as

$$\sigma_{R, v_i}^2 = R_{ii}^{(R)}(t, 0)$$

which is a function of the dispersion time. For a "point"-source release, one finds that since

$$\sigma_{R,v_i}^2 = \langle v_i^2 \rangle + \langle \bar{v}_i^2 \rangle - 2 \langle v_i \bar{v}_i \rangle \quad (6.4 - 9a)$$

then, in the limit of very small times, where $v_i \simeq \bar{v}_i$, it will be

$$(\text{for } t \rightarrow 0) \quad \sigma_{R,v_i}^2 \simeq 0 \quad (6.4 - 9b)$$

whereas for large times, where v_i and \bar{v}_i are independent

$$(\text{for } t \rightarrow \infty) \quad \sigma_{R,v_i}^2 \rightarrow 2\sigma_{v_i}^2 \quad (6.4 - 9c)$$

Thus we see that σ_{R,v_i}^2 grows from zero to a value twice that of $\sigma_{v_i}^2$ (or $\sigma_{u_i}^2$) as the dispersion process evolves.

A most important point has to be stressed in relation to equation (6.4-9b): the fact that the relative velocity variance is zero at the beginning of the time coordinate for a point release allows one to identify the process of relative or two-particle diffusion with the *conditioned* diffusion of a single particle, i.e. that at $t = 0$ has a deterministic velocity (zero variance); we will elaborate further on this point in the next sub-section.

The non-stationarity of $R_{ij}^{(R)}$ implies that Taylor's theorem does not hold for relative dispersion; one thus has

$$\Sigma_{ij}^{(R)} = \int_0^t \int_0^{t'} \left[R_{ij}^{(R)}(t', \tau) + R_{ji}^{(R)}(t', \tau) \right] d\tau dt' \quad (6.4 - 10a)$$

and for $i = j$

$$\Sigma_{ii}^{(R)} = \sigma_{R_i}^2 = 2 \int_0^t \int_0^{t'} R_{ii}^{(R)}(t', \tau) d\tau dt' \quad (6.4 - 10b)$$

Lagrangian time scales for relative diffusion are also functions of t :

$$T_{ij}^{(R)} = \frac{1}{(\sigma_{R,v_i}^2 \sigma_{R,v_j}^2)^{1/2}} \int_0^t \left[R_{ij}^{(R)}(t, \tau) + R_{ji}^{(R)}(t, \tau) \right] d\tau \quad (6.4 - 11)$$

$T_{ij}^{(R)}(t)$ is characteristic of those eddies that contribute to relative dispersion at time t after a (point) release; these are expected to be mainly the ones comparable to the typical fluid particle separation in the dispersing cloud, i.e. approximately comparable to the cloud size (Csanady, 1973).

• *Relative Dispersion II*

General Asymptotic Results

The general relations (6.4-10ab) allow derivation of a direct asymptotic result only in the case of very large times. Using (6.4-9c) one can write for the final phase of dispersion

$$\sigma_{R_i}^2 = 2\sigma_{v_i}^2 \overline{T_{ii}^{(R)}} t \quad (6.4 - 12)$$

where

$$\overline{T_{ii}^{(R)}} = \frac{1}{\sigma_{v_i}^2} \lim_{t' \rightarrow \infty} \frac{1}{t'} \int_0^{t'} \int_0^\infty R_{ii}^{(R)}(t, \tau) d\tau dt \quad (6.4 - 13)$$

is an averaged integral time scale of relative velocities in the i -th direction. One must note that an *implicit* assumption appearing in most works relevant to two-particle dispersion is that

$$\overline{T_{ii}^{(R)}} = T_i^L$$

• *Relative Dispersion III*

Dimensional Analysis for the Inertial Subrange

For small and intermediate diffusion times Batchelor (1949, 1952) applied Kolmogorov's hypothesis and dimensional analysis to determine $\Sigma_{ij}^{(2P)}$ for dispersion taking place at scales that belong in the inertial subrange of turbulence. He argued that in this subrange $d\Sigma_{ij}^{(2P)}/dt$ depends only on the initial separation of the fluid particles, the rate of turbulent energy dissipation ϵ and the time t for "small" diffusion times ($t < t^*$), but it depends only on ϵ and t for "intermediate" times. Batchelor's analysis is summarized, for example, in Seinfeld (1975, pp.313-316) and will not be repeated here. We only state briefly its main results (formulated in the meandering frame we consider here) for ready reference:

After a “molecular phase”, that will take place when the initial dimensions of the dispersing cloud are smaller than the Kolmogorov microscale $\ell_K = (\nu^3/\epsilon)^{1/3}$, and in which the species under consideration will spread only due to molecular diffusion, one has (recall also the discussion in Section 6.3.1)

(I) *the Short Time Inertial Subrange Dispersion* or simply *Initial Stage*, where

$$\sigma_{R_i}^2 = \sigma_{0_i}^2 + \beta_i^{(I)} (\epsilon \sigma_{0_i})^{2/3} t^2 \quad (6.4 - 14a)$$

$$K_i^{(R)} = \beta_i^{(I)} (\epsilon \sigma_{0_i})^{2/3} t \quad (6.4 - 14b)$$

and

(II) *the Intermediate Time Inertial Subrange Dispersion* or *Accelerated Dispersion Phase*, or simply *Inertial Stage*, where the quasi-asymptotic motion of fluid particles (Section 6.3.1) takes place in the inertial subrange and

$$\sigma_{R_i}^2 = \beta_i^{(II)} \epsilon (t - t^*)^3 \quad (6.4 - 15a)$$

$$K_i^{(R)} = \frac{3}{2} \beta_i^{(II)} \epsilon (t - t^*)^2 \quad (6.4 - 15b)$$

t^* being a (small) correction for an effective “inception of dispersion” that is often set equal to zero. Relation (6.4-15b) can also be written as

$$K_i^{(R)} = \frac{3}{2} \left(\beta_i^{(II)} \epsilon \right)^{1/3} \sigma_{R_i}^{4/3} \quad (6.4 - 15c)$$

which is of course typically referred as *Richardson's 4/3 power law*, and is mentioned that it was first proposed by Richardson (1926) on purely empirical grounds. However, if we want to be precise, we must mention that Richardson proposed his 4/3-law with respect to some actual, observable (and therefore stochastic), dimension of an expanding puff, and not with respect to the deterministic statistical property σ_{R_i} ; in fact the latter formulation is due to the (independent) work of Batchelor and Obukhov (see, e.g., Monin and Yaglom, 1975). The major differences of these formulations have already been discussed in sub-section 6.3.1.

• *Relative Dispersion IV*
Quasi-Asymptotic Results

Lin (1960ab) (see also Lin and Reid, 1963, p.513; Monin and Yaglom, 1975, pp.547-551) extended the 4/3 power diffusion law beyond the inertial subrange on the assumption that the mean-square relative particle acceleration is statistically homogeneous and stationary and has a short-ranged autocorrelation. Stating the homogeneity and stationarity assumptions in terms of the velocity relative to the center of mass and setting

$$\mathbf{a}^{(R)} = \frac{d\mathbf{v}^{(R)}}{dt} \quad (6.4 - 16a)$$

and

$$A_{ii}^{(R)}(\tau) = \left\langle a_i^{(R)}(t+\tau) a_i^{(R)}(t) \right\rangle \quad (6.4 - 16b)$$

one finds that

$$\begin{aligned} \Sigma_{ij}^{(R)} = \frac{1}{3} \left(t^3 \int_0^t A_{ii}^{(R)}(\tau) d\tau - \frac{3}{2} t^2 \int_0^t \tau A_{ii}^{(R)}(\tau) d\tau + \right. \\ \left. + \frac{1}{2} \int_0^t \tau^3 A_{ii}^{(R)}(\tau) d\tau \right) \end{aligned} \quad (6.4 - 17)$$

subject to the conditions of zero initial separation and

$$v_i^{(R)}(0) = 0, \quad a_i^{(R)}(0) \neq 0$$

From equation (6.4-17) one immediately has that, if $A_{ii}^{(R)}$ is effectively zero for $t > t_a$, i.e. if the acceleration covariance is sufficiently short-ranged, then for $t \gg t_a$ it follows that $\sigma_{R_i}^2 \sim t^3$. The coefficient of proportionality in this relation is easily found to be equal to the integral time scale of $a_i^{(R)}$.

One also has for sufficiently long dispersion times

$$A_{ii}^{(R)}(\tau) = 2A_{ii}^L(\tau)$$

where A_{ii}^L is the covariance of the single particle (fixed frame) acceleration.

The general behavior of both absolute and relative dispersion parameters, based on the asymptotic results of the preceding paragraphs, is summarized schematically in Figure 6-2.

• *Relative Dispersion V*

Empirical Information

Empirical information for relative dispersion parameters is very limited compared to that for absolute dispersion (see, e.g., Hanna et al. 1982, pp.41-45, and Pasquill and Smith, 1983, pp.220-232; note that these works focus on puff rather than on instantaneous plume dispersion). Thus, nothing equivalent to the Pasquill-Gifford curves (or any of the other general semiempirical, stability dependent, schemes for absolute σ_i 's) is available for the estimation of σ_{R_i} 's. Nevertheless, available observations support the dimensional analysis results (6.4-14a), (6.4-15a), the latter actually for ranges extending significantly beyond the inertial subrange. Indeed, these observations suggest that (6.4-14a) is valid for dispersion times typically less than 10^2 sec (approximately 1 min) whereas (6.4-15a) is valid for times up to 10^3 to 10^4 sec, i.e. approximately of the order of 1 hr (see Hanna et al., 1982, pp.43-44, for relevant references).

The currently available information regarding the constants $\beta^{(I)}$, $\beta^{(II)}$, for atmospheric conditions, can be roughly summarized as follows (typically for neutral and unstable conditions):

$$\beta_1^{(I)} \simeq \beta_2^{(I)} \simeq \beta_3^{(I)} \simeq 1$$

$$\beta_2^{(II)} \simeq 0.4 \text{ to } 2.0, \quad \beta_3^{(II)} \simeq (0.5 \text{ to } 1.0) \beta_2^{(II)}$$

with $t^* = 0$ (see also Hanna, 1984, p.1099). The effect of atmospheric stability is introduced through the value of the local (average) energy dissipation rate in (6.4-14a), (6.4-15a). A typical estimate of the time after which the influence of the source size is no longer important is $t \simeq \sigma_{0_i}^{2/3} / \epsilon^{1/3}$. However it must be mentioned here that σ_{0_i} does not necessarily correspond to an actual dimension of the source (and also reflects effects of initially enhanced dispersion due to momentum and buoyancy fluxes)

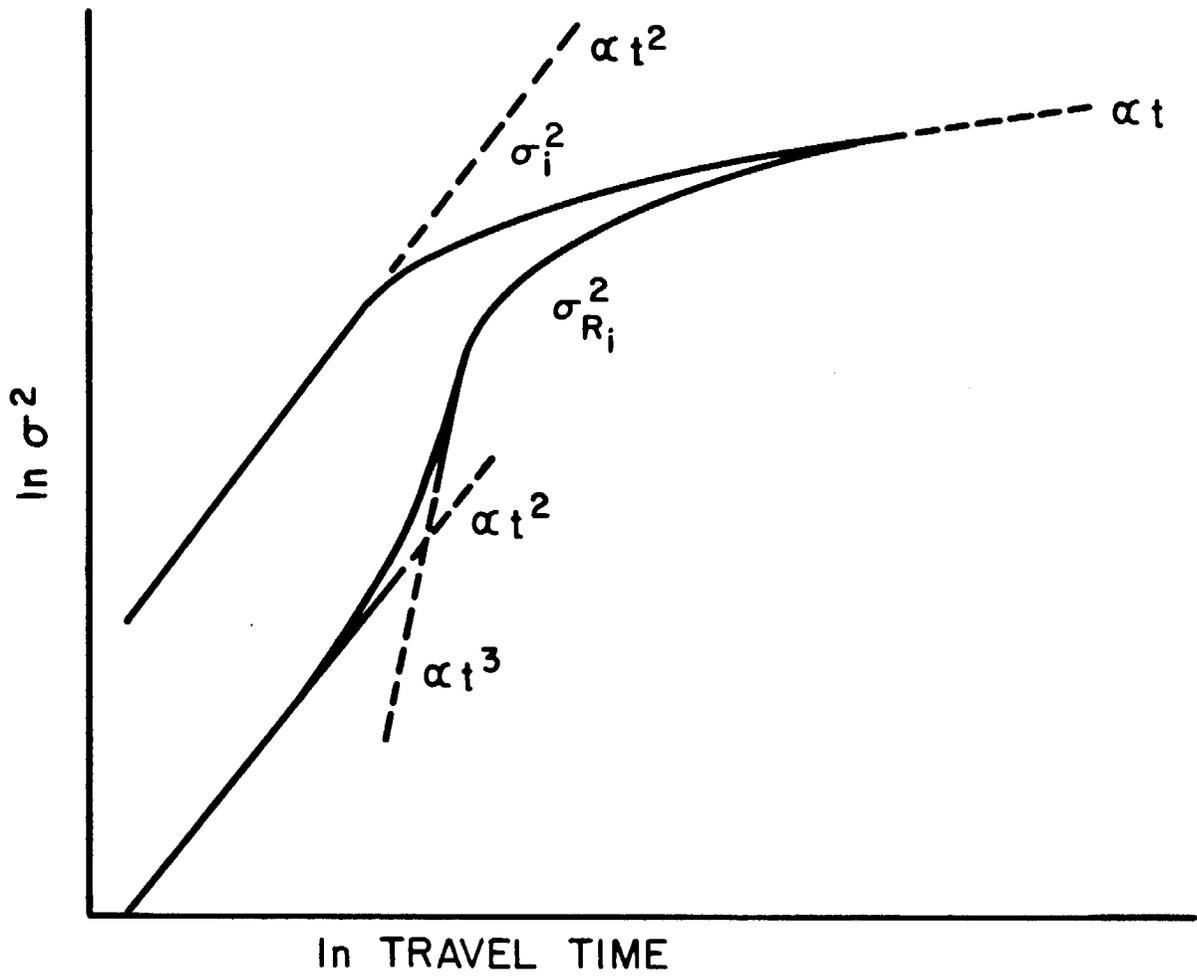


Figure 6-2
 Asymptotic Behavior
 of Absolute (σ_i) and Relative (σ_{R_i}) Dispersion Parameters

and thus is typically treated as a parameter that is fitted to the data for applying (6.4-14a); hence, a priori estimates involving this quantity are more or less meaningless. Another interesting time point is that when the relative dispersion parameter in the i -th direction equals that of meandering; according to Hanna (1984) available data show this time to vary in general from 0.5 to $1.5T_i^L$.

6.4.2 Conditioned Single Particle Motion and Its Relationship to Relative Dispersion

In this sub-section we discuss briefly the close relationship between (inertial sub-range) fluid particle dispersion observed in a non-inertial frame fixed to another fluid particle (or to the center of mass of a cloud of particles) and in an inertial frame moving with a constant velocity that results from a Galilean transformation of the instantaneous initial velocity of the particle. (*) Although this relationship was derived in the early 1960's (Novikov, 1963; Lin and Reid, 1963 – see also Monin and Yaglom, 1975, p.546) and was touched upon by Smith (1968) in his analysis of the statistics of conditioned particle motion, it has only recently come in the focus of relative dispersion modeling as a means for addressing atmospheric diffusion problems, basically in the context of the Langevin equation and related Monte Carlo methods (see sub-section 6.4.3). Schemes based on this relationship, commonly referred to as “one-particle models for relative dispersion,” were applied by Gifford (1982) to horizontal dispersion from a continuous point-source, and by Lee and Stone (1983ab) to diffusion from a finite-size, finite-duration source. The approach adopted in these schemes was criticized by Smith (1983), defended by Gifford (1983), discussed by Sawford (1984), and further discussed and compared with two-particle models by Lee et al. (1985).

To summarize the theoretical basis of the method let us consider the ensemble of random realizations of the initial (fixed frame) velocity of an arbitrary fluid particle $\mathbf{v}(0,0)$. Then we consider an inertial reference frame moving with fixed in time (for a given realization) velocity \mathbf{v}_0 relative to $\mathbf{v}(0,0)$ in the fixed frame. Thus the velocity of the new reference frame, $\mathbf{v}(0,0) - \mathbf{v}_0$, is constant for each realization, but different from realization to realization. However, in this frame the “tagged” arbitrary fluid particle has the same initial velocity \mathbf{v}_0 in all realizations; thus a *conditioned* ensemble

* This can equivalently be considered as the relationship between relative dispersion and conditioned absolute dispersion, i.e. dispersion of single fluid particles that are constrained to have the same initial velocity.

of fluid particle motions is defined. Let the random position vector and velocity of the particle in this frame be $\mathbf{y}^{(C)}(t)$ and $\mathbf{v}^{(C)}(t)$ respectively, where

$$\mathbf{v}^{(C)}(t) = \mathbf{v}(t) - \mathbf{v}(0) + \mathbf{v}_0$$

the superscript (C) indicating conditioned motion. Now, one can write for the elements of the tensor of fluid particle displacements in this frame (Monin and Yaglom, 1975, p.533)

$$\Sigma_{ij}^{(C)}(t) \equiv \langle y_i^{(C)}(t) y_j^{(C)}(t) \rangle = \int_0^t t' D_{ij}^L(t') dt' \quad (6.4 - 19)$$

where D_{ij}^L is the Lagrangian *structure function* for homogeneous-stationary turbulence, defined in general as (see, e.g., Monin and Yaglom, 1975)

$$\begin{aligned} D_{ij}^L(\tau) &\equiv D^L(\tau) \delta_{ij} = \\ &= \left\langle \left(v_i^{(C)}(t + \tau) - v_i^{(C)}(t) \right) \left(v_j^{(C)}(t + \tau) - v_j^{(C)}(t) \right) \right\rangle \end{aligned}$$

However, in every inertial frame of reference

$$D^L \tau = C_0 \epsilon \tau \quad (6.4 - 20)$$

for dispersion in the inertial subrange (Monin and Yaglom, 1975, p.359), where C_0 is a universal constant. Thus (6.4-19) gives

$$\Sigma_{ij}^{(C)}(t) = \frac{1}{3} C_0 \epsilon t^3 \quad (6.4 - 21)$$

which is equivalent to (6.4-15a) with $\beta^{(II)} = 3C_0$. Thus single-particle dispersion with fixed initial velocity is equivalent to dispersion relative to the center of mass.

Further discussion of conditioned dispersion models is presented in the next-subsection, after summarizing the fundamentals of Langevin equation methods.

6.4.2 Langevin Equation Methods

Langevin equation methods (well known through their application to Brownian motion problems) constitute “dynamic extensions” of the direct kinematic approach, described in the previous sub-sections, by introducing explicitly random force effects in the study of (fluid or other) particle motions. Langevin equations essentially are convenient models (approximations) of Newton’s second law where the force (per unit mass) acting on the particle is assumed to consist of a “restoring” component, dependent on the random instantaneous velocity, and an uncorrelated part (the so called *Langevin force*).

Although generalized Langevin equations with nonlinear restoring forces or with memory kernels (i.e. of integrodifferential form) have been used to describe the dynamics of random motions (see, e.g., van Kampen, 1981, Chapter VIII) the term “Langevin equation” is most commonly assigned to a linear stochastic differential equation whose nonhomogeneity or Langevin force (forcing term) $n(t)$ constitutes *white noise*. Its typical one-dimensional (without any loss of generality) form is

$$\frac{dv(t)}{dt} + \gamma v(t) = n(t) \quad (6.4 - 22a)$$

where by definition

$$\langle n(t) \rangle = 0, \quad \langle n(t) n(t') \rangle = \alpha \delta(t - t')$$

Because a stochastic process with the above properties of $n(t)$ does not formally exist (in the sense of an ordinary function) many researchers prefer to use instead the integral of $n(t)$, which is the Wiener process (or Wiener-Lévy process or simply “Brownian motion”) $b(t)$,

$$b(t) = \frac{1}{\sigma_b} \int_0^t n(t') dt'$$

with

$$\sigma_b = \sqrt{\alpha}$$

where division with σ_b produces the *standard* or *normalized* Wiener process (*), and, since the latter is nowhere (mean-square) differentiable, they write

$$dv(t) + \gamma v(t) dt = \sigma_b db(t) \quad (6.4 - 22b)$$

where

$$\langle b(t) \rangle = t, \quad \langle b(t) b(t') \rangle = \min(t, t')$$

(Note that σ_b has units of acceleration).

The solution of (6.4-22ab) is given by

$$v(t) = v_0 e^{-\gamma t} + \int_0^t e^{-\gamma(t-\tau)} \sigma_b db(\tau) \quad (6.4 - 23)$$

$$y(t) = y_0 + \frac{v_0}{\gamma} (1 - e^{-\gamma t}) + \frac{1}{\gamma} \int_0^t (1 - e^{-\gamma(t-\tau)}) \sigma_b db(\tau) \quad (6.4 - 24)$$

Avoiding all discussion of the deep mathematical subtleties involved in the formal interpretation of the above equations and of their solutions we limit ourselves here to some brief comments concerning the physical meaning of the processes and parameters appearing in them. At first we must note that when the white noise $n(t)$ is Gaussian (which is implicitly assumed in practically all applications), then the Langevin equation is equivalent to a Fokker-Planck equation for the random *velocity* process (see, e.g., Van Kampen, 1981, for details). The latter process is Markovian, and is characterized by a Gaussian transition density, whereas the fluid particles' positions $y = \int_0^t v(t') dt'$ are *not* Markovian processes (although the joint vector process

* The Wiener process is a nonstationary Markovian process – and also a martingale – with Gaussian independent increments and Gaussian transition probability density. It constitutes a model of the positions of particles undergoing Brownian motion (recall however that the Langevin equation produces non-Markovian positions) and has been studied extensively, essentially giving rise to many of the fundamental concepts of the modern theory of stochastic processes such as the Wiener measure, stochastic integration, etc. For an elementary introduction to the Wiener process one may consult, e.g., Papoulis (1965). A somewhat more advanced – but very readable – treatment can be found in Arnold (1974). From the extensive advanced mathematical literature relevant to the subject of Brownian motion, we mention the monograph of Chung (1982) and the three-volume treatise of Gihman and Skorohod (1974, 1975, 1979) – in particular volume III. Finally, the reader interested in the fractal aspects of Brownian motion can find a fascinating relevant discussion in the monograph of Mandelbrot (1983).

(v, y) is Markovian in phase space). This fact constitutes the relative advantage of this approach compared to the eddy diffusion models (with either constant or dispersion time dependent diffusivities), that result from either gradient transport hypotheses or as Fokker-Planck equations for the mean concentration (or, equivalently, the transition function). Indeed, these models (essentially all parabolic transport equations) are based on the Markovian property for the fluid particles' positions (see also our discussion in Section 6.3.2 of the present chapter, in the derivation of the modified ADE, and Seinfeld, 1975, Chapter 6). The improvement of dispersion modeling obtained through the Langevin description lies in the fact that now velocity is allowed to change over a finite time scale, possibly comparable to the time scale over which the concentration changes (whereas, as is well known, this is not the case with equations like the ADE). This is achieved by assigning the Markov property to the derivative of the process y instead to y itself (see also Durbin, 1983).

The parameter γ is a characteristic reciprocal time scale for the v -process. Furthermore the temporal velocity correlation is found to be (for $t > t'$)

$$\langle v(t) v(t') \rangle = \frac{\sigma_b^2}{2\gamma} \left(1 - e^{-2\gamma t'} \right) e^{-(t-t')}$$

and letting

$$\langle v^2(0) \rangle = \langle v_0^2 \rangle = \sigma_{0,v}^2$$

one obtains (setting $t' = 0$)

$$\sigma_b^2 = \alpha = 2\gamma\sigma_{0,v}^2$$

This is a significant result that relates what is essentially an initial condition to the statistical properties of the external forcing field. (Actually this last equation is the simplest form of the general *fluctuations-dissipation theorem* of statistical mechanics; see van Kampen, 1981, p.238, for a relevant discussion).

We further see that for $t \gg 1/\gamma$ the random function $v(t)$ tends to a process that besides being Gaussian-Markovian is also stationary (i.e. it is an Ornstein-Uhlenbeck process), independent of initial conditions, with zero mean, variance $\sigma_b^2/2\gamma$,

and covariance $R(\tau) = \sigma_b^2/2\gamma \exp(-\gamma|\tau|)$. Here we must note that one can formally define the Langevin model in such a way that it directly produces a stationary $v(t)$. This can be done either by setting the initial conditions at $t = -\infty$ instead of $t = 0$, or by a suitable transformation of the time coordinate and the time scale (see, e.g., Syski, 1967). Alternatively this can be controlled by the initial conditions: if one assumes that the statistical distribution of $v(0) = v_0$ is equal to the above large-time limiting distribution, then the distribution of $v(t)$ itself is independent of t and equals the limiting distribution (a direct consequence of the Markov property).

Now, in the case of turbulent fluid particle dispersion γ is typically taken to be the inverse of the Lagrangian time scale (see, e.g., Durbin, 1983; Sawford, 1984, 1985) and thus, in a given direction, the corresponding Langevin equation can be written as

$$dv_i(t) = -\frac{v_i(t) dt}{T_i^L} + \sigma_{0,v_i} \sqrt{\frac{2}{T_i^L}} db(t) \quad (6.4 - 26)$$

Pasquill and Smith (1983, p.138) note that when the velocity autocorrelation is not of exponential form then the appropriate time scale (characteristic of the rate of exchange of momentum between fluid particle and environment) will not be equal to the Lagrangian time scale. (Recall however that in the theoretical case of an Ornstein-Uhlenbeck process the autocorrelation is necessarily exponential).

Although the analogy between Brownian motion and turbulent dispersion was implicit in Taylor's (1921) concept of the "diffusion by continuous movements," and has been theoretically discussed by Obukhov (1959) and Lin and Reid (1963), it has only relatively recently (after 1975) become popular as a means for studying dispersion phenomena (and in particular atmospheric), mainly as the basis of Monte Carlo computer simulations (see also Pasquill and Smith, 1983; pp.133-141 *).

* It must be noted here that Pasquill and Smith (1983, p. 133) refer to these approaches as "Markovian random walk methods." However it is clear from the above discussion that the Markov property is used in various other occasions in models of turbulent dispersion, typically in relevance to the trajectories of the particles; thus it must be stressed that this explicit use of the term Markovian property refers to the random velocities.

The majority of these simulations have used the Langevin equation concept (often only implicitly) to model single-particle, i.e. absolute, dispersion statistics in fixed coordinate frames and for time averaged mean concentration fields. (e.g. Reid, 1979; Durbin, 1980; Durbin and Hunt, 1980; Wilson et al., 1981; Lamb, 1982; Legg, 1983, etc. – see also Seinfeld, 1983; Sawford, 1985). Although such numerical models do not always offer significant fundamental improvements over techniques using Taylor's theorem (see, for example, Panofsky and Dutton, 1984, p.247, for relevant comments), since in both cases Lagrangian velocity correlations (or some equivalent restrictions concerning the nature of the velocity field) have typically to be assumed a priori, they are much more versatile, allowing for complicated boundary conditions. Furthermore they are not restricted to homogeneous-stationary turbulence and can be used with dispersion time dependent velocity correlations (although most numerical experiments adopt stationary velocity correlations of the exponential type). For a study of applications of the Langevin equation to "non-ideal" turbulence we refer the reader to the works of Durbin (1983) and Sawford (1985).

In the numerical Monte Carlo simulations one estimates the "actual" random positions of many particles; thus not only the variance but many other statistical characteristics of the trajectories can be derived. Starting point of the numerical models is typically a linear recursive relation for $v(t)$, which in the case of one-dimensional homogeneous-stationary turbulence ($\sigma_v = \sigma_{0,v}$) has the form (Smith, 1968)

$$v(t + \tau) = \rho(\tau) v(t) + \hat{v}(t) \quad (6.4 - 27)$$

with

$$\rho(\tau) = \frac{R^L(\tau)}{\sigma_v^2}$$

typically assumed of exponential form. The variance of \hat{v} (the latter typically assumed Gaussian) is taken to be

$$\sigma_{\hat{v}}^2 = \sigma_v^2 (1 - \rho^2(\tau))$$

so that the variance of successive v 's remains the same. Thus in practice trajectories

are calculated numerically by selecting wind velocities randomly (but so that their statistics obey some restrictions imposed either by theory or by results of numerical turbulence models), choosing \hat{v} from a Gaussian distribution of prescribed variance, and finally calculating successive positions y from (6.4-27). A point worthy of noting here is that (6.4-27), with the variance of \hat{v} as above, constitutes a so called *First Order Autoregressive (AR1)*, Stochastic Time Series Model. It is in fact in the context of such a time series that many of the Monte Carlo models have been formulated, without explicit reference to the relation with the underlying Langevin equation (for the limit of continuous time). This relation can be shown to hold in the limit of small time lags. Indeed, for small τ (say $\tau = \tau_s$) (6.4-27) (after expanding in a series of powers of τ and discarding higher order terms) reduces to

$$\frac{dv(t)}{dt} + \frac{[1 - \rho(\tau_s)]}{\tau_s} v(t) = \frac{\hat{v}(t)}{\tau_s}$$

which is an approximate Langevin equation with

$$\gamma = \frac{[1 - \rho(\tau_s)]}{\tau_s}$$

and

$$\alpha = \frac{\sigma_v^2 [1 - \rho^2(\tau_s)]}{\tau_s}$$

One can see that for $\rho(\tau_s) = \exp(-\gamma\tau_s) \simeq 1 - \gamma\tau_s$ the equality $\alpha = 2\gamma\sigma_v^2$ that relates the parameters of the Langevin equation holds (approximately) for the first order autoregressive series model. Thus, for Gaussian Markovian stationary processes there is a strong connection between AR1 models and Langevin equations.

Let us now focus on the problem of relative dispersion in the perspective of the Langevin approach. As already mentioned this problem has been pursued along two different lines. One group of models considers the motion and separation of two fluid particles and is based on a set of two coupled Langevin equations governing the dynamics of each particle, that is essentially solved numerically (Durbin, 1980; Lamb, 1981; Sawford, 1982ab). The basic aspects of these models have been discussed by

Sawford (1983, 1985). As he points out, apart from points of detail, the fundamental difference between individual models lies in assumptions regarding the rate of two-particle separation: In both Sawford's and Lamb's models the instantaneous rate of separation of the pair of particles is a function of the ensemble-mean-square pair separation, with the result that the distribution of separations is Gaussian (for a Gaussian velocity distribution) and the two-particle displacement probability density is bivariate Gaussian. On the other hand in Durbin's model the instantaneous rate of separation is a function of the instantaneous separation, an assumption that leads to a non-Gaussian distribution of separations. These differences correspond respectively to the already discussed differences between Batchelor's (1952) notion that it is only the statistical tendency for particles to separate which is related to the size of the eddies, and Richardson's (1926) concept in which the probability density of separations depends on an eddy diffusivity that is a function of separation. For further details the reader is referred to the aforementioned publications and in particular to Sawford (1983, 1985). Finally we mention the more recent works of Faller and Choi (1985) and Faller (1985) who also use a two-equations Monte Carlo formalism to model relative dispersion in both the inertial subrange of three-dimensional turbulence and in the enstrophy(*) cascade of large-scale two-dimensional turbulence; however it must be noted that according to Sawford (1984, p.2408) "the Langevin equation is specifically applicable to three-dimensional turbulence" and "it is likely that ... it does not model the two-dimensional enstrophy cascade inertial range." In fact there are various unresolved problems in this area.

Another group of models for relative dispersion that use the Langevin equation is based on the equivalence between conditioned single particle dispersion and relative dispersion, that was discussed in the previous sub-section. As mentioned in that sub-section, recent interest in this conditioned dispersion method started with the

* Enstrophy is defined as the mean square vorticity of turbulence (see, e.g., Lin, 1972)

proposal of Gifford (1982) of using a simple formula for both σ_i^2 and $\sigma_{R_i}^2$:

$$\frac{\sigma_i^2}{2K_i(\infty) T_i^L} = \frac{t}{T_i^L} - \left[1 - \exp\left(-\frac{t}{T_i^L}\right) \right] - \frac{1}{2} \left(1 - \frac{\sigma_{0,v_i}^2}{\sigma_{v_i}^2} \right) \left[1 - \exp\left(-\frac{t}{T_i^L}\right) \right]^2 \quad (6.4-28)$$

where σ_{0,v_i}^2 is the fluid particle velocity variance at the source, and, of course,

$$K_i(\infty) = \sigma_{v_i}^2 T_i^L$$

Thus as σ_{0,v_i}^2 approaches $\sigma_{v_i}^2$ (6.4-28) σ_i^2 is found to describe absolute diffusion, (as predicted for an exponential velocity autocorrelation),

$$\frac{\sigma_i^2}{2K_i(\infty) T_i^L} = \frac{t}{T_i^L} - \left[1 - \exp\left(-\frac{t}{T_i^L}\right) \right]$$

whereas as σ_{0,v_i}^2 approaches zero, i.e. as the dispersion becomes conditioned by the fixed random initial value, one obtains the 4/3 diffusion power law, appropriate for relative dispersion (without initial size effects).

Equation (6.4-28) is obtained directly from the general solution (6.4-23) of the Langevin equation after squaring and ensemble averaging. Smith (1983) has pointed out that his (1968) statistical relations may also be used to give exactly the same equation and further discussed the problem of its proper interpretation in relation to observational data, a matter that is not simple (see also Pasquill and Smith, 1983, pp.122-123, for relevant comments). Lee and Stone (1983ab) extended Gifford's model to clusters of particles from finite-size, finite-duration sources. Lee et al. (1985) further discussed this approach, also comparing their earlier calculations with results from a two-particles, two-equations scheme they developed. The validity of the conditioned dispersion approach in relevance to atmospheric relative dispersion modeling was also reviewed and discussed by Sawford (1984) who stressed the generality of the equivalence (in the sense that it does not rely a priori on a Langevin model) between conditioned single particle motion and particle pair motion in the inertial subrange of atmospheric turbulence.

Sawford (1984, 1985) also discussed in general the applicability of Langevin type equations to atmospheric relative dispersion modeling and in particular the agreement of equation (6.4-28) with atmospheric observations. Although open to some questions, his major conclusions seem to summarize the most important points of our current knowledge in this area and for this reason are briefly reproduced here:

- Langevin type equations are good models for Lagrangian velocities only in high Reynolds number three-dimensional turbulence where the particle acceleration autocorrelation is short-ranged (a typical case being the inertial subrange where the equivalence between conditioned and relative dispersion holds),
- Langevin equations seem not applicable to relative dispersion on the very large (global) scales of atmospheric turbulence, at least partly because of the quasi-two-dimensionality of motion on these scales,
- For horizontal dispersion at smaller scales the application of equations like (6.4-28) is complicated by the lack of a well defined upper limit to the scale of the turbulent kinetic energy,
- Conditioned single particle models cannot appropriately model higher moments (or the pdf) of the separation; a pair of Langevin equations is needed for this task.

In conclusion, modeling of relative dispersion through Langevin equations (either a single one or a pair) is currently an active – and relatively controversial – field of research. Although several questions remain unresolved and the interpretation of various assumptions is not always universally accepted, many useful concepts have been recently clarified (and the present sub-section attempted to further organize and relate them), and some powerful mathematical tools have been brought to the attention of those interested in environmental dispersion. From a more practical (and perhaps narrower) perspective we point out the potential of (6.4-28) as a simple model for relative dispersion for the stages of quasi-asymptotic and asymptotic fluid particle motion.

6.5 RELATIVE DISPERSION ANALYSIS: II. SPECTRAL METHODS

In this section we present a new method for estimating relative dispersion parameters from (observed) atmospheric turbulence spectra. This method is based on the association of the relative dispersion and meandering processes with appropriately defined space-time scales. This allows the computation of specified dispersion parameters from the spectral form of Taylor's theorem after filtering out the frequencies at scales that do not contribute to the process under consideration. The parameters for the appropriate high-pass filter functions, required for the calculation of in-plume phenomena, are not assumed a priori but are determined through an iterative integral technique. The basic steps of this method were outlined briefly in Chapter 2. In the present section we explain the rationale behind these steps, discuss various relevant questions, and present some typical results obtained with this method. It must be mentioned at this point that since typically Eulerian and not Lagrangian atmospheric spectra are available with sufficient accuracy (and for a variety of atmospheric conditions), there arises the need to use a transformation technique in order to use the former spectra in conjunction with Taylor's theorem.

6.5.1 General Considerations

Scale of Atmospheric Motions and Plume Spread

Let us now briefly recall some aspects of the concepts of averaging and sampling times and of the associated scales, in relevance to plume dispersion (see also Appendix A6.1). A continuous plume from a point source in the atmosphere encounters a wide range of atmospheric motions associated with different scales, which we associate with the concept of eddies. Now, the very large eddies contribute to changes in the instantaneous wind vector while the smallest eddies cause slight dispersive spreading of the plume. The eddies of about the same size as the local plume width

are the most effective in producing turbulent plume dispersion. Eddies larger than the instantaneous plume width but smaller than the characteristic horizontal scale of the region of interest (typically the downwind distance from the source) produce the meandering characteristic of the instantaneous plume. Thus if L_E is a characteristic eddy dimension, x is the characteristic horizontal scale of the region (typically the downwind distance) and D_P is an (ensemble) average *instantaneous* plume width, then the role of eddies in plume dispersion is given by (see, e.g., Seinfeld, 1983, p.262)

- (1) $L_E \ll D_P$, slight plume dispersion; internal plume mixing
- (2) $L_E \sim D_P$, most effective in plume dispersion
- (3) $D_P < L_E \leq x$, produces plume meandering
- (4) $L_E > x$, produces changes in the wind vector

Since $D_P = D_P(x)$, it is obvious that as the plume is advected downwind the effect (on its spread) of atmospheric motions associated with a *given* spatial scale becomes qualitatively different. Furthermore, although in general eddies of a very wide range of scales are expected to be present in the atmosphere, they are not expected to be found with the same probability (i.e. the spectrum of eddies will be more "dense" in certain scales – more precisely in frequency or wavenumber bands – and less in others) this variation also holding for different directions. It is therefore imperative, in relating relative dispersion parameters to atmospheric turbulence properties, such as turbulent energy (i.e. fluctuating velocity variance), to discern between the contributions to these properties from different scales, of motion and, furthermore, to take into account the change of this contribution with advection time.

Turbulence Spectra (versus Correlations)

Comments and Definitions

In principle correlation functions and spectral densities contain the same information regarding the distribution of the variance of a given quantity over different spatial scales and frequencies (or eddy sizes). However, in practice, spectra are more useful than correlations or other statistics because (besides possible computational advantages) they give directly the distribution of the variance of interest (in our case

of turbulent energy, either total or in a given direction) with respect to frequency (or wavenumber), in a way such that the effects of particular frequency bands are independent from the effects of other frequency bands. This important advantage is shown schematically in Figure 6-3 (from Panofsky and Dutton, 1984) that shows a time series of data with an approximately linear macroscopic (i.e. low frequency) trend. The respective correlation functions and spectral densities are also given, calculated both without and with removal of this trend. One sees that whereas the values of the two correlation functions, for a given time lag, differ significantly, even for small time lags, the behavior of the spectral densities at large frequencies is independent of the slow variations (see Panofsky and Dutton, 1984, pp.174-176, for further relevant discussion).

In this work we adopt the following definitions for the frequency spectrum (*) $F_\alpha(\omega)$ of the *fluctuations* of the random quantity α (that is either Eulerian or Lagrangian with temporal autocorrelation $R_\alpha(\tau)$), following Monin and Yaglom (1975):

$$F_\alpha(\omega) = \frac{1}{\pi} \int_0^\infty R_\alpha(\tau) \cos \omega\tau d\tau \quad (6.5 - 1)$$

(We will not consider spectra corresponding to cross-correlations in the present work). Regarding the notation, it must be mentioned that, in the present work, when an $i = 1, 2, 3$ index notation is used for the velocities, then the index alone is used to specify the correlation (i.e. we write $R_i(\tau)$ instead of $R_{u_i}(\tau)$ - see previous sections).

For symmetric $R_\alpha(\tau)$ (i.e. stationary α') one can alternatively use the spectrum $E_\alpha(\omega) = 2F_\alpha(\omega)$, defined for $0 \leq \omega < \infty$ instead of $-\infty < \omega < \infty$, and thus the correlation $R_\alpha(\tau)$ will be given by

$$R_\alpha(\tau) = \int_{-\infty}^\infty F_\alpha(\omega) \exp(i\omega\tau) d\omega = \int_0^\infty E_\alpha(\omega) \cos \omega\tau d\omega \quad (6.5 - 2)$$

We also use the absolute spectral density in terms of "arithmetic frequency" $n = \omega/2\pi$

$$S_\alpha(n) = 2\pi E_\alpha(2\pi n) \quad (6.5 - 3)$$

* The reader is reminded that there are some differences in the definitions of turbulent spectra adopted by various authors; the major of these differences are summarized in Appendix A6.1.

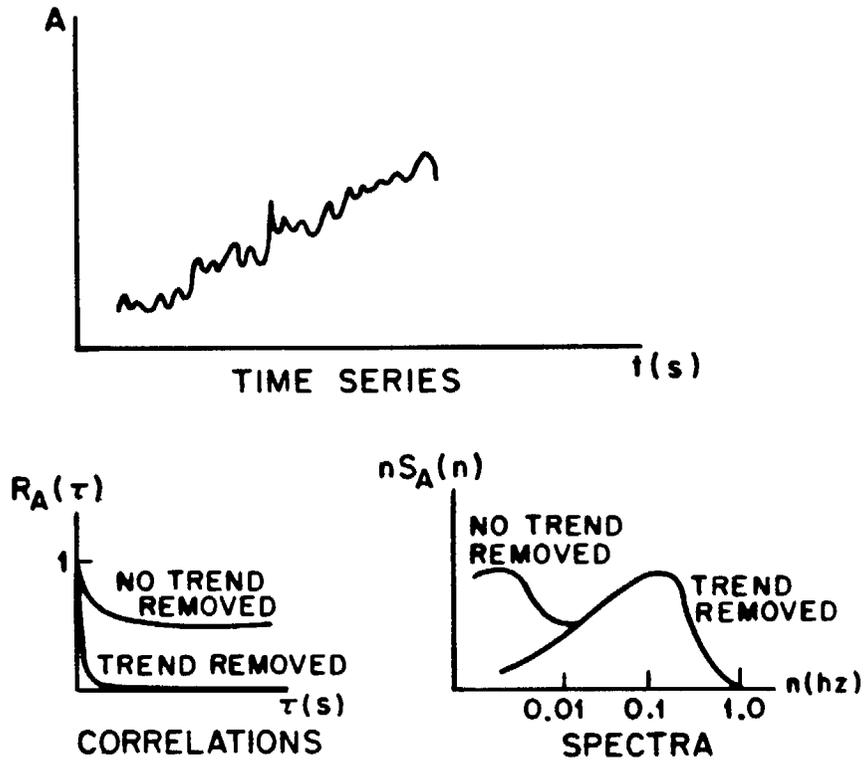


Figure 6-3
Effect of Trend Removal
on Correlation Functions and Spectral densities
(from Panofsky and Dutton, 1984)

which gives

$$\int_0^{\infty} S_{\alpha}(n) dn = \int_0^{\infty} E_{\alpha}(\omega) d\omega = \sigma_{\alpha}^2 \quad (6.5 - 4)$$

and note the identity

$$\int_0^{\infty} S_{\alpha}(n) dn = \int_0^{\infty} n S_{\alpha}(n) d \ln n \quad (6.5 - 5)$$

according to which the area under the curve defined by the function $nS_{\alpha}(n)$, which is often called the “logarithmic frequency spectrum,” plotted against $\ln n$ represents variance and $nS_{\alpha}(n)$ represents the variance per unit logarithm frequency interval. This identity is useful in the computations through the iterative algorithm proposed later in this section.

We further denote with $\hat{S}_{\alpha}(n)$, $\hat{R}_{\alpha}(\tau)$, the normalized spectral density and the temporal autocorrelation coefficient respectively

$$\hat{S}_{\alpha}(n) = \frac{S_{\alpha}(n)}{\sigma_{\alpha}^2}, \quad \hat{R}_{\alpha}(\tau) = \frac{R_{\alpha}(\tau)}{\sigma_{\alpha}^2} \quad (6.5 - 6)$$

(Note also that we will use the superscripts E and L to discriminate between Eulerian and Lagrangian spectra, as we have done with the correlations).

In the following α will be identified exclusively with the fixed-point wind velocity component in the i -th direction, u_i , or with the lagrangian fluid particle component v_i . Thus the direction i will suffice in characterizing the turbulent frequency spectra $S_{ii}^E(n)$ and $S_{ii}^L(n)$. As far as (one-dimensional) spatial spectra are concerned, we assume that they are directly related to the frequency spectra through Taylor’s “frozen turbulence” hypothesis, if, e.g., they are available and are to be used as a substitute of frequency spectra.

Another quantity, extensively used in atmospheric applications, also useful in our work, is the so called *meteorological frequency*, f , which is dimensionless and is defined as

$$f = n \frac{z}{\bar{u}} \quad (6.5 - 7)$$

where z is the height above the ground and \bar{u} is the mean wind velocity (sometimes substituted by the mean square-root-sum $\langle \sqrt{u_1^2 + u_2^2 + u_3^2} \rangle$ that is larger than the mean wind but is the quantity that is often measured in practice – see Panofsky and Dutton, 1984, p.98). The reason for using f is that, as we will briefly discuss later, on the basis of simple dimensional considerations for the surface layer, the spectra of any particular wind component are expected to scale with f (i.e. to be invariant, for given atmospheric stability conditions, when expressed in terms of f).

Spectral Form of Taylor's Theorem

Direct application of the Fourier transform to Taylor's theorem for single particle dispersion in homogeneous-stationary turbulence – equation (6.4-1a) – and for $i = j$ gives

$$\sigma_i^2(t) = \sigma_{v_i}^2 t^2 \int_0^\infty \hat{S}_{ii}^L(n) \frac{\sin^2 \pi n t}{(\pi n t)^2} dn \quad (6.5-8)$$

It is easy to see that in the above expression, where – as always in this chapter – $\sigma_{v_i}^2$ is assumed to correspond to the theoretical value, obtained for infinite sampling time and zero averaging time, the term containing the dispersion time t essentially plays the role of a low-pass filter that cuts out the high frequencies. Indeed, t is acting as the equivalent of an averaging time T_a that “smooths out” effects of the random v_i corresponding to time scales shorter than t and thus produces the statistic σ_i^2 . In the notation of Appendix A6.1, where $\sigma_\alpha^2 [T_s, T_a]$ denotes the value of σ_α^2 evaluated for sampling time T_s and averaging time T_a , equation (6.5-8) can be written as

$$\sigma_i^2 = t^2 \sigma_{v_i}^2 [\infty, t] \quad (6.5-9)$$

The implicit sampling time is infinite, thus allowing (in principle) even the slowest variations in the turbulent field to affect the value of σ_i^2 . In practice the concept of an infinite sampling time in the evaluation of turbulence statistics must correspond to intervals “long enough to accommodate all turbulent variations” but “short compared to the time scales of variations in the mean motions.”

The Relation of Eulerian and Lagrangian Properties

Before proceeding to discuss the application of (6.5-8) in describing turbulent dispersion properties we must stress the (already mentioned) need to transform observed Eulerian spectra to the corresponding Lagrangian densities appearing in this equation. However, relating Eulerian and Lagrangian spectra or, equivalently, correlations, is a most complicated (and in general unresolved) problem, the detailed discussion of which is beyond the scope of this work. A brief introduction to the methods used for tackling this problem (and in general for measuring Lagrangian properties), can be found in Pasquill and Smith (1983, pp.81-87; see also pp.127-128) while for a more comprehensive analysis of such methods one may consult the report of Koper and Sadeh (1975). Some more recent discussions of the subject can be found in Lee and Stone (1983b), Li and Meroney (1985ab) and Sadeh and Koper (1985).

In the present work we have already given equation (6.2-10), which is perhaps the most fundamental relationship among Eulerian and Lagrangian correlations, derived directly on the basis of Corrsin's (1959) independence hypothesis. The limits of the validity of this equation are discussed in Weinstock (1976). As we mentioned, the applicability of (6.2-10) to real situations is limited since it requires the a priori assumption of the transition density G . The most widely used alternative to the formal approaches based on this equation is the application of the so called *Hay-Pasquill hypothesis* (Hay and Pasquill, 1959) which states that Lagrangian and Eulerian correlations and spectra are similar in shape but are displaced by a scale factor β equal to the ratio of (typically the maximum) Lagrangian and Eulerian integral time scales $\beta = T^L/T^E$ (see Figure 6-4).

Thus

$$nS^L(n) = \beta nS^E(\beta n) \quad (6.5 - 10a)$$

$$R^L(\beta\tau) = R^E(\tau) \quad (6.5 - 10b)$$

Although this approach is strictly not valid in the high frequency range (inertial sub-range), where the spectra have different limiting slopes, it appears to be a satisfactory

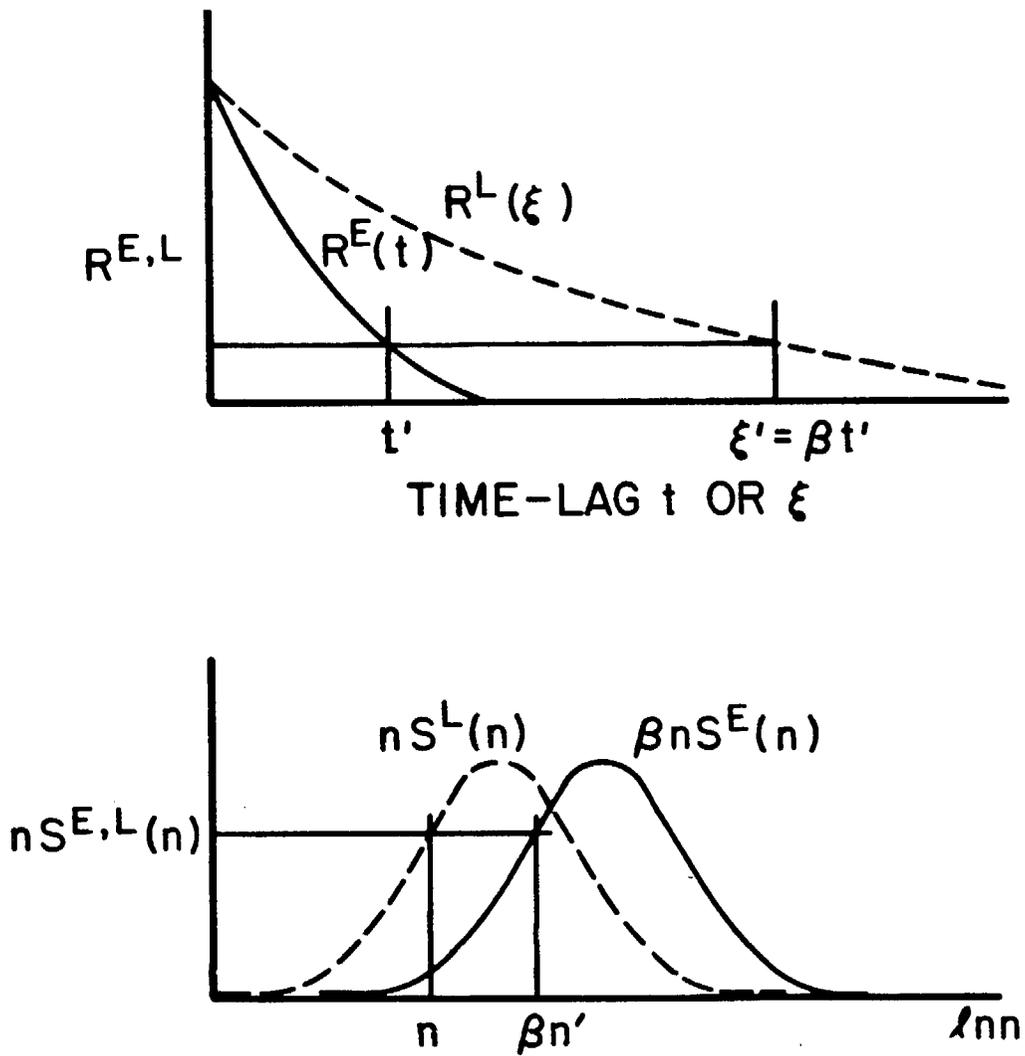


Figure 6-4
 Relation of Lagrangian and Eulerian Spectra and Correlations
 According to the Hay-Pasquill Hypothesis

approximation for the largest part of the spectrum according to available observations (see, e.g., Hanna, 1982). Thus it is adopted in the present work as the standard means for transforming observed Eulerian statistics to Lagrangian ones (especially when the calculations are relevant to the energy range).

Given the correlations or spectra, the only parameter required for applying the Hay-Pasquill hypothesis is β . Various methods have been proposed for its estimation. One approach has used equation (6.2-10) to infer some qualitative results concerning the Eulerian-Lagrangian time-scale relationship: Assuming *isotropic turbulence*, a Gaussian G with variance related to R^L through Taylor's theorem, and convenient forms of R^E , Saffman (1963) and Philip (1967) estimated the ratio of Lagrangian and Eulerian integral time scales $\beta = T^L/T^E$ as a function of the intensity of turbulence $\hat{\sigma}_{u_i} = \sigma_{u_i}/\bar{u}$, and found that, for small $\hat{\sigma}_{u_i}$,

$$\beta = \frac{T^L}{T^E} = \frac{\hat{\beta}}{\hat{\sigma}_{u_i}} \quad (6.5 - 11)$$

The estimated values of the constant $\hat{\beta}$ were 0.8 (Saffman) and 0.35 (Philip).

Relation (6.5-11) was also proposed by Corrsin (1963), who, in a simplified analysis, assumed that the Eulerian and Lagrangian spectra are represented by their well known inertial subrange forms (obtained through dimensional/similarity analysis)

$$S_{ii}^E(n) = A_i \bar{u}^{2/3} \epsilon^{2/3} n^{-5/3} \quad (6.5 - 12a)$$

$$S_{ii}^L(n) = B_i \epsilon n^{-2} \quad (6.5 - 12b)$$

for $n \geq n^E = 1/T^E$ and $n \geq n^L = 1/T^L$ respectively, and are equal to zero for $n < n^E$, $n < n^L$. Indeed, integrating the above equations from 0 to ∞ and taking into account that for homogeneous turbulence $\sigma_{u_i}^2 = \sigma_{v_i}^2$, one obtains (6.5-11) again, with

$$\hat{\beta} = \left(\frac{3}{2}\right)^{3/2} \frac{A_i^{3/2}}{B_i}$$

More realistic forms of the spectra, with finite values at small frequencies, have produced similar results with $\hat{\beta}$ in general in the range 0.35-0.8 (see Pasquill and Smith,

1983, p.84). Current information regarding the value of $\hat{\beta}$ (for time scales along the mean wind direction), based on available observations, narrows the above range to 0.4–0.6, with the value 0.44 ($= \sqrt{\pi}/4$ – see Panofsky and Dutton, 1984) being the most common suggestion. Thus, typical values of β (calculated for typical values of $\hat{\sigma}_{u_i}$) will be $\beta \simeq 4$ in neutral conditions, $\beta \simeq 2$ in the typical unstable daytime planetary boundary layer, and $\beta \simeq 10$ in stable conditions (Hanna, 1982). The value $\beta = 4$ has often been adopted as a representative average of β , independent of stability conditions.

6.5.2 An Iterative Spectral Algorithm for Estimating Relative Dispersion Parameters

General Discussion

The spectral form of Taylor's theorem for absolute dispersion, that shows explicitly the filtering role of travel time – and in particular expression (6.5-8a) which exemplifies the fact that absolute dispersion is (in principle) related to infinite sampling times – are the starting steps for developing a practical scheme for the estimation of relative dispersion parameters. The essence of our proposal is the following: at a given downwind distance (i.e. at a given dispersion time) apply the spectral formula (6.5-8) *modified so that it corresponds not to "infinite" sampling time but to a time period that is just long enough to take into account the effects of eddies of sizes smaller or comparable to a representative instantaneous "diameter" of the plume.* In this way, according to our discussion in the beginning of sub-section 6.5.1, meandering processes are excluded and the resulting σ_i^2 will be relevant only to relative dispersion processes.

In fact, the concept of finite sampling time, its effect on observed spectra, and the nature of dispersion parameters corresponding to such sampling times, have been the subject of study and discussion since the 1950's with the work of Ogura (1957, 1959) – see also Smith (1962), Hino (1968), Rowe (1979). In direct relation to relative dispersion parameter estimation, the most important work, formulated on conceptually

similar grounds, has been that of Smith and Hay (1961), specifically in the context of the *growth of a finite cluster of particles*. (See also the discussion in Pasquill and Smith, 1983, pp.154-158). Their analysis, *valid exclusively for isotropic conditions* and for clusters with a priori assumed *Gaussian mean concentration distribution* about their center of mass, essentially starts from the differential form of equation (6.4-10b), makes use of the Hay-Pasquill hypothesis for the relation among Eulerian and Lagrangian correlations and spectra, and results in the following expression for the rate of growth of the isotropic cluster (with standard deviation σ_R from the center of mass)

$$\frac{d\sigma_R}{dt} = \frac{2}{3} \frac{\beta}{\bar{u}} \int_0^\infty \int_0^{\bar{u}t/\beta} E_{(3D)}(\kappa) \frac{\sin \kappa s}{\kappa s} \frac{1 - \exp(-\sigma_R^2 \kappa^2)}{\sigma_R} ds d\kappa \quad (6.5 - 13a)$$

which for $\bar{u}t/\beta > \sigma_R$ simplifies to

$$\frac{d\sigma_R}{dt} = \frac{\pi}{3} \frac{\beta}{\bar{u}} \int_0^\infty E_{(3D)} \frac{1 - \exp(-\sigma_R^2 \kappa^2)}{\sigma_R \kappa} d\kappa \quad (6.5 - 13b)$$

where $E_{(3D)}$ is the integrated three dimensional Eulerian spectrum in terms of the magnitude of the wavenumber vector κ and β is the Hay-Pasquill parameter. Based on the above expressions and making various simplifying assumptions Smith and Hay (1961) proposed a simple working approximation for the range of the expansion where the size of the cluster is of the same order of magnitude as the Eulerian integral length scale of turbulence (or – Pasquill and Smith, 1983, p.157 – where the downwind distance from the source of an initially small cloud is 10 to 80 times the Eulerian scale):

$$\frac{1}{\bar{u}} \frac{d\sigma_R}{dt} = \frac{2}{3} \beta \hat{\sigma}_u^2 \quad (6.5 - 14a)$$

or, approximately (and for $\beta = 4$) (*)

$$\frac{d\sigma_R}{dt} \simeq 0.3 \sigma_u \quad (6.5 - 14b)$$

* Note that Pasquill and Smith, 1983, p.230, suggest a factor of about 0.22 instead of 0.3 in this expression.

(which – after squaring – suggests that in this range only about a ninth of the total variance of turbulence contributes in the dispersion of the cluster). This expression corresponds to the maximum of the $d\sigma_R/dt$ slope predicted by the Smith-Hay model and requires that $\sigma_R^2 \sim t^2$. It should be observed at a “central stage” of dispersion (Panofsky and Dutton, 1984, p.252), as the exponent of t in $\sigma_{R_i}^2(t)$ drops from the value of 3.0 in the inertial stage to the value of 1.0 in the final stage of dispersion. The model of Smith and Hay (in its simplified form) was reviewed and compared with atmospheric data by Sawford (1982a) who indeed identified a certain range of agreement between predictions and observations; for further information the reader is referred to this paper and also to a relevant discussion in Pasquill and Smith (1983, pp.230-232).

An important thing to observe at this point is that the general equation of Smith and Hay (6.5-13a) resembles the general spectral form of Taylor’s single particle theorem with the additional presence of a low-pass filter function, of the form $[1 - \exp(-\sigma_R^2 \kappa^2)] / \sigma_R$. This particular form of this weighting function is due to assumptions concerning the two-particle velocity correlations in isotropic turbulence. In fact both the concept of isotropy and these assumptions constitute important restrictions on the generality of the Smith-Hay scheme; these restrictions are also, of course, extended to the permissible form of the spectrum that can be used in this scheme. As far as the simple approximate equation (6.5-14a) – which is actually the form of the model that has been used the most in applications – is concerned, it has been derived on the assumption of a specific, very simple (exponential type) Eulerian correlation. It is therefore obvious that the (even approximate) applicability of the Smith-Hay model to dispersion in the highly anisotropic energy range of atmospheric turbulence, with spectra that are sensitive functions of stability and height, is questionable.

So there arises naturally the problem of extending the Smith-Hay approach to more realistic situations. However, although the above approach is now twenty five years old there have not been – to our knowledge – any significant steps towards a

practical generalization. An attempt to combine the theoretical scheme with information from actual atmospheric measurements was presented by Sheih (1980) who applied the approach of Smith and Hay directly to observed, Eulerian, one-dimensional, atmospheric frequency spectra. This attempt, which used isotropic theory results to model anisotropic conditions and directly substituted the one-dimensional frequency spectrum for the integrated three-dimensional wavenumber spectrum, contained some obviously serious errors and produced predictions that disagree with observations. However, it is still worth mentioning, at least because of the discussion it caused in the literature; indeed, Gifford (1981), who strongly criticized the model of Sheih, and also Mikkelsen and Troen (1981) and Rowe (1981), not only pointed out various problems and errors of Sheih's scheme but also provided some interesting comments regarding the spectral description of the relative dispersion problem.

Model Formulation

In the present work we avoid use of the Smith-Hay formula and propose a scheme based directly on the spectral form of Taylor's dispersion theorem, as stated in the beginning of the present subsection. The use of a theoretical result relevant to single-particle dispersion as a starting point might at first seem as an inappropriate step but in fact it is consistent with the relative dispersion concept (through the equivalence between relative-to-the-center-of-mass and two-particle dispersion). Indeed, filtering out the relatively low frequencies, that correspond to meandering, by using a small sampling time, is essentially equivalent to adopting a meandering frame (that follows the motion of the center of mass), since "an observer" moving with this frame does not "feel" exactly these frequencies.

The general relation for σ_i^2 , for finite sampling time T_s (see also Appendix A6.1), is

$$\sigma_i^2(t; T_s) = \sigma_{v_i}^2 \int_0^\infty \hat{S}_{ii}^L(n) \frac{\sin^2 \pi n t}{(\pi n t)^2} \left(1 - \frac{\sin^2 \pi n T_s}{(\pi n T_s)^2} \right) dn \quad (6.5 - 15)$$

a result that was discussed by Smith (1962).

In terms of the Eulerian spectrum (and assuming the Hay-Pasquill hypothesis is

valid) equation (6.5-15) becomes

$$\sigma_i^2(t; T_s) = \sigma_{v_i}^2 \int_0^\infty \hat{S}_{ii}^E(n) \frac{\sin^2 \pi n t / \beta}{(\pi n t / \beta)^2} \left(1 - \frac{\sin^2 \pi n T_s}{(\pi n T_s)^2} \right) dn \quad (6.5 - 16)$$

In order to calculate $\sigma_i^2(t; T_s) = \sigma_{R_i}^2(t)$ one must set T_s set equal to the maximum sampling time that still corresponds to the instantaneous or fluctuating plume, a typical estimate of which is

$$T_s = \frac{2\sqrt{2}\sigma_{R_i}}{\bar{u}} \quad (6.5 - 17)$$

(clearly T_s will be different in the horizontal and vertical directions). An important point to note here is that the proper characteristic velocity appearing in the definition (6.5-17) does not have always to be exactly equal to the mean wind speed; in fact we define it here as being always identical to the characteristic velocity scale that appears in the definition of the meteorological frequency, and that results in invariant representations of the Eulerian spectra.

Of course T_s defined in through (6.5-17) is a function of the unknown σ_{R_i} , that is to be estimated, and hence (6.5-16) becomes a nonlinear integral equation for σ_{R_i} . The solution to this equation is obtained through an iterative algorithm as follows:

Step 1: Given the spectrum function $\hat{S}_{ii}^E(n)$ calculate the absolute diffusivity σ_i (corresponding to $T_s = \infty$) for given t :

$$\sigma_i^2(t) = \sigma_{v_i}^2 t^2 \int_0^\infty \hat{S}_{ii}^E(n) \frac{\sin^2 \pi n t / \beta}{(\pi n t / \beta)^2} dn \quad (6.5 - 18)$$

Step 2: Use σ_i as a first estimate of σ_{R_i} for given t

$$\sigma_{R_i}^{(1)}(t) = \sigma_i(t)$$

and set

$$T_{s,i}^{(1)}(t) = \frac{2\sqrt{2}\sigma_{R_i}^{(1)}}{\bar{u}}$$

to calculate

$$[\sigma_{R_i}^2(t)]^{(2)} = \sigma_{v_i}^2 t^2 \int_0^\infty \hat{S}_{ii}^E(n) \frac{\sin^2 \pi n t / \beta}{(\pi n t / \beta)^2} \left(1 - \frac{\sin^2 \pi n T_{s,i}^{(1)}}{(\pi n T_{s,i}^{(1)})^2} \right) dn \quad (6.5 - 19)$$

Step 3: Use the value $\sigma^{(2)}(t)$ obtained from the previous step to calculate $T_{s,i}^{(2)}$ that improves the filter function, and introduce in the last equation above to obtain a refined estimate of $\sigma_{R_i} = \sigma_{R_i}^{(3)}$. Repeat until convergence is obtained (e.g., until two successively calculated values of σ_{R_i} do not differ by more than, say, 5%). We note here that an obvious requirement for this iterative process to converge is the absolute diffusivity to be a "sufficient" approximation for σ_{R_i} , a condition that might be violated very close to the source (in which case a fraction of σ_i might be used as a first estimate for σ_{R_i}).

Actually, numerical integration of the spectral formulas above is better performed with respect to $\ln n$ since the logarithmic frequency spectrum has a much smoother graph. Universal results (for given stability conditions) are obtained through the use of the meteorological frequency. An example of such calculations is given in the following paragraphs.

Model Application: An Example

The most important step in the implementation of the computational algorithm just described is the selection of the appropriate Eulerian spectral density. A variety of empirical and semiempirical models of $\hat{S}_{ii}^E(n)$ that fit extensive sets of observations have been proposed and tested during recent years. Excellent comprehensive reviews of the information and references relevant to these models can be found in Caughey (1982), Pasquill and Smith (1983, Chapter 2), Panofsky and Dutton (1984, Chapter 8), and – in a somewhat more concise form – in Jensen and Busch (1982). In particular, worthy of reference are the spectral function models proposed by Kaimal (1973) and Højstrup (1982), for stable and neutral-unstable conditions respectively, that seem to be based on the currently most comprehensive data bases.

An extensive discussion of the spectral properties of atmospheric turbulence (which are covered satisfactorily in the works mentioned above) is beyond our present objectives. However, it is useful to recall briefly some important points: First, it must be clear that the interest here is in the spectra corresponding to the energy range of

atmospheric turbulence. Observed inertial subrange spectra are in general found to follow the similarity analysis predictions, as given by equation (6.5-12a), in a satisfactory manner, the constants of this equation being approximately equal to

$$A_1 \simeq 0.15, \quad A_2 \simeq A_3 \simeq 0.20$$

Of course a sound general model for the energy range must produce the inertial subrange characteristics at high frequencies, i.e.

$$n\hat{S}_{ii}^E(n) \sim n^{-2/3} \quad (\text{large } n)$$

On the other hand, for very low frequencies $\hat{S}_{ii}^E(n)$ must tend to unity, i.e.

$$n\hat{S}_{ii}^E(n) \sim n \quad (\text{small } n)$$

A plot of $n\hat{S}_{ii}^E(n)$ is expected to have these two asymptotes with a maximum (or "spectral peak") in between. This maximum is attained at a frequency n_m corresponding to the scale at which the predominant production of turbulent energy takes place. For an observer at height z above the ground this scale is expected to be proportional to \bar{u}/z in the surface layer (see, e.g., Jensen and Busch, 1982, p.204). Thus the spectra $S_{ii}^E(n)$ of any particular velocity component are expected to scale with respect to the dimensionless meteorological frequency $f = nz/\bar{u}$, and, furthermore, $n\hat{S}_{ii}^E(n)$ at any height are expected to fall on a universal curve when plotted against f . (An interesting point to note is that the inertial subrange is typically always well confirmed for $f > 10$ and often for $f > 1$).

Perhaps the most simple spectral function that obeys the asymptotic rules stated above is given by

$$n\hat{S}_{ii}^E(n) = \frac{nS_{ii}^E(n)}{\sigma_{u_i}^2} = \frac{af}{(1+bf)^{5/3}} \quad (6.5-20)$$

Although the above expression contains two parameters, a and b , integration from 0 to ∞ on one hand and differentiation for determining the position of the spectral extremum on the other, show immediately that

$$a = \frac{1}{f_m}, \quad b = 1.5f_m \quad (6.5-20a)$$

where f_m is the meteorological frequency corresponding to the maximum of the logarithmic spectrum, a parameter that is directly obtained from observations.

Introducing the spectral function (6.5-20) one calculates the ratio

$$\frac{\sigma_{R_i}^2}{\sigma_{u_i}^2}$$

as follows:

Step 1: Calculate the absolute diffusivity σ_i^2 over $\sigma_{u_i}^2$, for given dimensionless $t^* = t\bar{u}/z$:

$$\left(\frac{\bar{u}}{z}\right)^2 \frac{\sigma_i^2}{\sigma_{u_i}^2} = t^{*2} \int_0^\infty \frac{af}{(1+bf)^{5/3}} \frac{\sin^2 \pi ft^*/\beta}{(\pi ft^*/\beta)^2} d \ln f \quad (6.5-18^*)$$

Step 2: Use $\sigma_i^2/\sigma_{u_i}^2$ as a first estimate of $\sigma_{R_i}^2/\sigma_{u_i}^2$, for given t^* and set

$$T_{s,i}^*(t) = \frac{2\sqrt{2}\sigma_{R_i}^2}{z\sigma_{u_i}^2/\bar{u}}$$

to calculate

$$\left(\frac{\bar{u}}{z}\right)^2 \frac{\sigma_{R_i}^2}{\sigma_{u_i}^2} = t^{*2} \int_0^\infty \frac{af}{(1+bf)^{5/3}} \frac{\sin^2 \pi ft^*/\beta}{(\pi ft^*/\beta)^2} \left(1 - \frac{\sin^2 \pi f T_{s,i}^*}{(\pi f T_{s,i}^*)^2}\right) d \ln f \quad (6.5-19^*)$$

Step 3: Use the value of $\sigma_{R_i}^2/\sigma_{u_i}^2$ obtained from the previous step to refine the estimate of $T_{s,i}^*$, and introduce again in the last equation above to obtain a new value of $\sigma_{R_i}^2/\sigma_{u_i}^2$. Repeat until convergence is obtained.

Comments: (i) In practice a general infimum and a general supremum for the lower and upper limits of integration respectively are $f = 10^{-3}$ and $f = 10^3$; in most cases however minimum and maximum values of f equal to 10^{-2} and 10^2 are sufficient. (ii) To obtain absolute values of σ_{R_i} , the relevant values of $\sigma_{u_i}^2$ are needed. Current knowledge regarding these values is reviewed in various sources, such as Nieuwstadt and van Dop (1982), Panofsky and Dutton (1984), and Weil (1985).

Given the frequency of the spectral maximum, f_m , the above procedure gives us $\sigma_{R_i}^2/\sigma_{u_i}^2$ as a function of the dispersion time t . As an example we present here

calculations for both $\sigma_i^2/\sigma_{u_i}^2$ and $\sigma_{R_i}^2/\sigma_{u_i}^2$ for dispersion in the vertical ($i = 3$), with f_m given by the following equations, based on atmospheric measurements (Panofsky and Dutton, 1984, p.189):

$$f_m = 0.183 \quad \left(\frac{z}{L} < -0.7 \right)$$

$$f_m = 0.482 + 0.437 \frac{z}{L} \quad \left(-0.7 \leq \frac{z}{L} < 0 \right)$$

$$f_m = 0.482 + 0.87 \frac{z}{L} \quad \left(\frac{z}{L} > 0 \right)$$

where L is the Monin-Obukhov length. Figures 6-5a, 6-5b, and 6-5c contain the results for $z/L = 0.0$ (neutral atmosphere), $z/L = -1.0$ (unstable atmosphere), and $z/L = 1.0$ (stable atmosphere). Typical values of $\beta = 4, 2,$ and 10 were used respectively for these three cases.

It is easy to see that these figures show quite good agreement – at least on a qualitative basis – with the known asymptotic results from similarity theory: $\sigma_i^2 \sim t^2$ for small times and $\sigma_i^2 \sim t$ for large times; also $\sigma_{R_i}^2 \sim t^3$ in the beginning of the calculations for the σ_{R_i} and $\sigma_{R_i}^2 \sim \sigma_i^2$ at large dispersion times. (Recall that the early, source-dependent, phase of the relative dispersion process is not modeled by the present algorithm). As expected, the effect of meandering is much more profound in unstable atmospheric conditions and reduces significantly with increasing atmospheric stability. For intensely unstable atmospheres σ_i seems to be a bad first approximation for σ_{R_i} for a significant downwind distance; thus, if for an application σ_{R_i} cannot simply be neglected with respect to meandering (which dominates dispersion there), it seems that one should calculate relative dispersion from some semiempirical formula that involves an effective source size.

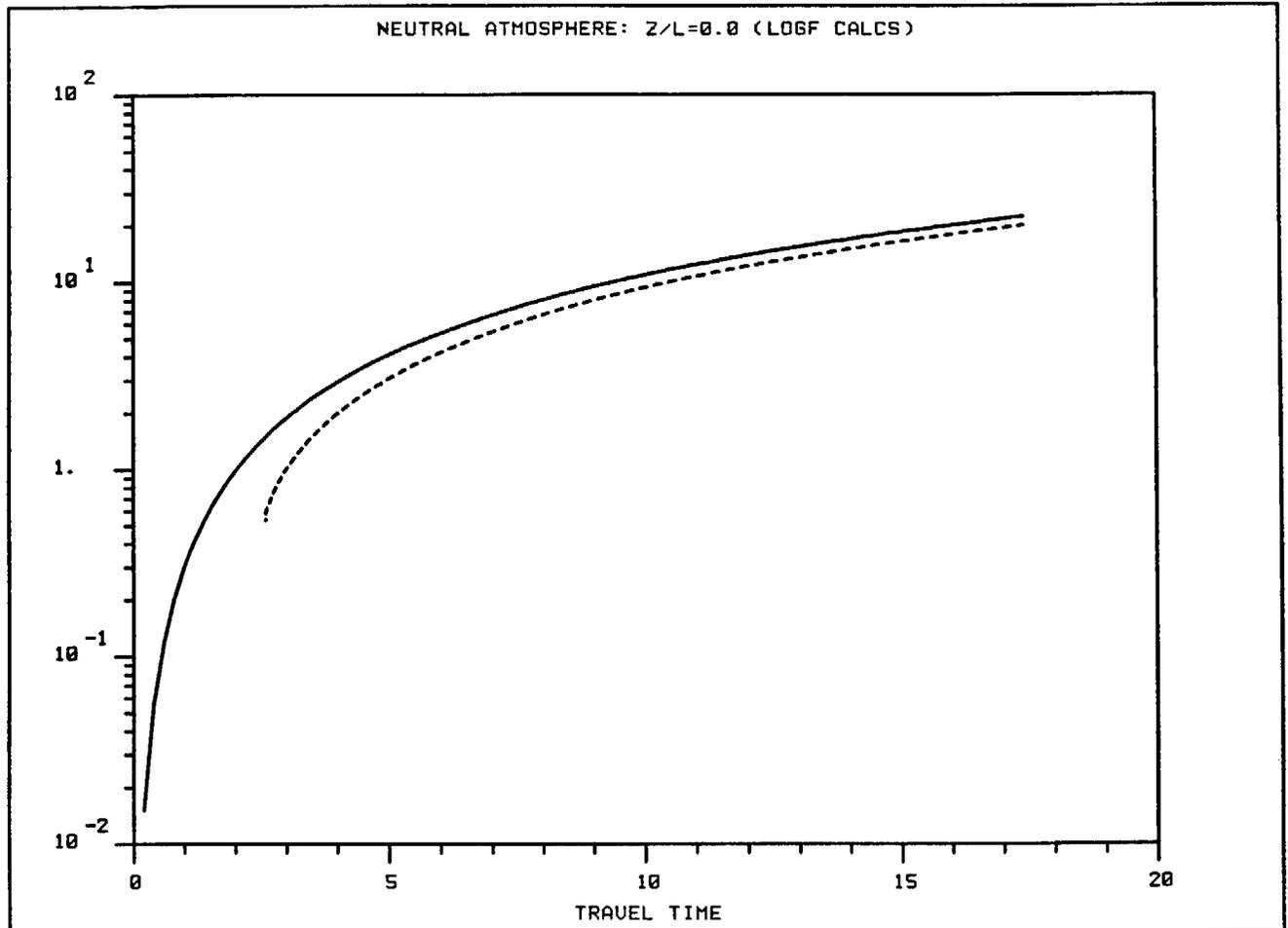


Figure 6-5a

Absolute and Relative Dispersion Parameters over $\sigma_{u_i}^2 (z/\bar{u})^2$
 (Solid and Dashed line respectively)
 in the Vertical Direction, versus $t\bar{u}/z$,
 for Neutral Atmospheric Conditions ($z/L = 0.0$),
 Calculated through Iterative Filtering of the Turbulent Spectrum

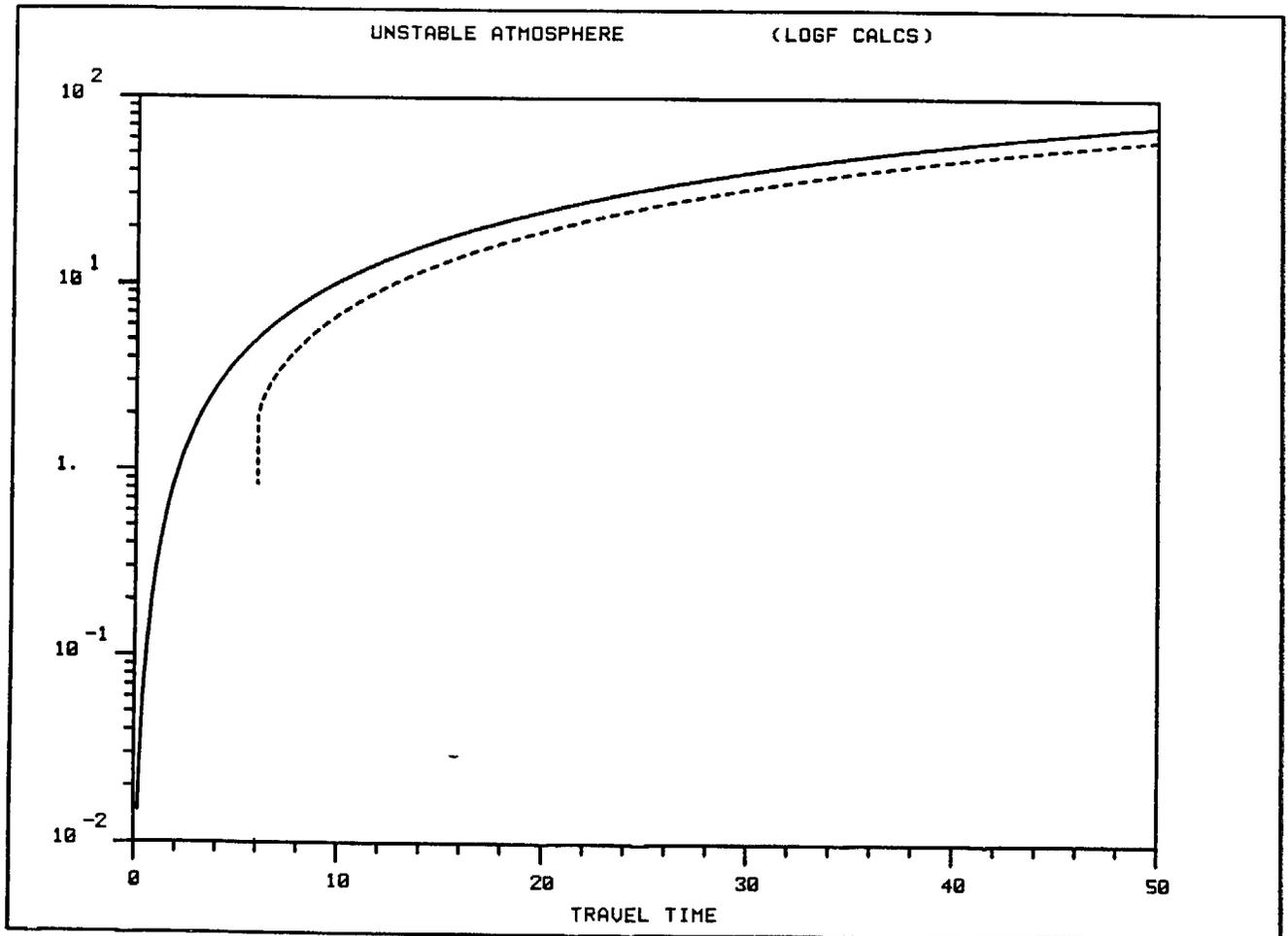


Figure 6-5b

Absolute and Relative Dispersion Parameters over $\sigma_{u_i}^2 (z/\bar{u})^2$
 (Solid and Dashed line respectively)
 in the Vertical Direction, versus $t\bar{u}/z$,
 for Unstable Atmospheric Conditions ($z/L = -1.0$),
 Calculated through Iterative Filtering of the Turbulent Spectrum

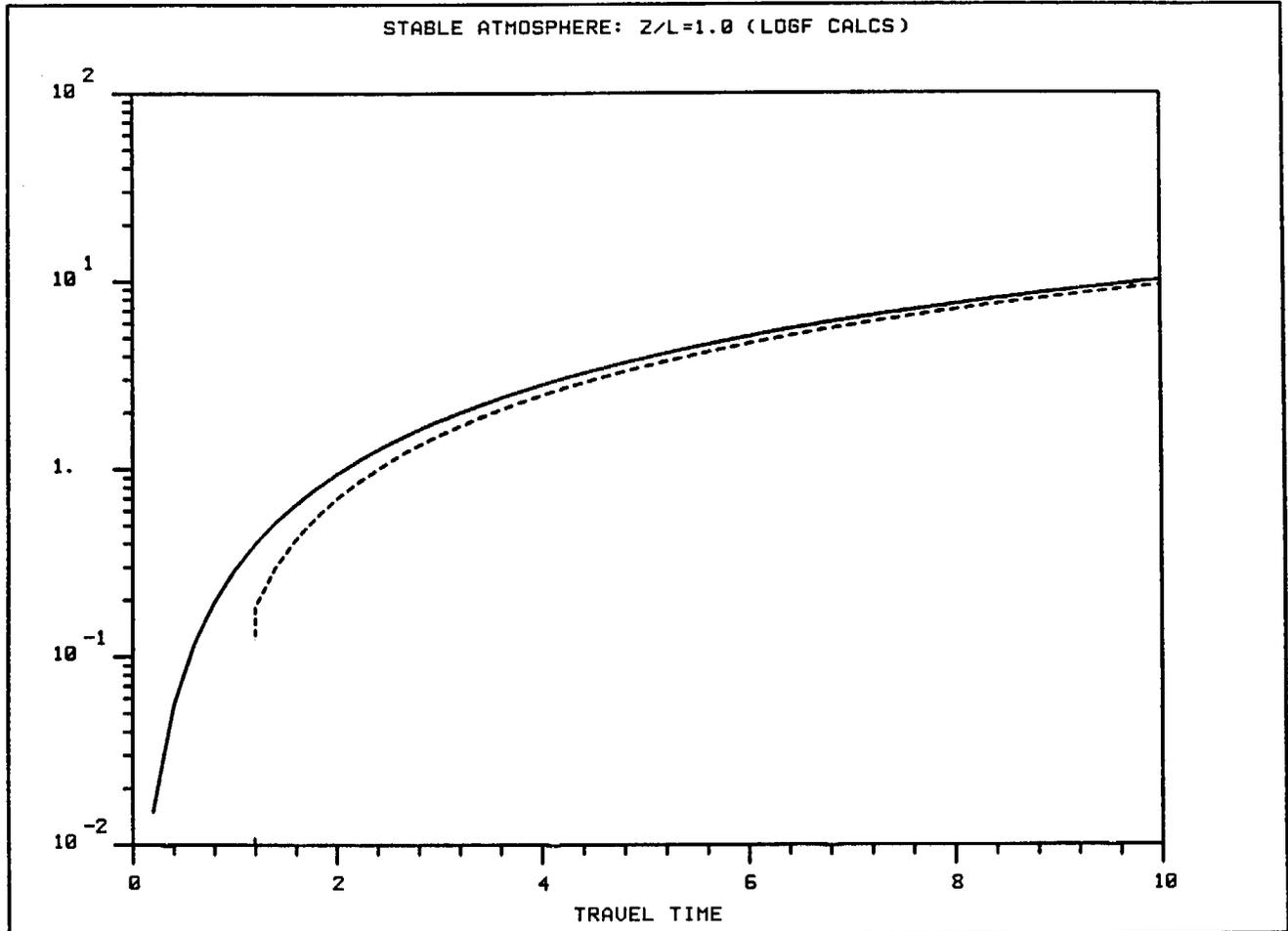


Figure 6-5c

Absolute and Relative Dispersion Parameters over $\sigma_{u_i}^2 (z/\bar{u})^2$
 (Solid and Dashed line respectively)
 in the Vertical Direction, versus $t\bar{u}/z$,
 for Stable Atmospheric Conditions ($z/L = 1.0$),
 Calculated through Iterative Filtering of the Turbulent Spectrum

6.6 CONCLUSIONS

The discussion in this chapter attempted an overview of different concepts and methods employed in the description of relative dispersion, focusing in particular on their interrelationships. A point that was stressed here is that various important questions, regarding sometimes widely applied hypotheses, remain unresolved and waiting for definitive answers. However, the attention that is given to the subject of relative dispersion has been steadily increasing in recent years (partly due to realizing its importance in modeling short term incidental releases of hazardous gases and to the problems related to concentration fluctuations), and a better understanding of the problems involved is a certain fact. It is hoped in particular that comparison of both the underlying fundamental assumptions and of the results from different methods employed to study relative dispersion will significantly improve the insight on the ambiguous points.

Among the methods presented here, those based on stochastic ordinary differential equations (Langevin equations) and their discrete counterparts (autoregressive time series models) seem to have the potential for improving our fundamental understanding of phenomena related to relative dispersion process in a more tractable manner than formulations dealing directly with the dynamics of transition functions. Nevertheless, the generality of the formalism that is developed in connection with the dynamics of the (stochastic and deterministic) transition functions allows us to see the various practical models of dispersion from a more broad perspective, derive and classify them in an elegant and general manner, and identify the connection of the assumptions involved in their formulations. In particular the discussion in this chapter tried to show that the use of time-dependent diffusion coefficients in an ADE-type equation is not an "illogical concept," as it is often claimed, but constitutes an – admittedly artificial – compromise that turns the parabolic partial differential equation of transport into a non-local scheme, avoiding the introduction of integrodifferential

models that formally account for the non-localness of the turbulent dispersion process.

From a more practical point of view, application of appropriate filtering techniques on observed turbulent spectra seems to offer a promising method for estimating dispersion parameters, with the effects of sampling and averaging time explicitly incorporated in their estimation. In this way these parameters reflect the action of the random fluid motions associated with a particular range of temporal and spatial scales. Thus not only the nature of the different "components" of dispersion is made clear, but also a means for exactly identifying the scales relevant to "mixing" and "advection" on a quantitative basis is possible. Of course various problems associated with this method expect some future improvement in their treatment; perhaps the most important are related to the Lagrangian-Eulerian spectra relationship and to the incorporation of an effective source size in the overall scheme of calculations.

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APPENDIX A6.1

**Frequency Spectra
and the Statistical Effects of
Finite Sampling and Averaging Times**

The apparent statistical properties of random fluctuating aerometric quantities such as wind velocity components, temperature, concentrations etc., are implicit functions of the averaging time T_a and the sampling duration T_s involved in their measurement or estimation. In the modeling schemes of the present work we employ mainly the variances, temporal autocorrelations, and frequency spectra of such quantities. Here we focus on the effects of finite sampling and averaging time on the variance, considering its spectral representations.

Let $\sigma_\alpha^2 [T_s, T_a]$ represent the apparent variance of the (Eulerian or Lagrangian) quantity α obtained by averaging measurements over the time interval T_a and sampling for time T_s . The fluctuation of α about its mean value is assumed to be a stationary stochastic function of time; thus the "theoretical" ensemble variance of α will be

$$E\{\alpha'^2\} = \langle \alpha'^2 \rangle = \sigma_\alpha^2 = \sigma_\alpha^2 [\infty, 0]$$

where $\alpha' = \alpha - \langle \alpha \rangle$.

Let $R_\alpha(\tau)$ be the temporal autocorrelation coefficient of α'

$$R_\alpha(\tau) = E\{\alpha'(t) \alpha'(t + \tau)\}$$

and $F_\alpha(\omega)$ be its (cyclic) frequency spectrum. At this point it is necessary to summarize a few remarks regarding the definition of spectral functions in studies of turbulence. (It must be noted of course that although the present discussion considers temporal single-point autocorrelations and related frequency spectra these remarks also apply to cross-correlations in both space and time and to all relevant frequency or wave-number spectral functions and tensors).

The majority of works in turbulence (see, e.g., Monin and Yaglom, 1975; Tennekes and Lumley, 1972; Townsend, 1976; Batchelor, 1953) defines $F_\alpha(\omega)$ as the non-symmetric Fourier transform of $R_\alpha(\tau)$ with the $1/2\pi$ factor in the transform partner of the pair

$$F_\alpha(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} R_\alpha(\tau) \exp(-i\omega\tau) d\tau \quad (A6.1-1)$$

which for symmetric $R_\alpha(\tau)$, i.e. stationary α' (as it was assumed) becomes

$$F_\alpha(\omega) = \frac{1}{\pi} \int_0^{\infty} R_\alpha(\tau) \cos \omega\tau d\tau \quad (A6.1-1a)$$

This allows use of the spectrum $E_\alpha(\omega) = 2F_\alpha(\omega)$, defined for $0 \leq \omega < \infty$ instead of $-\infty < \omega < \infty$, and thus

$$R_\alpha(\tau) = \int_{-\infty}^{\infty} F_\alpha(\omega) \exp(i\omega\tau) d\omega = \int_0^{\infty} E_\alpha(\omega) \cos\omega\tau d\omega \quad (\text{A6.1-2})$$

This notation comes in contrast with the common convention of (electrical mainly) engineering literature where the $1/2\pi$ factor is included in the inverse transform partner of the pair. However notational confusion does not stop at this point. Some works which are standard references in atmospheric turbulence and atmospheric diffusion theory do not follow the majority of turbulence literature but adopt different definitions:

Pasquill and Smith (1983: third edition of the classic monograph of Pasquill) adopt the definition (also used by Hinze, 1975)

$$F_\alpha^{(PS)}(\omega) = 2 \int_{-\infty}^{\infty} R_\alpha(\tau) \exp(-i\omega\tau) d\tau = 4 \int_0^{\infty} R_\alpha(\tau) \cos\omega\tau d\tau$$

and therefore

$$R_\alpha(\tau) = \frac{1}{4\pi} \int_{-\infty}^{\infty} F_\alpha^{(PS)}(\omega) \exp(i\omega\tau) d\omega = \frac{1}{2\pi} \int_0^{\infty} F_\alpha^{(PS)}(\omega) \cos\omega\tau d\omega$$

whereas Panofsky and Dutton (1984) set

$$F_\alpha^{(PD)}(\omega) = \frac{1}{\pi} \int_{-\infty}^{\infty} R_\alpha(\tau) \exp(i\omega\tau) d\tau = \frac{2}{\pi} \int_0^{\infty} R_\alpha(\tau) \cos\omega\tau d\tau$$

and

$$R_\alpha(\tau) = \frac{1}{2} \int_{-\infty}^{\infty} F_\alpha^{(PD)}(\omega) \exp(-i\omega\tau) d\omega$$

In other words

$$F_\alpha^{(PD)}(\omega) = E_\alpha(\omega)$$

It is therefore imperative that great care is taken when, e.g., an empirical spectral function is used in calculations, to be sure to what definition it corresponds.

Here we adopt the "mainstream" definition as in Monin and Yaglom (1975), using both $F_\alpha(\omega)$ and $E_\alpha(\omega)$. We also introduce the absolute spectral density in terms of "arithmetic frequency" $n = \omega/2\pi$

$$S_\alpha(n) = 2\pi E_\alpha(2\pi n) \quad (\text{A6.1-3})$$

which gives

$$\int_0^{\infty} S_\alpha(n) dn = \int_0^{\infty} E_\alpha(\omega) d\omega = \sigma_\alpha^2 \quad (\text{A6.1-4})$$

With this definition our spectral density $S_\alpha(n)$ is identical to both the function $S(n)$ defined in Pasquill and Smith (1983, p. 23) and to the function $S(f)$ defined in Panofsky and Dutton (1984, p. 85). A useful thing to note here is the identity

$$\int_0^\infty S_\alpha(n) dn = \int_0^\infty n S_\alpha(n) d \ln n$$

Thus the area under the curve $n S_\alpha(n)$ plotted against $\ln n$ represents variance. Thus $n S_\alpha(n)$ represents the variance per unit logarithm frequency interval.

Let further $\hat{S}_\alpha(n)$, $\hat{R}_\alpha(\tau)$, be the normalized spectral density and the temporal autocorrelation coefficient respectively

$$\hat{S}_\alpha(n) = \frac{S_\alpha(n)}{\sigma_\alpha^2}, \quad \hat{R}_\alpha(\tau) = \frac{R_\alpha(\tau)}{\sigma_\alpha^2}$$

Then it is easy to show that

$$\sigma_\alpha^2[\infty, T_\alpha] = \frac{2\sigma_\alpha^2}{T_\alpha} \int_0^{T_\alpha} \left(1 - \frac{\tau}{T_\alpha}\right) \hat{R}_\alpha(\tau) d\tau \quad (\text{A6.1-6})$$

(see, e.g., Tennekes and Lumley, 1972, p. 212; see also Chapter 5).

In terms of the spectral density one has (see, e.g., Pasquill and Smith, 1983, p. 26)

$$\sigma_\alpha^2[\infty, T_\alpha] = \sigma_\alpha^2 \int_0^\infty \hat{S}_\alpha(n) \frac{\sin^2 \pi n T_\alpha}{(\pi n T_\alpha)^2} dn \quad (\text{A6.1-7})$$

Thus, as T_α is increased, more of the spectrum is cut off and $\sigma_\alpha^2[\infty, T_\alpha]$ is reduced.

The complementary effect of sampling over finite time T_s can also be derived (Pasquill and Smith, 1985, p. 26):

$$\sigma_\alpha^2[\infty, 0] = \sigma_\alpha^2[T_s, 0] + \sigma_\alpha^2[T_s, 0]_\infty \quad (\text{A6.1-8})$$

where the subscript ∞ implies averaging of the variances estimated from consecutive periods T_s over infinite time. Substituting from (A6.1-7) one has

$$\sigma_\alpha^2[T_s, 0]_\infty = \sigma_\alpha^2 \int_0^\infty \hat{S}_\alpha(n) \left(1 - \frac{\sin^2 \pi n T_s}{(\pi n T_s)^2}\right) dn \quad (\text{A6.1-9})$$

For very large T_α the weighting function cuts off all but the very low frequencies, for which $\hat{S}_\alpha(n) \rightarrow 4T^*$ with $T^* = \int_0^\infty R_\alpha(\tau) d\tau$, effectively independent of n . Then, in (A6.1-7) $\hat{S}_\alpha(n)$ can be taken outside the integral sign and therefore

$$\lim_{T_\alpha \rightarrow \infty} \sigma_\alpha^2[\infty, T_\alpha] T_\alpha = 2\sigma_\alpha^2 T^* \quad (\text{A6.1-10})$$

(A6.1-10) is also the limiting form of Taylor's relations

$$\frac{d}{dT_\alpha} \{\sigma_\alpha^2[\infty, T_\alpha] T_\alpha\} = 2\sigma_\alpha^2 \int_0^{T_\alpha} R_\alpha(\tau) d\tau \quad (\text{A6.1-11a})$$

$$\sigma_{\alpha}^2 [\infty, t] t^2 = 2\sigma_{\alpha}^2 \int_0^t \int_0^{T_a} R_{\alpha}(\tau) d\tau dT_a \quad (\text{A6.1} - 11b)$$

which are applicable to any stationary random function of time.

When available data correspond to both finite sampling and averaging time the effect of the two in combination depends on the order in which the averaging and sampling operation are carried out. The two alternative procedures are described by Pasquill and Smith (1983, p. 28):

- (I) for samples of length T_s , averages are taken over subintervals T_a which do not overlap (T_s/T_a must be an integer),
- (II) averages are taken over intervals of length T_a and from the smoothed time series constructed in this way samples of length T_s are formed. In this case averages may be taken in an overlapping manner.

The combined effects of finite sampling and averaging times are given by the following relations (Pasquill and Smith, 1983) for procedures (I) and (II) respectively:

$$\sigma_{\alpha}^2 [T_s, T_a]_{(I)} = \sigma_{\alpha}^2 \int_0^{\infty} \hat{S}_{\alpha}(n) \left(\frac{\sin^2 \pi n T_a}{(\pi n T_a)^2} - \frac{\sin^2 \pi n T_s}{(\pi n T_s)^2} \right) \quad (\text{A6.1} - 12a)$$

$$\sigma_{\alpha}^2 [T_s, T_a]_{(II)} = \sigma_{\alpha}^2 \int_0^{\infty} \hat{S}_{\alpha}(n) \frac{\sin^2 \pi n T_a}{(\pi n T_a)^2} \left(1 - \frac{\sin^2 \pi n T_s}{(\pi n T_s)^2} \right) \quad (\text{A6.1} - 12b)$$

Thus, in case (I) the resultant effect is equivalent to subtracting the separate weighting functions for averaging over T_a and T_s , while in case (II) it is equivalent to applying the product of the separate weighting functions.

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for Appendix A6.1

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CHAPTER 7

Chapter 7 contains

- *a discussion of the initial phases of plume dispersion, and the scales and properties that are relevant to each phase,*
- *a brief overview of methods employed to model plume rise,*
- *a presentation of the models of Briggs and Schatzmann that are suggested as the “simple” and “comprehensive” alternatives, respectively, for use with the TRPM.*

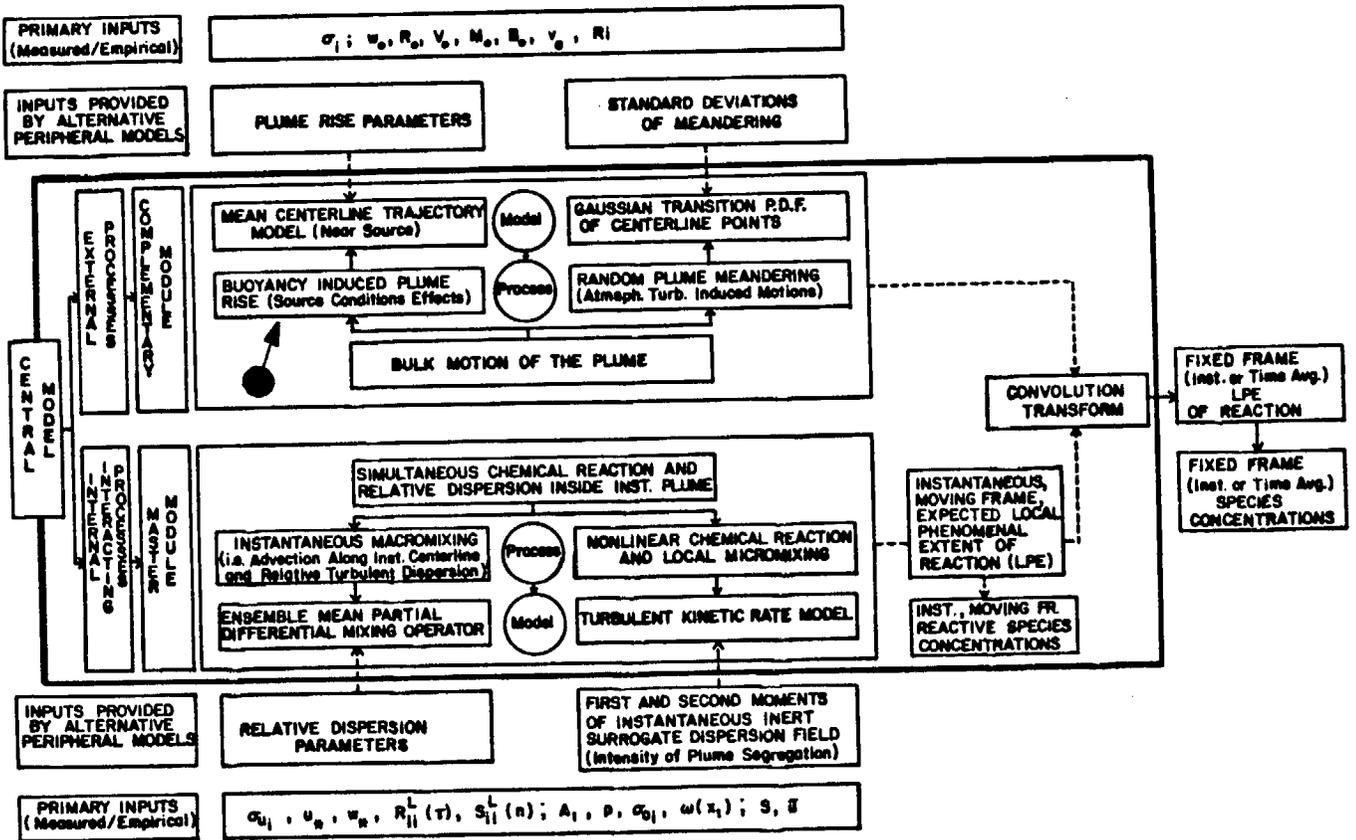


Figure 2-1d
TRPM Components Discussed in Chapter 7

CHAPTER 7

NEAR FIELD PLUME DYNAMICS

7.1 INTRODUCTION

In the development of the Turbulent Reacting Plume Model (TRPM) it was assumed that the processes of plume mixing that interact with chemistry are solely due to the action of the ambient, atmospheric, turbulence. Thus, as was mentioned in Chapters 2 and 3, the details of the early stages of plume dispersion, where the exit flow of gases from a stack (or any other "point" source) "merges" with the ambient cross-flow, are neglected (*). This was done on the basis of the argument that this process of flow merging is very fast compared to the time scales of both molecular diffusion processes and of nonlinear chemical interactions between plume and ambient species, of the type this work mainly focused on.

Nevertheless, source conditions play a significant role, not only by determining the rate and quality of early plume mixing but, more importantly, by affecting the dispersion and mixing parameters far beyond the stage where the plume exists as a separate fluid mechanical entity, distinct from the ambient flow. More specifically, initial conditions, in combination with the state of ambient stability, determine the

(*) It must be noted that the description of mixing and dispersion in the present basic operational version of the TRPM does not involve any geometric, kinematic or thermal parameters of the source, such as stack diameter, effluent exit temperature or velocity, etc.; actually the species emission rate is the only input associated with the source that is required directly by the master module of the TRPM.

evolution of the ascending path of the mean plume centerline and its final total rise, i.e. the height where atmospheric dispersion of the emissions essentially starts. Knowledge of the position of the mean centerline is essential not only for "placing" the results of local reaction-dispersion calculations at the actual mean spatial coordinates to which they are relevant (and therefore for integrating the results of the TRPM with calculations from larger scale models), but also because the dispersion rate of the plume may depend on its actual rise. A most extreme example of this dependence is associated with the existence of elevated temperature inversions. In such a case the buoyancy of the emissions may be able to cause (at least partial) penetration of this inversion layer. This will result in a significant reduction of near ground-level concentrations as well as of plume dispersion rates just above the inversion. A more general quantitative measure of the effects of near-field plume rise on plume dispersion can be obtained by examining the maximum ground level concentration which is roughly proportional to the inverse square of the effective source height. Experience suggests that this effective height is typically 2 to 10 times the actual stack height (Hanna et al., 1982); plume rise can therefore reduce (even without causing penetration of an inversion) ground level concentration by a factor of as much as 100. One must therefore conclude that a reliable scheme for the estimation of plume rise is a required component of any "realistic" reacting plume model.

It is nevertheless clear that the problem of near field plume (or jet) dynamics can often be of overwhelming complexity as it involves the simultaneous transfer of mass, momentum and heat, coupled with boundary conditions that can be highly complicated. Thus, intricate flow patterns and mixing mechanics are to be expected, except in the most trivial of cases (see also Figure 7-1). Analytical (exact or approximate) results are available for point sources of momentum and/or heat in a calm environment, resulting in laminar jets and plumes (see, e.g., Seinfeld, 1975; Yih, 1977). Extensive information is also available regarding the internal flow structure of turbulent jets and plumes in calm backgrounds (see, e.g., Hinze, 1975). In the case of discharges in turbulent cross flows the physics of the problem become very difficult to

handle and available experimental data and numerical computations reveal complex schemes of mixing and flow development (see, e.g., Moussa et al., 1977; Crabb et al., 1981). It is beyond the scope of the present work to discuss the vast range of research, both theoretical and experimental, that is relevant to turbulent jets and plumes; a relatively recent review of the current state of the field can be found in List (1982) – see also Fischer et al. (1979), Chen and Rodi (1980), Rodi (1982).

In the case of atmospheric plumes in particular, buoyancy is typically much more important than initial momentum (see next section) and hence it is mainly the former that determines plume evolution in the near field. This leads to the “line thermal analogy” for plume rise, according to which the internal motion of a point source plume resembles the convective motion induced by an instantaneous line source of heat corresponding to the projection of the mean plume centerline on the horizontal plane at source height. Csanady (1973; Chapter 6) and Scorer (1978; Chapter 10) contain informative introductions to the fundamental theory of buoyancy dominated plumes; for further analysis of the fundamentals of buoyancy effects in fluids one should consult the relevant monograph of Turner (1973); finally, useful introductions to the techniques of plume modeling can be found in Seinfeld (1975), Eskinazi (1975), Fischer et al. (1979) and Gebhard et al. (1984). Proceeding from the fundamental concepts, that are exposed in the above references, to computational models that realistically predict plume rise under atmospheric conditions (for given ambient stability) is far from being a trivial or even straightforward step. Indeed, although many models start from a common fundamental (and simplified) “picture” of the plume (see Section 7.3) they produce different working formulas (and results that vary significantly for the same inputs) as they adopt different assumptions regarding the action of atmospheric and plume turbulence.

The field of atmospheric plume rise modeling has been reviewed extensively and periodically by Briggs (see, e.g. Briggs 1969, 1975, 1984) who compared and classified

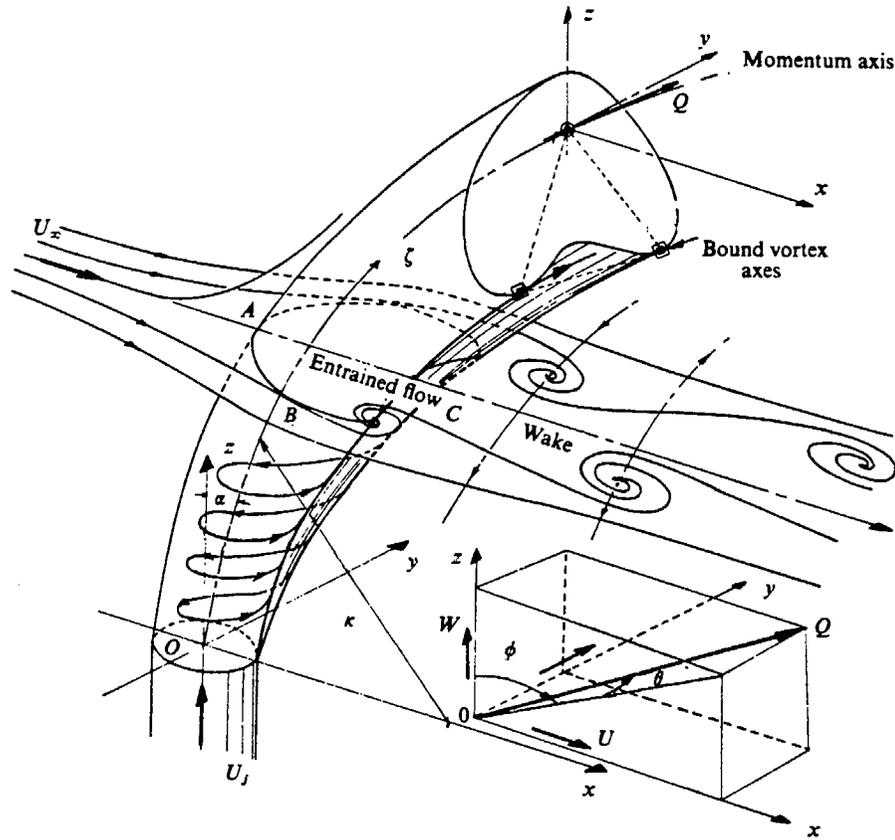


Figure 7-1

Rising Plume in a Cross-Flow

(Source: Moussa et al., 1977)

a variety of modeling approaches(*) as well as available data to finally reach a set of formulas (also periodically updated) that today are the most widely used means of calculating the rise of atmospheric plumes (see Section 7.4). Another extensive review, focusing on models for the prediction of cooling tower plume rise from natural-draft cooling towers, was presented by Carhart et al. (1982) who evaluated the theory and performance of 16 such models. Finally, a concise but general overview and discussion of the subject of plume rise modeling can be found in Schatzmann and Policastro (1984) who classify and analyze a wide range of assumptions commonly involved in this modeling.

In the present chapter, after a discussion of the main qualitative features of near field plume dynamics, and a general classification of the approaches that have employed to model these dynamics (a classification that contains some information more recent than what can be found in the latest works of Briggs), we present the two alternative options suggested for use with the TRPM. These are the widely used semiempirical algebraic equations of Briggs, and a more general scheme (a self similarity model of plume rise) resulting in a set of ordinary differential equations that require numerical solution, based on the work of Schatzmann and his coworkers; the latter is presented in relative detail in Appendix A7.2.

(*) In his 1975 review Briggs lists and discusses the basic features of about 50 models of atmospheric plume rise.

7.2 QUALITATIVE CONSIDERATIONS

7.2.1 Phases of Plume Dispersion

In order to provide perspective on the qualitative dynamics of atmospheric plumes we consider the following typical case of a plume “bent over” by the wind (Slawson and Csanady, 1967, 1971; Csanady, 1973): Effluent gases leave an industrial stack with temperature differences from the ambient environment of the order of 100-300 °C and vertical velocities w_0 of the order of 10 m s⁻¹, entering a cross wind of speed u_∞ that is of similar order of magnitude. Thus, the effluent gases from the stack “carry” both momentum and buoyancy “of their own” and therefore constitute a buoyant jet (or a forced plume) entering a turbulent atmospheric crossflow. Rapid mixing with the ambient air takes place and the plume axis bends over into the wind as the effluent gases acquire the horizontal momentum of the ambient air. Observations show that the transfer of horizontal momentum is usually essentially complete within a few stack diameters from the exit (Csanady, 1973). Thus very quickly portions of the plume start to travel horizontally at the mean speed of the ambient wind. Nevertheless, their vertical velocity relative to the ambient fluid however does not disappear so quickly, because of the continued action of the buoyancy forces.

Csanady (1973) reports that from several observations of the near-source size of chimney plumes it may be inferred that the effective mass of effluent gases increases through vigorous mixing with ambient air by something like a factor of 30 within a distance of 3 to 5 source diameters. By this time the deficiency of horizontal momentum compared to ambient air is therefore a negligible 3%. The vertical velocity w_M due to initial velocity is also about 3% of the original w_0 , that is for $w_0 \simeq 10 \text{ m s}^{-1}$ w_M is of the order of 30 cm s⁻¹. However, if the chimney diameter is not much less than say 3 m, the buoyancy force has had several seconds to act in the time the gases have moved 3 to 5 diameters (that is 9 to 15 m). A

typical order of magnitude for the initial buoyant acceleration of industrial stacks is 10 m s^{-2} , and although this also reduces through mixing in the same proportion as initial momentum, it generates an appreciable vertical velocity within the first few seconds. Indeed if the average acceleration between leaving the chimney top and a 30-fold increase in mass is only 1 m s^{-2} , and if this initial adjustment phase lasts at least 1 s, the buoyant contribution to vertical velocity becomes 1 m s^{-1} , or 3 about times larger than that due to the initial momentum. Csanady (1973) notes that such a conclusion holds only for chimneys discharging substantial quantities of heat. An initial buoyancy caused acceleration of the order of 10 m s^{-2} implies an initial excess temperature of the effluent gases of the order of $300 \text{ }^\circ\text{C}$. For a 3 m diameter chimney and an exit velocity $w_0 = 10 \text{ m s}^{-1}$ this corresponds to a considerable rate of heat release (order of 6000 kcal s).

These conclusions will not apply to much smaller chimneys (of order 1 m in diameter or less) nor to those which discharge their gases with a small buoyant acceleration. In such non-buoyant cases plume rise is due basically to initial momentum and is usually essentially complete within 10 chimney diameters or so. However, the vast majority of large industrial point sources produce buoyancy rather than momentum dominated plumes, as in the situation described here, and most effort in the field of atmospheric modeling has focused on these cases.

From the above example it becomes obvious that in buoyancy dominated plumes neither the radius of the stack, nor the initial vertical exit velocity are dominant in determining the path of the plume beyond the earliest mixing phase (often referred to as the "jet" or "momentum phase") that lasts for a distance of the order of a few stack diameters. The factor that quickly becomes of dominant importance is the total excess heat. However, beyond the jet phase of the plume this excess heat is small enough, even in plumes generated by large heat sources, and the Boussinesq approximation seems to be a valid assumption in most of the cases. These facts suggest that it is useful to identify successive stages in the evolution of a typical plume, where different sets of parameters are important and appropriate simplifications can

be made in the analytical description of the plume. The brief discussion that follows is based on the analysis of Slawson and Csanady (1967, 1971) who identified four phases (and classified them as the zeroth, first, second and third phase of plume evolution). An actual atmospheric plume is expected to conform better to this rather idealized qualitative model of behavior in near neutral atmospheres.

The Momentum (or Jet) Phase

This initial phase of plume evolution extends a few (say 3 to 5) stack diameters downwind and its dynamics are determined by source properties (stack radius, exit speed, density of effluent) and the ambient density and mean wind speed at source height. The inherent turbulence of the exit flow is much stronger than the ambient turbulence and dominates transport processes and the internal plume flow structure.

The Thermal Phase

In this phase the effect of source diameter and exit velocity become unimportant. Mean plume dynamics are determined by the flux of buoyancy of the plume and the ambient mean wind speed and stratification (i.e. the atmospheric potential temperature gradient). Inherent plume turbulence (generated by buoyant convective motion) still dominates the ambient and determines local turbulent properties and mixing. The total downwind extent of this phase is expected to be of the order of about a hundred stack diameters.

In a neutral atmosphere, or for suitably small vertical plume displacements, the flux of buoyancy may be regarded as approximately constant in this phase. However, in a stable atmosphere the potential temperature of the environment increases as the plume rises so that the plume's excess temperature (and hence its total buoyancy decreases). The converse is the case in an unstable atmosphere. (In highly unstable atmospheric conditions the vigorous convective motions of the ambient will most probably dominate very early the inherent motions of the plume and will play a more important role in determining its rise).

The term thermal phase is usually attributed to a rather smooth phase of buoyant plume dispersion, and is commonly associated with near-neutral conditions. In these

conditions most buoyancy dominated plumes retain smooth outlines and a moderate slope (about 0.2 or even less) against the horizontal for some distance during this phase, unless special ambient flow properties and source configuration cause characteristic irregularity phenomena known under the names of thermalling, downwashing (or flagging), downdraught, puffing and bifurcation (see Scorer, 1978; see also Appendix A7.1 for a brief glossary of terms describing plume behavior). It turns out to be reasonable in this phase to regard segments of the plume as if they were segments of a line thermal moving upward through quiescent surroundings (see, e.g., Turner, 1973).

The total plume rise in atmospheric crossflows during this phase is in principle predictable and the great majority of models used for this objective are relevant to the dynamics of this stage.

The Breakup Phase

Observation of buoyant plumes reveals that the relatively regular thermal phase of plume rise comes to a rather distinct end at some approximately predictable distance from the source as more vigorous mixing with the ambient air sets in and the plume often breaks up into several distinct parcels. In general, a stage, lasting for distances of the order of 100 m, where there is a distinct increase in mean plume width and mixing with the surrounding occurs mainly at large scales, is observed. This "breakup" phase of the plume is more pronounced in strong atmospheric turbulence and also occurs closer to the source when the ambient turbulence is more intense.

Obviously the large eddies which lead to the breakup are those naturally present in the wind (they are too large to be produced by the plume's own internal motion). Also their mixing action is dominant over the effects of the self-generated turbulence. When "breakup" is pronounced, it leads to an almost stepwise increase in plume diameter.

The dynamics of these phase are influenced by the scales and intensity of atmospheric turbulence (in addition to the mean wind speed and plume buoyancy flux).

The Atmospheric Diffusion Phase

A little further downwind the distinct parcels merge again into a larger, more diffuse plume, the subsequent growth of which is relatively slow. At this stage the various atmospheric diffusion theories become valid and this final phase of plume dispersion (which extends indefinitely downwind) is typically called the "atmospheric diffusion phase." Now the plume exists only in terms of the species emitted from the source; their fluctuating concentrations *define* the plume. Thus there is no separate flow structure associated with the plume phenomenon and we deal only with atmospheric fluid mechanics.

The actual height of plume rise above the actual source is affected by the randomness of the physical factors involved. The expected rise, is in general a function of the downwind distance from the source and a number of other physical parameters, different for each phase, as they were identified in the previous paragraphs. Recall that in the preceding discussion it was assumed that during the initial phases of plume dispersion no special aerodynamic phenomena such as downwash take place. It is further assumed that the source is sufficiently far above the ground so that the flow pattern within the plume is not disturbed by surface effects. Otherwise the effective height (that is the sum of plume rise plus the real source height) may influence further plume rise (see, e.g., Csanady, 1973, 6.15).

Figure 1-3 in Chapter 1 depicts schematically the downwind range relevant to the various phases that were discussed here together with the most important physical-chemical in-plume processes occurring at a given range.

Results regarding the expected plume dynamics during the "distinct" initial phases of dispersion can be obtained by simple dimensional analysis if the physical parameters recognized as important during each phase are taken into account. These simple results are summarized, together with some empirical information in List (1982). (In relation with the formulas listed there we must note that the effect of a solid boundary on the buoyant movements in a large plume has been ignored; also the atmospheric potential temperature distribution is represented through its gradients, but this in turn may be a function of height.) Finally it must be noted that the line-thermal analogy applies only to the second of the four phases of initial plume dispersion. This is the only phase for which we have a relatively adequate theory for the internal motion and concentration patterns of a buoyant plume. Appendix A7.3 summarizes the suggestions of Briggs (1975) for these internal patterns.

7.3 MODELING PLUME RISE: THE BASIC APPROACHES

Research in the field of plume rise over the past 30 years has led to a confusing proliferation of prediction schemes, that offer a variety of different answers for a specific problem, ranging from simple empirical or semiempirical formulas to complex numerical formulations. It is obvious from the discussion of Section 7.1 that compilation and discussion of a list of specific models representative of the entire spectrum of existing approaches would be a most ambitious task that certainly is beyond the scope of the present work. The reader who is seeking information of this kind is urged to consult List (1982), Briggs (1975, 1984) and Carhart et al. (1982). What is attempted here is a general classification of the various approaches on the basis of the first principles involved.

The two extreme forms of plume rise models, and in general of models of plume (or jet) dynamics, are:

(I) Simple algebraic relations giving the expansion, the trajectory (or final rise) etc., of plumes in either calm or turbulent environments, that are derived from dimensional analysis and empirical information. Typically, the construction of such relations starts with the identification of the important physical parameters involved in the problem (which may be different in the various phases of plume evolution, as discussed in Section 7.2), and, possibly, with assumptions regarding the behavior of some of these parameters. Self similarity is most commonly assumed for velocity, concentration and temperature profiles and simple self similarity laws are invoked. General correlations are then derived on dimensional grounds; qualitative consideration of the governing transport equations with an order of magnitude analysis of their terms, as well as of constraints imposed by conservation requirements, may facilitate or "enhance" this step. The correlations thus derived contain numerical parameters which must be determined on the basis of empirical information. Tutorial expositions of this

approach can be found for example in Seinfeld (1975; Appendix B), Csanady (1973; sections 6.12 and 6.13) and Fisher et al. (1979; Chapter 9).

(II) Numerical schemes that solve the sets of the coupled (partial differential) equations governing the fields of mean velocity, concentration, temperature and, possibly, fields of higher order moments or correlations of these variables. The most important step in the formulation of models following this approach is the construction of appropriate closure approximations for the turbulent correlation terms; both first and higher order closure assumptions have appeared in the relevant literature. Some formulations in this area limit attention to uniform environments; others attempt to take into account the effects of ambient turbulence, crossflow and stratification which complicate the problem significantly. For examples of this approach see, e.g., Mellor and Yamada (1977), Teske et al. (1978), Yamada (1979), Chen and Nikitopoulos (1979); see also List (1982) and Liu et al. (1982; Section 4) for discussions of relevant models.

The "gap" between the approaches described above is occupied by the class of the so-called "integral type" models, widely ranging in variety and complexity, that in general attempt a description of the problem based on more "physical" grounds than models of class (I) but lead to the formulation of schemes that are more tractable than the ones contained in class (II). The key element in the various integral type models is the reduction of the set of governing partial differential equations into a set or ordinary differential equations (essentially through self similarity assumptions and appropriate closure schemes). One can discern two major lines in the development of integral approximations:

(IIIa) The governing ordinary differential equations are formulated directly by considering an appropriate control volume of the evolving plume and constructing balances of momentum, mass, energy and species concentration. This "shell balance" approach (see, e.g., Bird et al., 1960) has been adopted by the majority of investigators starting from the works of Taylor (1945), Priestley (1953), Priestley and Ball (1955) and Morton et al. (1956). Typically "top-hat" profiles of concentration,

temperature, etc., are assumed inside the control volume (but more complicated self similarity is also possible). Quoting Csanady (1973), "the main idealization involved [in this approach] is that although in reality the flow and temperature patterns are continuous, an artificial distinction is introduced between an "identifiable plume" and the ambient fluid. The identifiable plume is assumed to grow by "entrainment" of the ambient fluid, the rate of entrainment being governed by an entrainment velocity at the perimeter of the plume." This constitutes the essence of what is generally referred to as the "Morton-Taylor approach" or "Taylor's entrainment hypothesis." This hypothesis replaces the "straightforward" turbulent transfer closure assumptions that are required to provide a closed set of governing equations.

The most simple models in this approach just reproduce the results of dimensional reasoning discussed earlier; more complicated models attempt detailed descriptions of plume evolution basically using more elaborate entrainment hypotheses. (For a critical discussion of the physical situation behind simple entrainment hypotheses see Netterville, 1985). A review and comparison of several models of this type can be found in Briggs (1975); Briggs' own suggestions (1969, 1975, 1984), which are summarized in Section 7.4 of this chapter, are typical simple applications of this integral approach. For an introduction to the essentials of this type of modeling one may consult the same basic references mentioned in (I). Typically, the Boussinesq approximation is invoked in application (see, e.g., Fan (1967); Abraham (1971) etc.). (IIIb) Alternatively, the original coupled partial differential equations that govern the transport processes in the plume-ambient system are reduced into ordinary differential equations via *Prandtl's integral approximation method* and appropriate self similarity assumptions. Examples of this approach are presented by Hirst (1972) and Schatzmann (1976) and in general provide a more powerful method for describing plume dynamics, starting from a more detailed consideration of the problem and introducing simplifications not a priori but gradually, based on an explicit analysis that requires rational justification of the assumptions involved. This approach (in particular Schatzmann's schemes) is discussed in detail in the following (Section 7.5

and Appendix A7.2). Again turbulent transport closure is conveniently provided by "entrainment hypotheses." For a recent analysis and review of relevant entrainment assumptions see Chiang and Sill (1985).

Finally we close this section by pointing attention to the main subjects that seem to receive currently the major interest in the area of near-field plume dynamics modeling: these are, besides the evaluation and refinement of entrainment hypotheses (also related to their justification on physical grounds), (a) modeling of cooling tower plumes, (b) modeling of the effects related to elevated inversion penetration (see, e.g., Mannins, 1979) and (c) modeling of plume rise in the convective planetary boundary layer (see, e.g., Lamb (1982) and Willis and Deardorff (1984)).

7.4 THE MODELS OF BRIGGS

(Briggs, 1969, 1975, 1984)

The following equations for the various phenomena of plume rise (associated with the momentum and thermal phases of plume dispersion) appear in the most recent reviews of Briggs (see, e.g., Briggs, 1984) and currently they seem to be the most widely accepted working formulas relevant to these phenomena. The brief exposition presented here follows mainly the conventions and the pattern of classification adopted in the *Handbook of Atmospheric Diffusion* of the Department of Energy (Hanna et al., 1982), with some changes in the notation; it should be viewed only as a collection of common definitions and practical formulas for direct application and is included in this work for ready reference. For detailed derivations of Briggs' formulas, extensions to other cases, discussion of the assumptions involved and of the associated uncertainties, as well as for information relevant to their relation to other approaches and their evolution to the currently accepted forms one should consult Briggs (1969, 1975, 1984).

Definitions

The basic geometric (shape) parameters involved in Briggs' formulas are shown schematically in Figure 7-3; a typical "vertical" and a "bent over" plume are shown. In practice a plume will be assumed vertical or bent over when the angle of its centerline with the horizontal is respectively larger or smaller than 45° ; according to Hanna et al. (1982) a plume is "more or less vertical" if wind speed is less than about 1m/s. A "plume volume flux" is defined by Briggs as

$$\dot{V} = w \hat{R}^2 \quad (\text{vertical}) \quad (7.4 - 1)$$

$$\dot{V} = u_\infty \hat{R}^2 \quad (\text{bent over}) \quad (7.4 - 2)$$

where w is the vertical speed of the plume (assumed uniform in a cross-section and therefore representing an average value), u_∞ is the mean ambient wind speed and \hat{R}

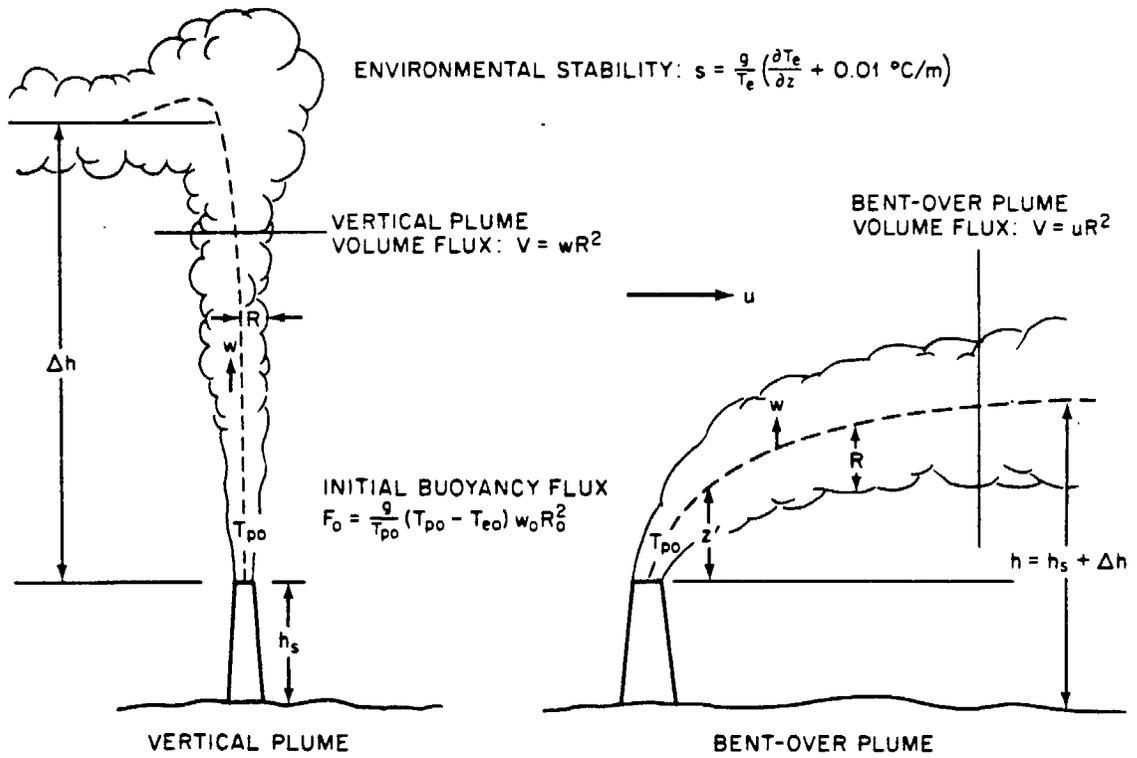


Figure 7-2

Basic Parameters of "Vertical" and "Bent Over" Plumes

Appearing in the Models of Briggs (1975, 1984)

(from Hanna et al., 1982 - the notation is that used in this ref.)

is an effective plume radius in a horizontal or vertical plane for vertical and bent over plumes respectively. (Note that in the formulation presented here the factor π does not appear explicitly anywhere; thus it is incorporated implicitly in the definition of the effective radius \hat{R}). Initial fluxes of volume, \dot{V}_0 , buoyancy \dot{B}_0 and momentum \dot{M}_0 are defined as

$$\dot{V}_0 = w_0 \hat{R}_0^2 \quad (7.4-3)$$

$$\dot{B}_0 = \frac{g}{T_0} (T_0 - T_{\infty 0}) \dot{V}_0 \quad (7.4-4)$$

$$\dot{M}_0 = \frac{\rho_0}{\rho_{\infty 0}} w_0 \dot{V}_0 \quad (7.4-5)$$

where subscript 0 indicates stack exit values and ∞ indicates ambient properties. Thus T_0 and ρ_0 are the plume temperature and density at the stack and $T_{\infty 0}$, $\rho_{\infty 0}$ are the corresponding ambient properties at stack height. (Implicit in (7.4-4) is that the mean molecular weight of the plume gases does not differ appreciably from that of ambient air; otherwise all temperatures in (this equation must be divided by the mean plume molecular weight). At an arbitrary height buoyancy and momentum flux are defined as

$$\dot{B} = \frac{g}{T} (T - T_{\infty}) \dot{V} \quad (7.4-6)$$

$$\dot{M} = w \dot{V} \quad (7.4-7)$$

The environmental stability (or stratification) parameter ζ is expressed in terms of the ambient potential temperature ($T_{\infty}^{(p)}$) gradient as

$$\zeta = \frac{g}{T_{\infty}} \frac{\partial T_{\infty}^{(p)}}{\partial z} \simeq \frac{g}{T_{\infty}} \left(\frac{\partial T_{\infty}}{\partial z} + 0.001^\circ C/m \right) \quad (7.4-8)$$

(the last factor is approximately the adiabatic lapse rate; one should note that ζ is also the square of the Brunt-Vaisala frequency). In many cases the appropriate field data for direct determination of ζ are not available; for these situations the approximate values of temperature gradients given in Table 7-1 can be used in (7.4-8).

Another concept that appears in Brigg's formulas is the ratio of the effective area influenced by the plume momentum to the cross-sectional area of the so-called

Table 7-1
Typical Temperature Stratification
Corresponding to the Pasquill-Gifford Stability Classes

<i>STABILITY CLASS</i>	AMBIENT TEMPERATURE GRADIENT $\partial T/\partial z$ ($^{\circ}\text{C}/100\text{m}$)	POTENTIAL TEMPERATURE* GRADIENT $\partial\theta/\partial z$ ($^{\circ}\text{C}/100\text{m}$)
<i>A (extremely unstable)</i>	<-1.9	<-0.9
<i>B (moderately unstable)</i>	-1.9 to -1.7	-0.9 to -0.7
<i>C (slightly unstable)</i>	-1.7 to -1.5	-0.7 to -0.5
<i>D (neutral)</i>	-1.5 to -0.5	-0.5 to 0.5
<i>E (slightly stable)</i>	-0.5 to 1.5	0.5 to 2.5
<i>F (moderately stable)</i>	>1.5	>2.5

* Calculated by assuming $d\theta/dz \approx dT/dz + \Gamma$, where Γ is the adiabatic lapse rate (0.986 $^{\circ}\text{C}/100\text{m}$).

thermal plume (Briggs, 1975), S , which is approximately equal to 2.3 for bent-over plumes.

Finally, the entrainment velocity v_e that appears in the closure scheme (Taylor's entrainment hypothesis)

$$\frac{d\dot{V}}{dz} = 2\hat{R}v_e$$

is related to plume vertical speed through

$$v_e = \alpha w \quad (\text{vertical plumes})$$

$$v_e = \beta w \quad (\text{bent-over plumes})$$

where β is larger than α .

Governing Equations:

Vertical Plumes

(i) Conservation of buoyancy

$$\frac{d\dot{B}}{dz} = -\zeta\dot{V} \quad (7.4 - 9)$$

(ii) Conservation of momentum

$$\frac{d\dot{M}}{dz} = \frac{\dot{B}}{w} \quad (7.4 - 10)$$

(iii) Entrainment hypothesis

$$\frac{d\dot{V}}{dz} = 2\alpha\hat{R}w = 2\alpha M^{\frac{1}{2}} \quad (7.4 - 11)$$

where $\alpha = 0.08$

Governing Equations:

Bent-Over Plumes

(i) Conservation of buoyancy

$$\frac{d\dot{B}}{dz} = -\frac{\zeta}{S}\dot{V} \quad (7.4 - 12)$$

with $S = 2.3$

(ii) Conservation of momentum

$$\frac{d\dot{M}}{dz} = \frac{\dot{B}}{w} \quad (7.4 - 13)$$

(iii) Entrainment hypothesis

$$\frac{d\dot{V}}{dz} = 2\beta\hat{R}u_\infty \quad (7.4 - 14)$$

or, if u_∞ is constant

$$\hat{R} = \beta z \quad (7.4 - 15)$$

where $\beta = 0.6$ for a buoyant plume and $\beta = 0.4 + 1.2(u_\infty/w_0)$ for a jet.

7.4.1 Near Source Rise

(Not Affected by Ambient Stability)

Typically ambient stability has little effect for dispersion times less than $\zeta^{-1/2}$ (between 10 and 100s) and ambient turbulence is not important for distances less than about ten stack heights (Hanna et al., 1982). For these short times the following results hold:

Vertical Plumes

$$\hat{R} = 0.6z, \quad w = 6.25 \frac{M^{1/2}}{z} \quad \left(t < \frac{M}{\dot{B}_0}\right) \quad (7.4 - 16)$$

$$\hat{R} = 0.15z, \quad w = 2.3 \left(\frac{\dot{B}_0}{z}\right)^{\frac{1}{3}} \quad \left(t > \frac{M}{\dot{B}_0}\right) \quad (7.4 - 17)$$

M/\dot{B}_0 is typically less than 10 s.

Bent-Over Plumes

The plume trajectory is given by

$$\Delta z = \left(\frac{3}{\beta_2^2} \frac{\dot{M}}{u_\infty^2} x + \frac{3}{2\beta_2^2} \frac{\dot{B}_0}{u_\infty^3} x^2 \right)^{\frac{1}{3}} \quad (t < t^*) \quad (7.4 - 18)$$

where $\beta_2 = 0.6$ and $\beta_1 = 0.4 + 1.2(u_\infty/w_0)$ and

$$\Delta z = 1.6 \frac{\dot{B}_0^{\frac{1}{3}}}{u_\infty} x^{\frac{2}{3}} \quad (t > t^*) \quad (7.4 - 19)$$

with $t^* = \dot{M}/\dot{B}_0$ which is typically of the order of 5s. The coefficient 1.6 is expected to be accurate within $\pm 40\%$ (Hanna et al., 1982).

7.4.2 Rise Limited by Ambient Stability (Stably Stratified Atmosphere)

Vertical Plumes

In a stably stratified atmosphere vertical plumes achieve an "equilibrium rise" Δz_{eq} that is equal to

$$\Delta z_{eq} = 2.44 \left(\frac{\dot{M}}{\zeta} \right)^{\frac{1}{4}} \quad (7.4 - 20)$$

if it is dominated by buoyancy, and

$$\Delta z_{eq} = 5.3 \frac{\dot{B}_0^{1/4}}{\zeta^{-3/8}} - 6R_0 \quad (7.4 - 21)$$

Bent-Over Plumes

The final rise of a buoyant plume is

$$\Delta h = 2.6 \left(\frac{\dot{B}_0}{u_\infty \zeta} \right)^{\frac{1}{3}} \quad (7.4 - 22)$$

The wind speed u_∞ in this formula is an average value between the heights h_s and $h_s + \Delta h$.

7.4.3 Penetration of an Elevated Inversion

An elevated inversion, approximated a jump $\Delta T^{(p)}$ in a constant potential temperature at a height Δz_{el} above the stack will be penetrated if the following conditions are met:

Vertical Buoyant Plume

$$\Delta z_{el} < 4.9 \dot{B}_0^{2/5} \left(\frac{g \Delta T^{(p)}}{T^{(p)}} \right)^{-\frac{3}{5}} \quad (7.4 - 23)$$

Vertical Momentum Plume

$$\Delta z_{el} < 6.2 \frac{\dot{B}_0 / M^{1/2}}{(g/T(p)) \Delta T(p)} \quad (7.4 - 24)$$

Buoyant Bent-Over Plume

$$\Delta z_{el} < 2.5 \left[\frac{\dot{B}_0}{u_\infty (g/T(p)) \Delta T(p)} \right]^{\frac{1}{2}} \quad (7.4 - 25)$$

(Bent-over jets have little ability to penetrate inversions.)

If the final plume rise (Δh is within a factor of 2 of the inversion height above the stack (Δz_{el}), only a fraction (P) of the plume will penetrate the inversion whereas a fraction $1 - P$ is reflected off the inversion and diffuses downward. Briggs (1975) suggested the formula $P = 1.5 - \Delta z_{el} / \Delta h$.

7.4.4 Rise Determined by Ambient Turbulence (Neutral and Unstable Atmospheres)

In this case plume rise comes to an end when the thermal phase of dispersion terminates in the breakup phase where ambient turbulence overcomes the internal turbulence of the plume. In Brigg's "breakup model" this occurs when the internal plume eddy dissipation, approximated by $1.5w^3/z$ equals the ambient eddy dissipation rate ϵ . The following simplified formulas for final plume rise are proposed:

Nearly Neutral Conditions

Buoyancy dominated plume

$$\Delta h = 1.54 \left(\frac{\dot{B}_0}{u_\infty u_*^2} \right)^{\frac{2}{3}} h_s^{\frac{1}{3}} \quad (7.4 - 26)$$

where u_* is the friction velocity.

Momentum dominated plume

$$\Delta h = 3D \left(\frac{w_0}{u_\infty} - 1 \right) \quad (7.4 - 27)$$

where D is the stack diameter

Convective Conditions

A tentative formula is

$$\Delta h = 3 \left(\frac{\dot{B}_0}{u_\infty} \right)^{\frac{3}{5}} \mathcal{K}^{-\frac{2}{5}} \quad (7.4 - 28)$$

where \mathcal{K} is the surface buoyancy flux defined as

$$\mathcal{K} = \frac{g}{T_\infty} \overline{w'T'_\infty}$$

(see, e.g., Hanna et al., 1982 – Section 1-4.4).

The formulas of Briggs are very similar to available results from dimensional analysis; as mentioned earlier, a summary of such results, together with of the empirical constants involved (according to various investigators) is given in List (1982).

7.5 THE PLUME RISE MODEL OF SCHATZMANN

(Schatzmann 1976, 1978, 1979ab; Schatzmann and Flick, 1977)

The approach of Schatzmann offers a formulation that is more comprehensive than those described in the previous section, as it takes into account the physics of the thermal phase of plume rise in much more detail. The resulting model, consists of a set of ordinary differential equations for mean centerline plume properties and other plume parameters, and has to be solved numerically. In its most general form it holds for arbitrary ambient stratifications of temperature as well as for large density differences between the emissions and the environment (*).

Thus, temperature inversions of any slope are taken naturally into account in the model calculations. A restriction is that the ambient wind velocity field is "locally" shear free; step changes are however allowed.

A rather general situation, involving an elevated temperature inversion layer, typical of the conditions that can be directly addressed by Schatzmann's basic model is depicted schematically in Figure 7-3.

Starting point of Schatzmann's models are the fundamental Eulerian transport equations for mass, momentum and conserved scalars (inert species concentrations and temperature) formulated in an orthogonal curvilinear coordinate system that is always tangential to the mean plume centerline, as it was first introduced by Hirst (1972). Reduction of this coupled set of partial differential equations (initially corresponding to random instantaneous quantities), and of the associated boundary conditions, to an initial value problem involving a set of ordinary differential equations for mean properties and parameters, proceeds through an elaborate sequence of mathe-

(*) The governing equations developed in this approach are reduced to a closed, solvable form without the introduction of the Boussinesq approximation. However, the currently available values of the empirical parameters appearing in the entrainment function have been determined, in both the cases of "dry" plumes (Schatzmann, 1979a) and "wet" plumes (Schatzmann and Policastro, 1984) only for conditions that are relevant to the Boussinesq approximation.

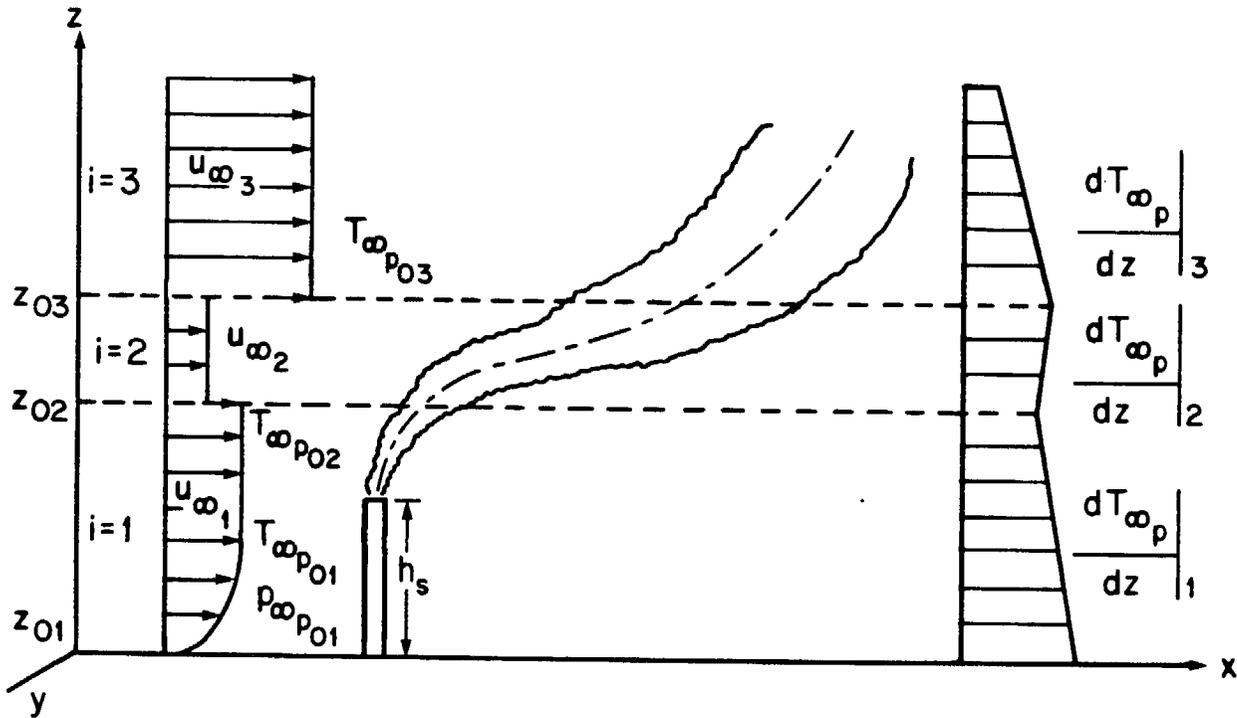


Figure 7-3
 Schematic Representation of Plume Rise
 in a Stratified Atmosphere,
 Typical of the Conditions Addressed by Schatzmann's Model
 (adapted from Schatzmann, 1977)

mathematical manipulations as well as of simplifying assumptions. Among these assumptions a most important one is that of self-similarity of the profiles of certain "mean excess" plume properties that finally allows integration of the governing equations into a simpler system. A complete exposition of the fundamental theory and the various assumptions involved in the aforementioned sequence can only be found scattered in a series of publications; the same holds for the determination of the empirical entrainment functions that provide closure to the turbulent transport equations and for applications and comparisons of the operational models with other approaches. For this reason, and to facilitate use of the existing models resulting from this approach (as well as in order to provide a basis for further work based on it) we present in Appendix A7.2 a concise but systematic derivation of the self-similarity ordinary differential equation system of Schatzmann (for both the two- and three-dimensional flow cases), listing in detail all the approximations involved. In the same appendix, as an additional step for providing a readily usable means for calculations, the "Schatzmann set" of equations is further reduced (from the coupled form in which it appears in the literature) into a scheme that is directly amenable to numerical treatment. All the necessary conditions and parameters for numerical application of a basic form of the model as well as a discussion relating this approach to other integral techniques can also be found there.

7.6 CONCLUSIONS

The subject of near-field plume dynamics (where plume momentum and buoyancy are significant) is a major area of atmospheric and in general fluid mechanical research and is covered by specialized monographs and an extensive literature (see, e.g., List, 1982; Briggs, 1984 for reviews). The present chapter (complemented by Appendices A7.1 to A7.4) attempted

- (i) a concise overview of the physical problems and the modeling approaches in this area, and
- (ii) an exposition of two alternatives (at different levels of complexity) that are appropriate for use with the TRPM model.

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APPENDIX A7.1

**A Brief Glossary of Terms
Describing Plume Behavior**

(For further information see Scorer, 1968, 1978)

Aerodynamic Downwash or Flagging: *A situation in which stack effluents are brought to ground level very close to the source and in undesirably high concentrations by being entrained into the eddies in the lee of the chimney.*

It occurs in the cases of strong winds or low source exit velocities as well as for very irregular airflows where eddies in the wake of the stack entrain some of the effluent. Rapid vertical movement occurs in the separated flow region behind the source and this usually communicates with larger similar regions behind industrial buildings which are close to the source. This results to downwash. Its avoidance is achieved through proper aerodynamic design and is usually carried out with aid of wind tunnel model studies of actual plants.

Bifurcation: *The phenomenon of a plume dividing into two distinct "branches" showing an overall cross section that resembles a strong cylindrical thermal.*

Bifurcation occurs in cases of strongly buoyant bent-over plumes due to the pattern of intense entrainment of clear air up the middle of their boundary. Coning plumes are the ones more likely to be bifurcated.

Coning: *The situation in which the plume has a steadily widening boundary in its atmospheric diffusion phase and does not exhibit significant sinuosities. It is characteristic of neutral atmospheric conditions.*

In the case of coning plumes dispersion is due mainly to eddies of size smaller than the local instantaneous plume width. Thus relative diffusion dominates meandering.

Downdraught: *A situation similar to Aerodynamic Downwash: Effluent is entrained from time to time in the lee of the building associated with the chimney; common in dwelling houses.*

Downwash: see *Aerodynamic Downwash.*

Fanning: *A situation of limited dispersion taking place mainly in the horizontal direction. It is typical*

of stable atmospheres.

A fanning plume achieves final rise (equilibrium level) very soon after emission. Significant concentration values are confined at this height.

Flagging: see *Aerodynamic Downwash*.

Fumigation: *A situation where the plume is dispersing downwards but not upwards. It occurs when the emission takes place below an inversion that is not penetrated.*

Lofting: *The inverse of Fumigation: The plume disperses only upwards. It occurs when the atmosphere is stable below the plume and neutral aloft.*

Lofting occurs when either the actual height of the stack is sufficient to place the effluent above the inversion (or the plume buoyancy strong enough to allow penetration of the inversion). Dominant mixing mechanism in the case of lofting plumes is the relative dispersion.

Looping: *The case where the plume exhibits large sinuosities compared to its instantaneous width. It occurs in unstable atmospheres.*

In the case of looping plumes the effect of meandering is most important. The averaged observed dispersion is predominantly caused by eddies with size large compared to that of the instantaneous plume.

Thermalling: *A phenomenon that takes place when thermal convection of the ambient is very strong (highly unstable atmospheres). The plume breaks up into distinct masses by the action of individual thermals of the atmosphere whose buoyancy dominates that of the plume. Another possibility is that masses from the chimney are directly entrained into natural thermals of the environment.*

References for Appendix A7.1

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APPENDIX A7.2

**Self Similarity Modeling
for the Thermal Phase of Plume Dispersion**

The evolution of a buoyant plume is governed by:

(i) the continuity equation of (total) mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (\text{A7.2-1})$$

(ii) the continuity equation of momentum

$$\rho \left[\frac{\partial \mathbf{u}}{\partial t} + \frac{1}{2} \nabla \mathbf{u} \mathbf{u} - \mathbf{u} \times (\nabla \times \mathbf{u}) \right] = (\rho - \rho_\infty) \mathbf{g} - \nabla p_d \quad (\text{A7.2-2})$$

(iii) the continuity equation for a passive scalar

$$\frac{\partial (\rho c)}{\partial t} + \mathbf{u} \cdot \nabla (\rho c) + \rho c \nabla \cdot \mathbf{u} = 0 \quad (\text{A7.2-3})$$

and (iv) the continuity equation of heat

$$\frac{\partial (\rho T)}{\partial t} + \mathbf{u} \cdot \nabla (\rho T) + \rho T \nabla \cdot \mathbf{u} = 0 \quad (\text{A7.2-3})$$

To describe plume rise the (s, r, ϕ) system of orthogonal curvilinear coordinates is employed (Figure A7.2-1). The base vectors $(\mathbf{i}_s, \mathbf{i}_r, \mathbf{i}_\phi)$ of this system are expressed in terms of the base vectors $(\mathbf{i}, \mathbf{j}, \mathbf{k})$ of the *locally fixed* Cartesian (x, y, z) system, with x in the direction of the mean ambient flow(*) and z opposite to the direction of the gravity force, as follows:

$$\mathbf{i}_s = \mathbf{i} \cos \theta_1 \cos \theta_2 + \mathbf{j} \sin \theta_1 \cos \theta_2 + \mathbf{k} \sin \theta_2$$

$$\begin{aligned} \mathbf{i}_r = & \mathbf{i} (-\sin \theta_1 \cos \phi - \cos \theta_1 \sin \theta_2 \sin \phi) \\ & + \mathbf{j} (\cos \theta_1 \cos \phi - \sin \theta_1 \sin \theta_2 \sin \phi) \\ & + \mathbf{k} \cos \theta_2 \sin \phi \end{aligned}$$

(*) Note that in Schatzmann's (1978, 1979ab) notation y is set parallel to the ambient flow; however here we follow the common convention that sets x parallel to the mean ambient flow.

$$\begin{aligned} \mathbf{i}_\phi &= \mathbf{i} (\sin \theta_1 \sin \phi - \cos \theta_1 \sin \theta_2 \cos \phi) \\ &+ \mathbf{j} (-\cos \theta_1 \sin \phi - \sin \theta_1 \sin \theta_2 \cos \phi) \\ &+ \mathbf{k} \cos \theta_2 \cos \phi \end{aligned}$$

The following analysis is restricted to the two-dimensional case $(\theta_1, \theta_2) = (0, \theta)$. Letting

$$\kappa = r \sin \phi \frac{d\theta}{ds}$$

the Lamé coefficients (scale factors) become

$$h_s = 1 - \kappa, \quad h_r = 1, \quad h_\phi = r$$

and the vector operations involved in the continuity equations are

$$\begin{aligned} \nabla a &= \frac{1}{1 - \kappa} \frac{\partial a}{\partial s} \mathbf{i}_s + \frac{\partial a}{\partial r} \mathbf{i}_r + \frac{1}{r} \frac{\partial a}{\partial \phi} \mathbf{i}_\phi \\ \nabla \cdot \mathbf{a} &= \frac{1}{1 - \kappa} \frac{\partial a_s}{\partial s} + \frac{1}{r} \frac{\partial (r a_r)}{\partial r} + \frac{1}{r} \frac{\partial a_\phi}{\partial \phi} - \frac{a_r \kappa}{1 - \kappa r} - \frac{a_\phi}{1 - \kappa r} \frac{1}{\partial \phi} \end{aligned}$$

and

$$\begin{aligned} \nabla \times \mathbf{a} &= \frac{1}{r} \left(\frac{\partial (r a_\phi)}{\partial r} - \frac{\partial a_r}{\partial \phi} \right) \mathbf{i}_s \\ &+ \left(\frac{1}{r} \frac{\partial a_s}{\partial \phi} - \frac{a_s}{1 - \kappa r} \frac{1}{\partial \phi} - \frac{1}{1 - \kappa} \frac{\partial a_\phi}{\partial s} \right) \mathbf{i}_r \\ &+ \left(\frac{1}{1 - \kappa} \frac{\partial a_r}{\partial s} - \frac{\partial a_s}{\partial r} + \frac{a_s \kappa}{1 - \kappa r} \right) \mathbf{i}_\phi \end{aligned}$$

In the above a is any scalar and $\mathbf{a} = a_s \mathbf{i}_s + a_r \mathbf{i}_r + a_\phi \mathbf{i}_\phi$ is any vector.

Substituting in the continuity equations for steady state conditions one has:

(i) total mass continuity equation

$$\begin{aligned} \rho \left[\frac{1}{1 - \kappa} \frac{\partial u}{\partial s} + \frac{1}{r} \frac{\partial}{\partial r} (rv) + \frac{1}{r} \frac{\partial}{\partial \phi} - \frac{v \kappa}{1 - \kappa r} - \frac{w}{1 - \kappa r} \frac{1}{\partial \phi} \right] \\ + \frac{u}{1 - \kappa} \frac{\partial \rho}{\partial s} + v \frac{\partial \rho}{\partial r} + \frac{w}{r} \frac{\partial \rho}{\partial \phi} = 0 \end{aligned} \quad (A7.2 - 4)$$

(ii) momentum equation in the s -direction

$$\begin{aligned} \rho \left\{ u \frac{\partial u}{\partial s} + v \frac{\partial u}{\partial r} (1 - \kappa) + \frac{1}{r} \left[w \frac{\partial u}{\partial \phi} (1 - \kappa) - uw \frac{\partial \kappa}{\partial \phi} - uv \kappa \right] \right\} = \\ = (1 - \kappa) (\rho_\infty - \rho) g \sin \theta - \frac{\partial p_d}{\partial s} \end{aligned} \quad (A7.2 - 5)$$

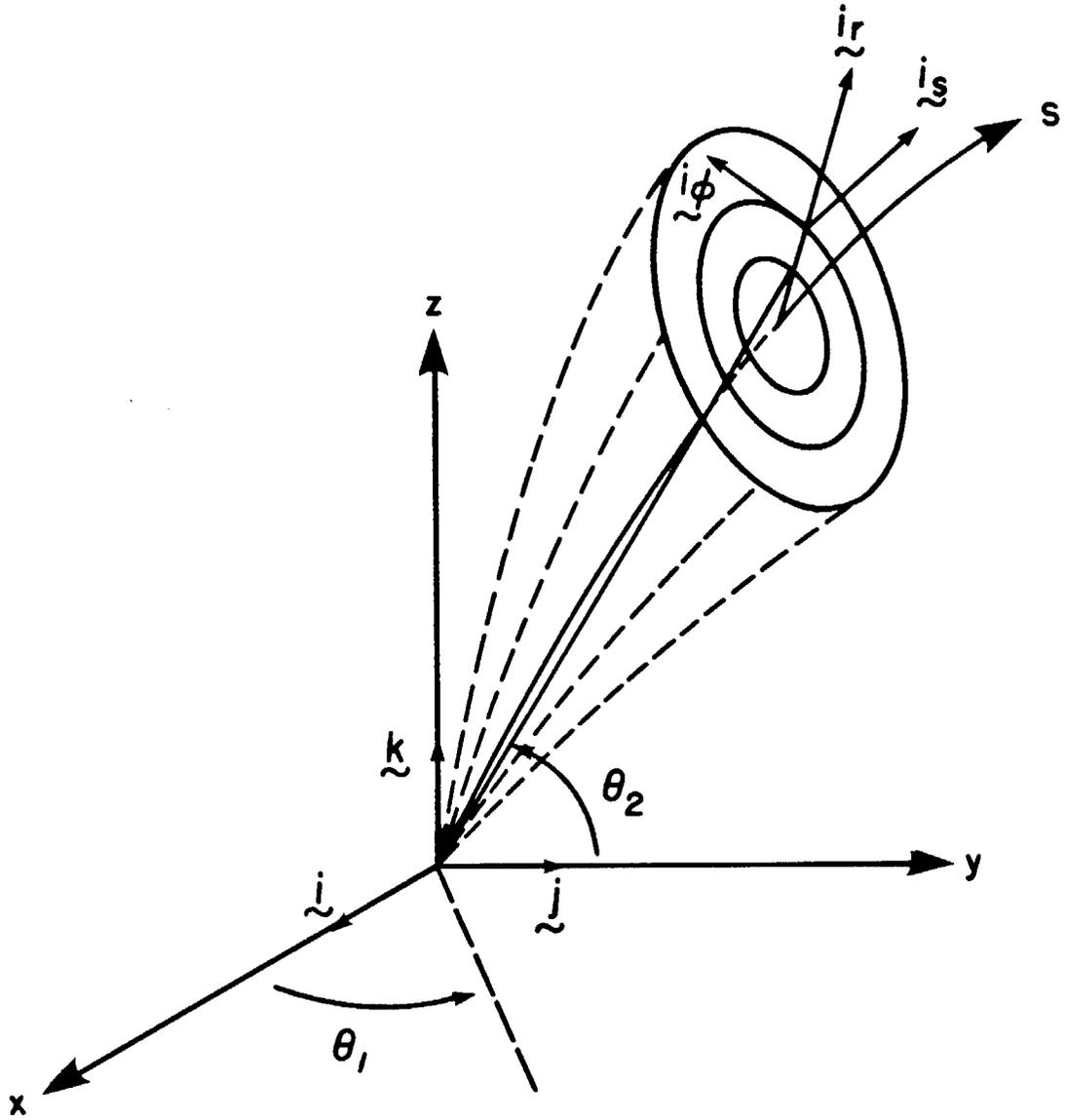


Figure A7.2-1
Coordinate System Employed in the Plume Rise Model

(iib) momentum equation in the y -direction

$$\begin{aligned}
& \rho \left\{ u \frac{\partial u}{\partial s} + v \frac{\partial u}{\partial r} (1 - \kappa) + \frac{1}{r} \left[w \frac{\partial u}{\partial \phi} (1 - \kappa) - uw \frac{\partial \kappa}{\partial \phi} - uv\kappa \right] \right\} \cos \theta \\
& - \rho \left\{ u \frac{\partial u}{\partial s} \sin \phi + v \frac{\partial v}{\partial r} (1 - \kappa) \sin \phi + u \frac{\partial w}{\partial s} \cos \phi + v \frac{\partial w}{\partial r} (1 - \kappa) \cos \phi \right. \\
& + \frac{1}{r} \left[w \frac{\partial v}{\partial \phi} (1 - \kappa) \sin \phi - w^2 (1 - \kappa) \sin \phi + u^2 \kappa \sin \phi + w \frac{\partial w}{\partial \phi} (1 - \kappa) \cos \phi \right. \\
& \left. \left. + uw (1 - \kappa) \cos \phi + u^2 \frac{\partial \kappa}{\partial \phi} \cos \phi \right] \right\} \sin \theta \\
& = -\frac{\partial p_d}{\partial s} \cos \theta + \frac{\partial p_d}{\partial r} (1 - \kappa) \sin \phi \sin \theta + \frac{1}{r} \frac{\partial p_d}{\partial \phi} (1 - \kappa) \cos \phi \cos \theta \tag{A7.2-5}
\end{aligned}$$

(iic) momentum equation in the z -direction

$$\begin{aligned}
& \rho \left\{ u \frac{\partial u}{\partial s} + v \frac{\partial u}{\partial r} (1 - \kappa) + \frac{1}{r} \left[w \frac{\partial u}{\partial \phi} (1 - \kappa) - uw \frac{\partial \kappa}{\partial \phi} - uv\kappa \right] \right\} \sin \theta \\
& \rho \left\{ u \frac{\partial v}{\partial s} \sin \phi + v \frac{\partial v}{\partial r} (1 - \kappa) \sin \phi + u \frac{\partial w}{\partial s} \cos \phi + v \frac{\partial w}{\partial r} (1 - \kappa) \cos \phi \right. \\
& \quad + \frac{1}{r} \left[w \frac{\partial v}{\partial \phi} (1 - \kappa) \sin \phi - w^2 (1 - \kappa) \sin \phi + u^2 \kappa \sin \phi \right. \\
& \quad \left. \left. + w \frac{\partial w}{\partial \phi} (1 - \kappa) \cos \phi + vw (1 - \kappa) \cos \phi + u^2 \frac{\partial \kappa}{\partial \phi} \cos \phi \right] \right\} \cos \theta \\
& = (\rho_\infty - \rho) g (1 - \kappa) - \frac{\partial p_d}{\partial s} \sin \theta - \frac{\partial p_d}{\partial r} (1 - \kappa) \sin \phi \cos \theta \\
& \quad - \frac{1}{r} \frac{\partial p_d}{\partial \phi} (1 - \kappa) \cos \phi \cos \theta \tag{A7.2-6}
\end{aligned}$$

(iii) continuity equation for concentration

$$u \frac{\partial c}{\partial s} + v \frac{\partial c}{\partial r} (1 - \kappa) + \frac{w}{r} \frac{\partial c}{\partial \phi} (1 - \kappa) = 0 \tag{A7.2-7}$$

(iv) continuity equation for temperature

$$u \frac{\partial T}{\partial s} + v \frac{\partial T}{\partial r} (1 - \kappa) + \frac{w}{r} \frac{\partial T}{\partial \phi} (1 - \kappa) = 0 \tag{A7.2-8}$$

Implicit in the derivation of the above steady state equations was the assumption of a divergence free flow (i.e. $\nabla \cdot \mathbf{u} = 0$).

Equations for Averages

It is assumed that

(1) Reynolds averaging (i.e. decomposition in an ensemble mean and a fluctuating part) is applicable for \mathbf{u} , ρ , p_d , c and T , and that time averages approximate ensemble means:

$$\mathbf{u} = \langle \mathbf{u} \rangle + \mathbf{u}' = \bar{\mathbf{u}} + \mathbf{u}', \quad \text{etc.}$$

and,

(2) the structure of turbulence is not influenced by the effects of compressibility (valid for flows with small Mach numbers) and therefore the terms containing density fluctuations ρ' are omitted.

Then, the mean quantities are decomposed into their background and excess components(*) (Figure A7.2-2):

$$\bar{u} = u_g + u_d$$

$$\bar{v} = v_g + v_d$$

$$\bar{w} = w_g + w_d$$

$$\bar{\rho} = \rho_\infty + \rho_d$$

$$\bar{T} = T_\infty + T_d$$

$$\bar{c} = c_\infty + c_d$$

where

$$u_g = u_\infty \cos \theta$$

$$v_g = -u_\infty \sin \theta \sin \phi$$

$$w_g = u_\infty \sin \theta \cos \phi$$

and the subscript ∞ denotes properties of the ambient flow field.

Introducing these assumptions in the governing equations one has:

(*) The excess components can be either positive or negative.

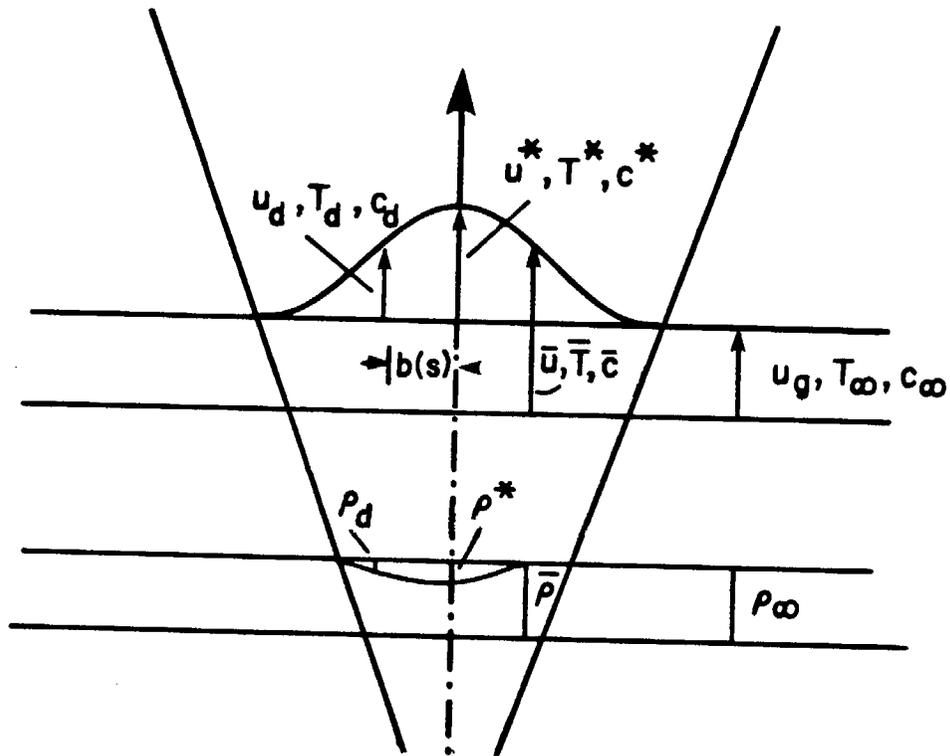


Figure A7.2-2
Definition of Background and Excess Quantities

(i) continuity of total mass

$$\begin{aligned}
& (\rho_\infty + \rho_d) \left\{ \frac{\partial(u_g + u_d)}{\partial s} + \frac{\partial v_d}{\partial r} (1 - \kappa) + \frac{1}{r} \left[\frac{\partial(w_g + w_d)}{\partial \phi} (1 - \kappa) + (v_g + v_d) (1 - 2\kappa) - (w_g + w_d) \frac{\partial \kappa}{\partial \phi} \right] \right\} \\
& + (u_g + u_d) \frac{\partial(\rho_\infty + \rho_d)}{\partial s} + (v_g + v_d) \frac{\partial \rho_d}{\partial r} (1 - \kappa) + \frac{1}{r} (w_g + w_d) \frac{\partial \rho_d}{\partial \phi} (1 - \kappa) = 0 \quad (A7.2-9)
\end{aligned}$$

(ii) momentum equation in the s -direction

$$\begin{aligned}
& (\rho_\infty + \rho_d) \left\{ (u_g + u_d) \frac{\partial(u_g + u_d)}{\partial s} + (v_g + v_d) \frac{\partial u_d}{\partial r} (1 - \kappa) \right. \\
& + \frac{1}{r} \left[(w_g + w_d) \frac{\partial u_d}{\partial \phi} (1 - \kappa) - (u_g + u_d) (w_g + w_d) \frac{\partial \kappa}{\partial \phi} - (u_g + u_d) (v_g + v_d) \kappa \right] \\
& + \frac{\partial \overline{u'^2}}{\partial s} + \frac{1}{r} \frac{\partial(r \overline{u'v'})}{\partial r} (1 - \kappa) + \frac{1}{r} \left[\frac{\partial \overline{u'w'}}{\partial \phi} (1 - \kappa) - 2\kappa \overline{u'v'} - 2\overline{u'w'} \frac{\partial \kappa}{\partial \phi} \right] \left. \right\} \\
& + \overline{u'^2} \frac{\partial(\rho_\infty + \rho_d)}{\partial s} + \overline{u'v'} \frac{\partial \rho_d}{\partial r} (1 - \kappa) + \frac{1}{r} \overline{u'w'} \frac{\partial \rho_d}{\partial \phi} (1 - \kappa) = \\
& = -\rho_d g (1 - \kappa) \sin \theta - \frac{\partial p_d}{\partial s} \quad (A7.2-10)
\end{aligned}$$

(iib) momentum equation in the y -direction

$$\begin{aligned}
& (\rho_\infty + \rho_d) \left\{ (u_g + u_d) \frac{\partial(u_g + u_d)}{\partial s} + (v_g + v_d) \frac{\partial u_d}{\partial r} (1 - \kappa) \right. \\
& + \frac{1}{r} \left[(w_g + w_d) \frac{\partial u_d}{\partial \phi} (1 - \kappa) - (u_g + u_d)(w_g + w_d) \frac{\partial \kappa}{\partial \phi} - (u_g + u_d)(v_g + v_d) \kappa \right] \\
& + \frac{\overline{\partial u'^2}}{\partial s} \frac{1}{r} \frac{\partial(r \overline{u'v'})}{\partial(1 - \kappa)} + \frac{1}{r} \left[\frac{\overline{\partial u'w'}}{\partial \phi} (1 - \kappa) - 2 \overline{u'v'} \kappa - 2 \overline{u'w'} \frac{\partial \kappa}{\partial \phi} \right] \\
& \left. \frac{1}{(\rho_\infty + \rho_d)} \left[\overline{u'^2} \frac{\partial(\rho_\infty + \rho_d)}{\partial s} + \overline{u'v'} \frac{\partial \rho_d}{\partial r} (1 - \kappa) + \overline{u'w'} \frac{1}{r} \frac{\partial \rho_d}{\partial \phi} (1 - \kappa) \right] \right\} \cos \theta \\
& - (\rho_\infty + \rho_d) \left\{ (u_g + u_d) \frac{\partial(v_g + v_d)}{\partial s} + (v_g + v_d) \frac{\partial v_d}{\partial r} (1 - \kappa) \right. \\
& + \frac{1}{r} \left[(w_g + w_d) \frac{\partial(v_g + v_d)}{\partial \phi} (1 - \kappa) - (w_g + w_d)^2 (1 - \kappa) + (u_g + u_d)^2 \kappa \right] \\
& + \frac{\overline{\partial u'v'}}{\partial s} + \frac{1}{r} \frac{\partial(r \overline{v'^2})}{\partial r} (1 - \kappa) + \frac{1}{r} \left[\frac{\overline{\partial v'w'}}{\partial \phi} (1 - \kappa) - \overline{w'^2} (1 - \kappa) + (\overline{u'^2} - \overline{v'^2}) \kappa - \overline{v'w'} \frac{\partial \kappa}{\partial \phi} \right] \\
& + \frac{1}{r} \left[\overline{u'v'} \frac{\partial(\rho_\infty + \rho_d)}{\partial s} + \overline{v'^2} \frac{\partial \rho_d}{\partial(1 - \kappa)} + \overline{v'w'} \frac{1}{r} \frac{\partial \rho_d}{\partial \phi} (1 - \kappa) \right] \left. \right\} \sin \phi \sin \theta \\
& - (\rho_\infty + \rho_d) \left\{ (u_g + u_d) \frac{\partial(w_g + w_d)}{\partial s} + (v_g + v_d) \frac{\partial w_d}{\partial r} (1 - \kappa) \right. \\
& + \frac{1}{r} \left[(w_g + w_d) \frac{\partial(w_g + w_d)}{\partial \phi} (1 - \kappa) + (v_g + v_d)(w_g + w_d) (1 - \kappa) + (u_g + u_d)^2 \frac{\partial \kappa}{\partial \phi} \right] \\
& + \frac{\overline{\partial u'w'}}{\partial s} + \frac{1}{r} \frac{\partial(r \overline{v'w'})}{\partial r} (1 - \kappa) + \frac{1}{r} \left[\frac{\overline{\partial w'^2}}{\partial \phi} (1 - \kappa) + \overline{v'w'} (1 - \kappa) + (\overline{u'^2} - \overline{w'^2}) \frac{\partial \kappa}{\partial \phi} - \overline{v'w'} \kappa \right] \\
& + \frac{1}{(\rho_\infty + \rho_d)} \left[\overline{v'w'} \frac{\partial(\rho_\infty + \rho_d)}{\partial s} + \overline{v'w'} \frac{\partial \rho_d}{\partial r} (1 - \kappa) + \overline{w'^2} \frac{1}{r} \frac{\partial \rho_d}{\partial \phi} (1 - \kappa) \right] \left. \right\} \cos \phi \sin \theta = \\
& = - \frac{\partial p_d}{\partial s} \cos \theta + \frac{\partial p_d}{\partial r} (1 - \kappa) \sin \phi \sin \theta + \frac{1}{r} \frac{\partial p_d}{\partial \phi} \cos \phi \sin \theta \tag{A7.2 - 11}
\end{aligned}$$

(iic) momentum equation in the z -direction

$$\begin{aligned}
& (\rho_\infty + \rho_d) \left\{ (u_g + u_d) \frac{\partial(u_g + u_d)}{\partial s} + (v_g + v_d) \frac{\partial u_d}{\partial r} (1 - \kappa) \right. \\
& + \frac{1}{r} \left[(w_g + w_d) \frac{\partial u_d}{\partial \phi} (1 - \kappa) - (u_g + u_d)(w_g + w_d) \frac{\partial \kappa}{\partial \phi} - (u_g + u_d)(v_g + v_d) \kappa \right] \\
& + \frac{\overline{u'^2}}{\partial s} \frac{1}{r} \frac{\partial(r \overline{u'v'})}{\partial r} + \frac{1}{r} \left[\frac{\partial \overline{u'w'}}{\partial \phi} (1 - \kappa) - 2 \overline{u'v'} \kappa - 2 \overline{u'w'} \frac{\partial \kappa}{\partial \phi} \right] \\
& \left. \frac{1}{(\rho_\infty + \rho_d)} \left[\overline{u'^2} \frac{\partial(\rho_\infty + \rho_d)}{\partial s} + \overline{u'v'} \frac{\partial \rho_d}{\partial r} (1 - \kappa) + \overline{u'w'} \frac{1}{r} \frac{\partial \rho_d}{\partial \phi} (1 - \kappa) \right] \right\} \sin \theta \\
& - (\rho_\infty + \rho_d) \left\{ (u_g + u_d) \frac{\partial(v_g + v_d)}{\partial s} + (v_g + v_d) \frac{\partial v_d}{\partial r} (1 - \kappa) \right. \\
& + \frac{1}{r} \left[(w_g + w_d) \frac{\partial(v_g + v_d)}{\partial \phi} (1 - \kappa) - (w_g + w_d)^2 (1 - \kappa) + (u_g + u_d)^2 \kappa \right] \\
& + \frac{\partial \overline{u'v'}}{\partial s} + \frac{1}{r} \frac{\partial(r \overline{v'^2})}{\partial r} (1 - \kappa) + \frac{1}{r} \left[\frac{\partial \overline{v'w'}}{\partial \phi} (1 - \kappa) - \overline{w'^2} (1 - \kappa) + (\overline{u'^2} - \overline{v'^2}) \kappa - \overline{v'w'} \frac{\partial \kappa}{\partial \phi} \right] \\
& + \frac{1}{r} \left[\overline{u'v'} \frac{\partial(\rho_\infty + \rho_d)}{\partial s} + \overline{v'^2} \frac{\partial \rho_d}{\partial r} (1 - \kappa) + \overline{v'w'} \frac{1}{r} \frac{\partial \rho_d}{\partial \phi} (1 - \kappa) \right] \left. \right\} \sin \phi \cos \theta \\
& - (\rho_\infty + \rho_d) \left\{ (u_g + u_d) \frac{\partial(w_g + w_d)}{\partial s} + (v_g + v_d) \frac{\partial w_d}{\partial r} (1 - \kappa) \right. \\
& + \frac{1}{r} \left[(w_g + w_d) \frac{\partial(w_g + w_d)}{\partial \phi} (1 - \kappa) + (v_g + v_d)(w_g + w_d) (1 - \kappa) + (u_g + u_d)^2 \frac{\partial \kappa}{\partial \phi} \right] \\
& + \frac{\partial \overline{u'w'}}{\partial s} + \frac{1}{r} \frac{\partial(r \overline{v'w'})}{\partial r} (1 - \kappa) + \frac{1}{r} \left[\frac{\partial \overline{w'^2}}{\partial \phi} (1 - \kappa) + \overline{v'w'} (1 - \kappa) + (\overline{u'^2} - \overline{w'^2}) \frac{\partial \kappa}{\partial \phi} - \overline{v'w'} \kappa \right] \\
& + \frac{1}{(\rho_\infty + \rho_d)} \left[\overline{v'w'} \frac{\partial(\rho_\infty + \rho_d)}{\partial s} + \overline{v'w'} \frac{\partial \rho_d}{\partial r} (1 - \kappa) + \overline{w'^2} \frac{1}{r} \frac{\partial \rho_d}{\partial \phi} (1 - \kappa) \right] \left. \right\} \cos \phi \cos \theta = \\
& = -\rho_d g (1 - \kappa) - \frac{\partial p_d}{\partial s} \sin \theta + \frac{\partial p_d}{\partial r} (1 - \kappa) \sin \phi \cos \theta + \frac{1}{r} \frac{\partial p_d}{\partial \phi} \cos \phi \cos \theta \quad (A7.2 - 12)
\end{aligned}$$

(iv) continuity equation for a scalar (c or T)

$$\begin{aligned}
& (u_g + u_d) \frac{\partial(c_\infty + c_d)}{\partial s} + (v_g + v_d) \frac{\partial c_d}{\partial r} (1 - \kappa) + (w_g + w_d) \frac{1}{r} \frac{\partial c_d}{\partial \phi} (1 - \kappa) \\
& + \frac{\partial \overline{u'c'}}{\partial s} + \frac{1}{r} \frac{\partial(r \overline{v'c'})}{\partial r} (1 - \kappa) + \frac{1}{r} \left[\frac{\partial \overline{w'c'}}{\partial \phi} (1 - \kappa) - \overline{v'c'} \kappa - \overline{w'c'} \frac{\partial \kappa}{\partial \phi} \right] \\
& \frac{1}{(\rho_\infty + \rho_d)} \left[\overline{u'c'} \frac{\partial(\rho_\infty + \rho_d)}{\partial s} + \overline{v'c'} \frac{\partial \rho_d}{\partial r} (1 - \kappa) + \overline{w'c'} \frac{1}{r} \frac{\partial \rho_d}{\partial \phi} (1 - \kappa) \right] = 0 \quad (A7.2 - 13)
\end{aligned}$$

Simplifications

(a) The Pressure Gradients

The difficulty of estimating the complex gradients of p_d is circumvented through the following method (Fan, 1967; Schatzmann, 1978): One arbitrarily sets

$$\frac{\partial p_d}{\partial s} = \frac{\partial p_d}{\partial r} = \frac{\partial p_d}{\partial \phi} = 0$$

and assigns the effects of these gradients to an empirical "drag function" for the pressure forces per plume segment ds after integration over the angular and radial directions

$$F_D(s) = c_D \frac{1}{2} \rho_\infty(s) (u_\infty \sin \theta)^2 2R(s) \quad (A7.2 - 14)$$

where c_D is an empirical coefficient.

(b) Shear Free Assumption

The ambient mean velocity is assumed uniform in the region of interest:

$$\frac{\partial u_\infty}{\partial x} = \frac{\partial u_\infty}{\partial y} = \frac{\partial u_\infty}{\partial z} = 0 \quad (A7.2 - 15)$$

Note however that the derivatives of the background velocity components u_g , v_g and w_g with respect to s and ϕ do not vanish.

(c) Axisymmetry Assumption

The plume flow is assumed to be axisymmetric during the phase under consideration with respect to the mean excess quantities and the turbulent correlations:

$$\begin{aligned} w_d &= 0 \\ \frac{\partial u_d}{\partial \phi} &= \frac{\partial v_d}{\partial \phi} = \frac{\partial w_d}{\partial \phi} = 0 \\ \frac{\partial \overline{u'^2}}{\partial \phi} &= \frac{\partial \overline{v'^2}}{\partial \phi} = \frac{\partial \overline{w'^2}}{\partial \phi} = \frac{\partial \overline{u'v'}}{\partial \phi} = \frac{\partial \overline{u'w'}}{\partial \phi} = \frac{\partial \overline{v'w'}}{\partial \phi} = 0 \\ \frac{\partial \overline{u'c'}}{\partial \phi} &= \frac{\partial \overline{v'c'}}{\partial \phi} = \frac{\partial \overline{w'c'}}{\partial \phi} = \frac{\partial \overline{u'T'}}{\partial \phi} = \frac{\partial \overline{v'T'}}{\partial \phi} = \frac{\partial \overline{w'T'}}{\partial \phi} = 0 \\ \frac{\partial \rho_d}{\partial \phi} &= \frac{\partial c_d}{\partial \phi} = \frac{\partial T_d}{\partial \phi} = 0 \end{aligned} \quad (A7.2 - 16)$$

The assumption of axisymmetry is expected to be valid for vertical plumes in calm environments. Deviations are expected for bent-over plumes in cross-flows, mainly due to the suppression of the counter rotating vortex pair; appropriate formulations for the entrainment function are used to compensate for this effect.

(d) Similarity Assumption

This is the most essential part of the general method described here. It allows separation of variables and subsequent integration in the radial direction that simplify the partial differential equations to ordinary differential equations. Self similarity of the profiles of mean quantities is in general expected to be valid after short distances ($s/D \simeq 6$) from the source (zone of flow establishment). Turbulent quantities in general assume fully developed profiles at larger distances, e.g. for $s/D > 50$ (Schatzmann, 1978). The following Gaussian forms are assigned to the mean excess quantities:

$$u_d(s, r) = u^*(s) \exp \left[- \left(\frac{r}{b(s)} \right)^2 \right] \quad (A7.2 - 17a)$$

$$T_d(s, r) = T^*(s) \exp \left[- \left(\frac{r}{\lambda b(s)} \right)^2 \right] \quad (A7.2 - 17b)$$

$$c_d(s, r) = c^*(s) \exp \left[- \left(\frac{r}{\lambda b(s)} \right)^2 \right] \quad (A7.2 - 17c)$$

$$\rho_d(s, r) = \rho^*(s) \exp \left[- \left(\frac{r}{\lambda b(s)} \right)^2 \right] \quad (A7.2 - 17d)$$

where the superscript * is used to denote centerline values and the "spreading ratio" λ (proportional to the turbulent Schmidt number) is introduced to account for the different rates of dispersion of momentum and of scalar quantities.

Radial Integration of the Continuity Equations

To integrate the continuity equations use is made of

- (i) Prandtl's boundary layer approximation, according to which the gradients in the direction of the flow are negligible compared to gradients perpendicular to this direction, and of
(ii) The boundary conditions

$$\begin{aligned} u_d = \rho_d = c_d = T_d = 0 \\ \overline{u'v'} = \overline{v'c'} = \overline{v'T'} = 0 \\ \overline{v'^2} = \overline{v_\infty'^2} \end{aligned} \quad (A7.2 - 18)$$

where the boundary is taken at $R = \sqrt{2}b$, or to $R \rightarrow \infty$ if the value of the quantity under consideration becomes zero at the nominal edge of the plume.

General Integral Forms of the Continuity Equations

Applying the Leibniz rule

$$\int_{\alpha(s)}^{\beta(s)} \frac{\partial [f(s, r)]}{\partial s} dr = \frac{d}{ds} \int_{\alpha(s)}^{\beta(s)} f(s, r) dr = \frac{d}{ds} [\beta(s)] f(s, \beta) + \frac{d}{ds} [\alpha(s)] f(s, \alpha)$$

and combining the y and z momentum equations to describe the variability of θ with s one obtains:

- (i) continuity equation for total mass

$$\frac{d}{ds} \int_0^\infty (\rho_\infty + \rho_d) u_d r dr + \frac{d}{ds} \left[u_g \int_0^\infty \rho_d r dr \right] + \frac{1}{2} R^2 u_g \frac{d\rho_\infty}{ds} = \rho_\infty E \quad (A7.2 - 19)$$

- (ii) momentum equation in the s direction

$$\frac{d}{ds} \int_0^\infty (\rho_\infty + \rho_d) u_d (u_g + u_d) r dr = - \int_0^\infty \rho_d g r dr \sin \theta \quad (A7.2 - 20)$$

- (iii) θ -equation

$$\frac{d\theta}{ds} = \frac{- \int_0^\infty \rho_d g r \cos \theta - \frac{1}{2} u_\infty \rho_\infty E \sin \theta - (\sqrt{2}/2\pi) c_D \rho_\infty b u_\infty^2 \sin^2 \theta}{\int_0^\infty (\rho_\infty + \rho_d) u_d (u_g + u_d) r dr - \rho_\infty b^2 v_\infty'^2} \quad (A7.2 - 21)$$

(iv) continuity equation for a scalar (c or T)

$$\frac{d}{ds} \int_0^\infty (\rho_\infty + \rho_d) c_d (u_g + u_d) r dr = -\frac{dc_\infty}{ds} \int_0^R (\rho_\infty + \rho_d) (u_g + u_d) r dr \quad (A7.2 - 22)$$

In the above equations E represents the volume of ambient air entrained into the plume due to turbulence and is defined by

$$E(s) = -\frac{1}{2\pi} \int_C v_d(R) dC = -v_d(R) R \quad (A7.2 - 23)$$

Integral Forms for Gaussian Profiles

Introducing the Gaussian self similarity profiles (A7.2 - 17a, b, c, d) the integration with respect to r can be performed, resulting in a set of five ordinary differential equations for seven unknowns $b(s)$, $\theta(s)$, $u^*(s)$, $\rho^*(s)$, $T^*(s)$, $c^*(s)$ and $E(s)$:

(i) continuity equation of total mass

$$\frac{d}{ds} (\rho_\infty u^* b^2) + 2b^2 u_\infty \cos \theta \frac{d\rho_\infty}{ds} + \lambda^2 \frac{d}{ds} (u_\infty \cos \theta \rho^* b^2) + \frac{\lambda^2}{\lambda^2 + 1} \frac{d}{ds} (\rho^* u^* b^2) = 2\rho_\infty E \quad (A2.7 - 24)$$

(ii) momentum equation in the s -direction

$$\frac{d}{ds} \left\{ u^* b^2 \left[u^* \left(\frac{1}{2} \rho_\infty + \frac{\lambda^2}{2\lambda^2 + 1} \rho^* \right) + u_\infty \cos \theta \left(\rho_\infty + \frac{\lambda^2}{\lambda^2 + 1} \rho^* \right) \right] \right\} = -\lambda^2 b^2 \rho^* g \sin \theta \quad (A7.2 - 25)$$

(iii) θ -equation

$$\frac{d\theta}{ds} = -\frac{\lambda^2 b^2 \rho^* g \cos \theta + u_\infty \rho_\infty E \sin \theta + (1/\pi) \sqrt{2} c_D \rho_\infty b u_\infty^2 \sin^2 \theta}{b^2 u^* \left(\frac{1}{2} \rho_\infty + \frac{\lambda^2}{2\lambda^2 + 1} \rho^* \right) + b^2 u^* u_\infty \cos \theta \left(\rho_\infty + \frac{\lambda^2}{\lambda^2 + 1} \rho^* \right) - 2b^2 \rho_\infty v_\infty^2} \quad (A7.2 - 26)$$

(iv) continuity equation for an inert scalar (concentration)

$$\begin{aligned} & \frac{d}{ds} \left[\lambda^2 b^2 \left(u_\infty \cos \theta \rho_\infty c^* + \frac{1}{2} u_\infty \cos \theta \rho^* c^* + \frac{1}{\lambda^2 + 1} u^* \rho_\infty c^* + \frac{1}{\lambda^2 + 2} u^* \rho^* c^* \right) \right] = \\ & = -\left(\frac{dc_\infty}{ds} \right) b^2 \left(2u_\infty \cos \theta \rho_\infty + \lambda^2 u_\infty \cos \theta \rho^* + u^* \rho_\infty + \frac{\lambda^2}{\lambda^2 + 1} u^* \rho^* \right) \end{aligned} \quad (A7.2 - 27)$$

(v) heat transport equation

$$\begin{aligned} & \frac{d}{ds} \left[\lambda^2 b^2 \left(u_\infty \cos \theta \rho_\infty T^* + \frac{1}{2} u_\infty \cos \theta \rho^* T^* + \frac{1}{\lambda^2 + 1} u^* \rho_\infty T^* + \frac{1}{\lambda^2 + 2} u^* \rho^* T^* \right) \right] = \\ & = -\left(\frac{dT_\infty}{ds} \right) b^2 \left(2u_\infty \cos \theta \rho_\infty + \lambda^2 u_\infty \cos \theta \rho^* + u^* \rho_\infty + \frac{\lambda^2}{\lambda^2 + 1} u^* \rho^* \right) \end{aligned} \quad (A7.2 - 28)$$

To obtain closure one must further provide:

- an equation of state $\rho = f_1(c, T)$,
- an entrainment hypothesis $E = f_2(b, \theta, u^*, \rho^*, c^*, T^*)$, and
- information concerning the variability of ambient properties T_∞ , c_∞ and $\overline{v'^2_\infty}$ with the streamwise coordinate s .

Finally the initial conditions (corresponding to the end of the zone of flow establishment $s = s_0$) $b(s_0)$, $\theta(s_0)$, $u^*(s_0)$, $T^*(s_0)$ and $c^*(s_0)$ must be specified for the numerical solution of the system (A7.2 – 23) to (A7.2 – 27). These subjects will be discussed in following sections. An extension of the basic system of equations to three dimensions is presented next.

Generalization to Three Dimensions

The general integral form of the continuity equations for total mass, conserved scalars (c and T), and momentum in the s -direction remain unchanged in the three-dimensional case, with u_g now given by

$$u_g = u_\infty \sin \theta_1 \cos \theta_2$$

The dependence of θ_2 and θ_1 on s is given by (Schatzmann, 1979b):

$$\frac{d\theta_2}{ds} = \frac{-\int_0^\infty \rho_d g r \cos \theta_2 - \frac{1}{2} u_\infty \rho_\infty E \sin \theta_1 \sin \theta_2 - (\sqrt{2}/2\pi) c_D \rho_\infty b u_\infty^2 \sin^2 \theta_1 \sin^2 \theta_2}{\int_0^\infty (\rho_\infty + \rho_d) u_d (u_g + u_d) r dr - \rho_\infty b^2 \overline{v'^2_\infty}} \quad (\text{A7.2} - 21')$$

and

$$\frac{d\theta_1}{ds} = \frac{\frac{1}{2} \rho_\infty E u_\infty \cos \theta_1 + (\sqrt{2}/2\pi) c_D \rho_\infty \beta u_\infty^2 \cos^2 \theta_1}{\int_0^\infty (\rho_\infty + \rho_d) u_d (u_g + u_d) r dr - \rho_\infty b^2 \overline{v'^2_\infty}} \quad (\text{A7.2} - 21'')$$

Introducing the Gaussian self similarity profiles (A7.2 – 17a, b, c, d) the integration with respect to r gives a set of six ordinary differential equations for eight unknowns $b(s)$, $\theta_1(s)$, $\theta_2(s)$, $u^*(s)$, $\rho^*(s)$, $T^*(s)$, $c^*(s)$ and $E(s)$:

(i) continuity equation of total mass

$$\begin{aligned} \frac{d}{ds} (\rho_\infty u^* b^2) + 2b^2 u_\infty \sin \theta_1 \cos \theta_2 \frac{d\rho_\infty}{ds} + \lambda^2 \frac{d}{ds} (u_\infty \sin \theta_1 \cos \theta_2 \rho^* b^2) \\ + \frac{\lambda^2}{\lambda^2 + 1} \frac{d}{ds} (\rho^* u^* b^2) = 2\rho_\infty E \end{aligned} \quad (\text{A2.7} - 24')$$

(ii) momentum equation in the s -direction

$$\frac{d}{ds} \left\{ u^* b^2 \left[u^* \left(\frac{1}{2} \rho_\infty + \frac{\lambda^2}{2\lambda^2 + 1} \rho^* \right) + u_\infty \sin \theta_1 \cos \theta_2 \left(\rho_\infty + \frac{\lambda^2}{\lambda^2 + 1} \rho^* \right) \right] \right\} = -\lambda^2 b^2 \rho^* g \sin \theta_2 \quad (A7.2 - 25')$$

(iii') θ_2 -equation

$$\frac{d\theta_2}{ds} = - \frac{\lambda^2 b^2 \rho^* g \cos \theta_2 + u_\infty \rho_\infty E \sin \theta_1 \cos \theta_2 + (\sqrt{2}/\pi) c_D \rho_\infty b u_\infty^2 \sin^2 \theta_1 \sin^2 \theta_2}{b^2 u^{*2} \left(\frac{1}{2} \rho_\infty + \frac{\lambda^2}{2\lambda^2 + 1} \rho^* \right) + b^2 u^{*2} u_\infty \sin \theta_1 \cos \theta_2 \left(\rho_\infty + \frac{\lambda^2}{\lambda^2 + 1} \rho^* \right) - 2b^2 \rho_\infty \overline{v'^2_\infty}} \quad (A7.2 - 26')$$

(iii'') θ_1 -equation

$$\frac{d\theta_1}{ds} = \frac{u_\infty \rho_\infty E \cos \theta_1 + (\sqrt{2}/\pi) c_D \rho_\infty b u_\infty^2 \cos^2 \theta_1}{b^2 u^{*2} \left(\frac{1}{2} \rho_\infty + \frac{\lambda^2}{2\lambda^2 + 1} \rho^* \right) + b^2 u^{*2} u_\infty \sin \theta_1 \cos \theta_2 \left(\rho_\infty + \frac{\lambda^2}{\lambda^2 + 1} \rho^* \right) - 2b^2 \rho_\infty \overline{v'^2_\infty}} \quad (A7.2 - 26'')$$

(iv) continuity equation for an inert scalar (concentration)

$$\begin{aligned} \frac{d}{ds} \left[\lambda^2 b^2 \left(u_\infty \sin \theta_1 \cos \theta_2 \rho_\infty c^* + \frac{1}{2} u_\infty \sin \theta_1 \cos \theta_2 \rho^* c^* + \frac{1}{\lambda^2 + 1} u^* \rho_\infty c^* + \frac{1}{\lambda^2 + 2} u^* \rho^* c^* \right) \right] = \\ = - \left(\frac{dc_\infty}{ds} \right) b^2 \left(2u_\infty \sin \theta_1 \cos \theta_2 \rho_\infty + \lambda^2 u_\infty \sin \theta_1 \cos \theta_2 \rho^* + u^* \rho_\infty + \frac{\lambda^2}{\lambda^2 + 1} u^* \rho^* \right) \quad (A7.2 - 27') \end{aligned}$$

(v) heat transport equation

$$\begin{aligned} \frac{d}{ds} \left[\lambda^2 b^2 \left(u_\infty \sin \theta_1 \cos \theta_2 \rho_\infty T^* + \frac{1}{2} u_\infty \sin \theta_1 \cos \theta_2 \rho^* T^* + \frac{1}{\lambda^2 + 1} u^* \rho_\infty T^* + \frac{1}{\lambda^2 + 2} u^* \rho^* T^* \right) \right] = \\ = - \left(\frac{dT_\infty}{ds} \right) b^2 \left(2u_\infty \sin \theta_1 \cos \theta_2 \rho_\infty + \lambda^2 u_\infty \sin \theta_1 \cos \theta_2 \rho^* + u^* \rho_\infty + \frac{\lambda^2}{\lambda^2 + 1} u^* \rho^* \right) \quad (A7.2 - 28') \end{aligned}$$

Closure Assumptions

Ambient Properties

A typical case of an atmosphere with three distinct layers (the middle one corresponding to an elevated inversion) is depicted schematically in Figure 7-3. Left subscripts (01), (02), and (03) refer to properties at the bases of these three layers; thus $(01)T_{p\infty}$ and $(01)\rho_{p\infty}$ are respectively the ground values of potential ambient temperature and density (all potential properties being denoted with the use of subscript p). Mean ambient velocities and turbulent intensities are typically assumed uniform inside each layer; the distributions of ambient temperature and concentration are assumed known. In the following discussion focuses on the two dimensional case $(\theta_1, \theta_2) = (0, \theta)$.

Equations of State

The (potential) local density defect at the plume axis is given by

$$\rho_p^* = -\rho_{p\infty} \frac{T_{p\infty}}{T_{p\infty} + T_p^*} \quad (\text{A7.2 - 29})$$

and its along axis variation will be

$$\begin{aligned} \frac{d}{ds} \rho_p^* = & - \left[\frac{\rho_{p\infty} + \rho_p^*}{T_{p\infty} + T_p} \right] \left[\frac{dT_p^*}{ds} + \frac{dT_{p\infty}}{dz} \sin \theta \right. \\ & \left. + \frac{\rho_{p\infty}}{T_{p\infty}} \frac{dT_{p\infty}}{dz} \sin \theta \right] \end{aligned} \quad (\text{A7.2 - 30})$$

The ambient potential density at height z from the ground is given by

$$\rho_{p\infty}(z) = (01)\rho_{p\infty} \frac{(01)T_{p\infty}}{T_{p\infty}(z)} \quad (\text{A7.2 - 31})$$

and will vary along the plume centerline according to

$$\frac{d}{ds} \rho_{p\infty} = -\frac{\rho_{p\infty}}{T_{p\infty}} \frac{dT_{p\infty}}{dz} \sin \theta \quad (\text{A7.2 - 32})$$

The potential temperature gradient is related to the actual atmospheric temperature gradient through

$$\frac{dT_{p\infty}}{dz} = \frac{T_{p\infty}(z)}{T_{\infty}(z)} \left(\frac{dT_{\infty}}{dz} + \frac{g}{C_P} \right)$$

and the quotient of the potential and actual temperature is

$$\frac{T_{p\infty}(z)}{T_{\infty}(z)} = \left(\frac{p_{p\infty}}{p_{\infty}(z)} \right)^{\frac{Rg}{C_P}}$$

Entrainment Hypothesis
(*Turbulent Transport Closure*)

Schatzmann (1979a) developed an entrainment function approximation starting from the integral equation for the mean kinetic energy of the plume

$$\begin{aligned} & \frac{d}{ds} \left[u^{*2} b^2 \left(u^* + \frac{3}{2} u_g \right) \right] = \\ & = -\frac{6}{\lambda^2 + 1} u^{*3} b \frac{\lambda^2 \sin \theta}{\mathcal{F}^2} - 24 u^* \frac{1}{b^2} \int_0^\infty \overline{u'v'} \exp \left(-\frac{r}{b} \right)^2 r^2 dr \end{aligned}$$

where \mathcal{F} is the local densimetric Froude number, defined by

$$\mathcal{F}^2 = \frac{u^{*2}}{\frac{\rho^*}{\rho_\infty} g b}$$

The cross correlation $\overline{u'v'}$ was expressed in terms of empirical function of $\eta = r/b$ and the Boussinesq approximation was invoked to obtain $\hat{E} = E/(u^*b)$ as

$$\hat{E} = \frac{\frac{d}{ds} b + \left(\frac{\lambda^2 - 2}{\lambda^2 + 1} - 12I_2 \right) \frac{\lambda^2 \sin \theta}{\mathcal{F}^2} + \left[\left(\frac{1}{4} - 12I_4 \right) \sin \theta \beta \frac{d}{ds} \theta + \frac{3}{2} \frac{d}{ds} b \right] \frac{u_\infty}{u^*}}{1 + 12I_1 + (1 + 24I_3) \frac{u_\infty}{u^*} \cos \theta} \quad (\text{A7.2 - 33})$$

where the I_i 's are dimensionless integration constants. Schatzmann (1979a) considered limiting cases of the above expression, introduced an additional entrainment term to compensate for the suppression of the action of the vortex pair by the assumption of axisymmetry, and used available experimental data bases and numerical experiments to fit parameters and to simplify equations. Thus he finally obtained the semi-empirical expression

$$\hat{E} = \frac{A_1 + A_2 \frac{\sin \theta}{\mathcal{F}^2}}{1 + 0.5 A_3 \frac{u_\infty}{u^*} \cos \theta} \left(1 + A_4 \frac{u_\infty}{u^*} \sin \theta \right) + A_5 \frac{L_\infty}{b} \frac{\sqrt{v_\infty'^2}}{u^*} \quad (\text{A7.2 - 34})$$

The factor containing the A_4 parameter is the term accounting for the additional entrainment mentioned above; the last term represents the interaction of the energy-containing eddies of atmospheric turbulence with the large scale structure of the plume turbulence (L_∞ stands for the value of an appropriate macroscale of these energy containing eddies) and will be significant only in some relatively far-field phase of dispersion. For the near field a reasonable approximation is $A_5 = 0$. The empirical constants A_1 to A_4 suggested by Schatzmann (1979a) are

$$A_1 = 0.057$$

$$A_2 = 0.67$$

$$A_3 = 10.0$$

$$A_4 = 2.0$$

**Preparation of the Continuity Equations
for Numerical Solution**

Equations (A7.2-23) to (A7.2-29), (A7.2-31) and (A7.2-34) provide a closed system for the evaluation of the eight unknowns $b(s)$, $\theta(s)$, $u^*(s)$, $T^*(s)$, $c^*(s)$, $\rho^*(s)$, $\rho_\infty(s)$ and $\hat{E}(s)$. To solve this system numerically it is transformed in the final form

$$\frac{dq}{ds} = f_i(s; q_1, q_2, \dots, q_n); \quad i = 1, 2, \dots, n$$

which (after non-dimensionalization) is ready for numerical solution.

First the above equations are transformed into explicit equations with respect to the unknown variables and their gradients. It can be shown that the variation of u^* , b and ρ^* with s does not depend on the gradients of T^* and neither on c^* or its gradients. Thus, finally, one has to solve simultaneously the system

$$\mathbf{A} \frac{d\mathbf{q}}{ds} = \mathbf{f}$$

and the equation

$$\frac{dT^*}{ds} = \frac{1}{a_{41}} \left(\frac{d\rho^*}{ds} - a_{42} \right)$$

where

$$\mathbf{q} = \left(\frac{du^*}{ds} \quad \frac{db}{ds} \quad \frac{d\rho^*}{ds} \right)^T$$

$$\mathbf{f} = (f_1 \quad f_2 \quad f_3)^T$$

and

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

with

$$a_{11} = \frac{b}{u^*} \left(1 + \lambda^2 \frac{\rho^*}{\rho_\infty} \right)$$

$$a_{12} = 2 \left(1 + \frac{\lambda^2}{\lambda^2 + 1} \frac{\rho^*}{\rho_\infty} + \lambda^2 \frac{\rho^*}{\rho_\infty} \frac{u_\infty}{u^*} \cos \theta \right)$$

$$a_{13} = \frac{\lambda^2 b}{\rho_\infty} \left(\frac{u_\infty}{u^*} \cos \theta + \frac{1}{\lambda^2 + 1} \right)$$

$$a_{21} = \frac{b}{u^*} \left(1 + \frac{u_\infty}{u^*} \cos \theta + \frac{2\lambda^2}{2\lambda^2 + 1} \frac{\rho^*}{\rho_\infty} + \frac{\lambda^2}{\lambda^2 + 1} \frac{\rho^*}{\rho_\infty} \frac{u_\infty}{u^*} \cos \theta \right)$$

$$a_{22} = 1 + 2 \frac{u_\infty}{u^*} \cos \theta + \frac{2\lambda^2}{1\lambda^2 + 1} \frac{\rho^*}{\rho_\infty} + \frac{2\lambda^2}{\lambda^2 + 1} \frac{\rho^*}{\rho_\infty} \cos \theta$$

$$\begin{aligned}
a_{23} &= \frac{b}{\rho_{\infty}} \left(\frac{\lambda^2}{2\lambda^2 + 1} \frac{\lambda^2}{\lambda^2 + 1} \frac{u_{\infty}}{u^*} \cos \theta \right) \\
a_{31} &= -\frac{T^*}{u^*} \left(\frac{1}{\lambda^2 + 1} + \frac{1}{\lambda^2 + 2} \frac{\rho^*}{\rho_{\infty}} \right) \\
a_{32} &= -\frac{T^*}{u^*} \left[2 \left(\frac{1}{\lambda^2 + 1} + \frac{u_{\infty}}{u^*} \cos \theta \right) + \left(\frac{2}{\lambda^2 + 2} + \frac{u_{\infty}}{u^*} \cos \theta \right) \frac{\rho^*}{\rho_{\infty}} \right] \\
a_{33} &= -\frac{T^*}{2\rho_{\infty}} \left(\frac{2}{\lambda^2 + 2} + \frac{u_{\infty}}{u^*} \cos \theta \right) \\
&\quad + \frac{\frac{1}{\lambda^2 + 1} + \frac{u_{\infty}}{u^*} \cos \theta + \frac{1}{2} \left(\frac{2}{\lambda^2 + 2} + \frac{u_{\infty}}{u^*} \cos \theta \right) \frac{\rho^*}{\rho_{\infty}}}{\frac{\rho_{\infty}}{T_{\infty}} \left(\frac{T_{\infty}}{T_{\infty} + T^*} \right) \left(1 + \frac{\rho^*}{\rho_{\infty}} \right)} \\
f_1 &= \frac{2\hat{E}}{u^*b} - \left(1 + 2 \frac{u_{\infty}}{u^*} \cos \theta \right) \frac{b}{\rho_{\infty}} \frac{d\rho_{\infty}}{ds} + \lambda^2 \frac{\rho^*}{\rho_{\infty}} \frac{u_{\infty}}{u^*} \sin \theta b \frac{d\theta}{ds} \\
f_2 &= -\lambda^2 \frac{\rho^*}{\rho_{\infty}} gb \frac{1}{u^{*2}} \sin \theta - \frac{1}{2} \left(1 + 2 \frac{u_{\infty}}{u^*} \cos \theta \right) \frac{b}{\rho_{\infty}} \frac{d\rho_{\infty}}{ds} + \left(1 + \frac{\lambda^2}{\lambda^2 + 1} \frac{\rho^*}{\rho_{\infty}} \right) \frac{u_{\infty}}{u^*} b \sin \theta \frac{d\theta}{ds} \\
f_3 &= \frac{T_{\infty}}{\rho_{\infty}} \left(\frac{1}{\lambda^2 + 1} + \frac{u_{\infty}}{u^*} \cos \theta \right) \frac{d\rho_{\infty}}{ds} - T^* \frac{u_{\infty}}{u^*} \sin \theta \left(1 + \frac{1}{2} \frac{\rho^*}{\rho_{\infty}} \right) \frac{d\theta}{ds} \\
&\quad - \frac{\frac{1}{\lambda^2 + 1} + \frac{u_{\infty}}{u^*} \cos \theta + \frac{1}{2} \left(\frac{2}{\lambda^2 + 2} + \frac{u_{\infty}}{u^*} \cos \theta \right) \frac{\rho^*}{\rho_{\infty}}}{\frac{\rho_{\infty}}{T_{\infty}} \left(\frac{T_{\infty}}{T_{\infty} + T^*} \right) \left(1 + \frac{\rho^*}{\rho_{\infty}} \right)} \left[\frac{b}{T_{\infty} + T^*} \left(1 + \frac{\rho^*}{\rho_{\infty}} \right) \frac{dT_{\infty}}{dz} \sin \theta + \frac{b}{\rho_{\infty}} \frac{d\rho_{\infty}}{ds} \right] \\
a_{41} &= -\rho_{\infty} \frac{1}{T_{\infty} + T^*} \left(1 + \frac{\rho^*}{\rho_{\infty}} \right) \\
a_{42} &= - \left[\frac{b}{T_{\infty} + T^*} \left(1 + \frac{\rho^*}{\rho_{\infty}} \right) \frac{dT_{\infty}}{dz} \sin \theta + \frac{b}{\rho_{\infty}} \frac{d\rho_{\infty}}{ds} \right]
\end{aligned}$$

Finally, c^* is calculated from

$$\frac{dc^*}{ds} = \frac{1}{a_{51}} \left(a_{52} \frac{dc_{\infty}}{ds} + a_{53} \frac{du^*}{ds} + a_{54} \frac{db}{ds} + a_{55} \frac{d\theta}{ds} + a_{56} \frac{d\rho^*}{ds} + a_{57} \frac{d\rho_{\infty}}{ds} \right)$$

where

$$\begin{aligned}
a_{51} &= \frac{1}{\lambda^2 + 1} + \frac{u_{\infty}}{u^*} \cos \theta + \frac{1}{2} \left(\frac{2}{\lambda^2 + 2} + \frac{u_{\infty}}{u^*} \cos \theta \right) \frac{\rho^*}{\rho_{\infty}} \\
a_{52} &= - \left[\frac{1}{\lambda^2} \left(1 + 2 \frac{u_{\infty}}{u^*} \cos \theta \right) + \left(\frac{1}{\lambda^2 + 1} + \frac{u_{\infty}}{u^*} \cos \theta \right) \frac{\rho^*}{\rho_{\infty}} \right] \\
a_{53} &= -\frac{c^*}{u^*} \left(\frac{1}{\lambda^2 + 1} + \frac{1}{\lambda^2 + 2} \frac{\rho^*}{\rho_{\infty}} \right) \\
a_{54} &= -\frac{c^*}{b} \left[2 \left(\frac{1}{\lambda^2 + 1} + \frac{u_{\infty}}{u^*} \cos \theta \right) + \left(\frac{2}{\lambda^2 + 2} + \frac{u_{\infty}}{u^*} \cos \theta \right) \frac{\rho^*}{\rho_{\infty}} \right]
\end{aligned}$$

$$a_{55} = c^* \frac{u_\infty}{u^*} \sin \theta \left(1 + \frac{1}{2} \frac{\rho^*}{\rho_\infty} \right)$$

$$a_{56} = -\frac{c^*}{1\rho_\infty} \left(\frac{2}{\lambda^2 + 2} + \frac{u_\infty}{u^*} \cos \theta \right)$$

$$a_{57} = -\frac{c^*}{\rho_\infty} \left(\frac{1}{\lambda^2 + 1} + \frac{u_\infty}{u^*} \cos \theta \right)$$

(Note: in the above equations temperatures and densities represent potential quantities; the subscript p has been neglected for simplicity.)

*Position
of the Mean Plume Centerline*

Finally, the position (x, z) of the plume centerline in fixed Cartesian coordinates, for a given s , is determined through the parametric equations

$$x(s) = \int_{s_0}^s \cos \theta(s) ds$$

$$z(s) = \int_{s_0}^s \sin \theta(s) ds$$

which must be integrated numerically.

Initial Conditions

Schatzmann (1976) and Schatzmann and Flick (1977) suggested the following relationships (initial conditions) between centerline quantities at the end of the zone of flow establishment (subscript 0) and their corresponding values at the source (subscript j):

$$u_0^* = u_j^* \quad (A7.2 - 35)$$

$$\theta_0 = \theta_j \left(1 - 1.22 \frac{u_\infty}{u_j^*} \right) \quad \text{for } \theta_j = 90^\circ, \frac{u_\infty}{u_j^*} < 0.7 \quad (A7.2 - 36a)$$

$$\theta_0 = 0.167\theta_j \quad \text{for } \theta_j = 90^\circ, \frac{u_\infty}{u_j^*} \geq 0.7 \quad (A7.2 - 36b)$$

$$b_0 = D_s \sqrt{\frac{1}{2} \frac{(u_j^* + u_\infty \cos \theta_0)}{(u_j^* + 2u_\infty \cos \theta_0)}} \quad (A7.2 - 37)$$

where D_s is the source diameter,

$$T_0^* = T_j^* \frac{\lambda^2 + 1}{2\lambda^2} \frac{u_j^* + 2u_\infty \cos \theta_0}{u_j^* + (\lambda^2 + 1) u_\infty \cos \theta_0} \quad (A7.2 - 38)$$

$$c_0^* = c_j^* \frac{\lambda^2 + 1}{2\lambda^2} \frac{u_j^* + 2u_\infty \cos \theta_0}{u_j^* + (\lambda^2 + 1) u_\infty \cos \theta_0} \quad (A7.2 - 39)$$

and

$$s_0 = 0 \quad \text{if } \frac{u_\infty}{u_j^*} > 0.3 \quad (A7.2 - 40a)$$

$$s_0 = D_s \left(6.2 - 20 \frac{u_\infty}{u_j^*} \right) \quad \text{if } \frac{u_\infty}{u_j^*} < 0.3 \quad (A7.2 - 40b)$$

**Simplifications
through the Boussinesq Approximation**

Introduction of the Boussinesq approximation in the continuity equations (A7.2-24) to (A7.2-28) gives the following reduced forms

(i) continuity equation of total mass

$$\frac{d}{ds} (u^* b^2) = 2E \quad (A7.2 - 24a)$$

(ii) momentum equation in the s -direction

$$\frac{d}{ds} [u^* b^2 (u^* + 2u_\infty \cos \theta)] = -\lambda^2 b^2 \frac{\rho^*}{\rho_0} g \sin \theta \quad (A7.2 - 25a)$$

(iii) θ -equation

$$\frac{d\theta}{ds} = -2 \left[\frac{\lambda^2 b^2 \frac{\rho^*}{\rho_0} g \cos \theta + u_\infty E \sin \theta + (\sqrt{21}/\pi) c_D b u_\infty^2 \sin^2 \theta}{b^2 u^* (u^* + 2u_\infty \cos \theta) - 4b^2 \overline{v'^2}} \right] \quad (A7.2 - 26a)$$

(iv) continuity equation for an inert scalar (concentration)

$$\frac{d}{ds} \{b^2 c^* [u^* (\lambda^2 + 1) u_\infty \cos \theta]\} = - \left(\frac{\lambda^2 + 1}{\lambda^2} \right) \frac{dc_\infty}{ds} [b^2 (u^* + 2u_\infty \cos \theta)] \quad (A7.2 - 27a)$$

(v) heat transport equation

$$\frac{d}{ds} \{b^2 T^* [u^* (\lambda^2 + 1) u_\infty \cos \theta]\} = - \left(\frac{\lambda^2 + 1}{\lambda^2} \right) \frac{dT_\infty}{ds} [b^2 (u^* + 2u_\infty \cos \theta)] \quad (A7.2 - 28a)$$

Comments

Using the Boussinesq approximation, and assuming the ambient fluid to be free of turbulence and of density stratification, the equations of Schatzmann can be compared directly with those published by Abraham (1971), Chan and Kennedy (1972), Fan (1967), Hoult, Fay and Forney (1969), Keffer and Baines (1963), Hirst (1972) and others, who also applied the integral method. Comparison, however, shows that the equations of these authors are not in general identical with the formulas presented here. According to Schatzmann (1978, 1979a) the differences are due to the following:

- (i) Hirst, in deriving his mathematical model, applied the Leibniz rule (for the differentiation of an integral with variable limits) in an erroneous way.
- (ii) All other above-mentioned investigators, who basically followed the classical vertical plume analysis of Morton, Taylor and Turner (1956) for plumes in a cross-flow, balanced the fluxes through the control surface incompletely.

Both errors lead to the same results. For example, the integral form of the continuity equation of mass becomes

$$\frac{d}{ds} \int_0^R (u_g + u_d) r dr = \frac{1}{2} \frac{d}{ds} [b^2 (u^* + 2u_\infty \cos \theta)] = E \quad (A7.2 - 41)$$

instead of the correct relation

$$\frac{d}{ds} \int_0^R u_d r dr = \frac{1}{2} \frac{d}{ds} (b^2 u^*) = E \quad (A7.2 - 41a)$$

Figure A7.2-3 shows the difference between (A7.2-41) and (A7.41a) for a plume in a co-flowing stream. The flux of ambient fluid $E = -v_d(R) R = -v_d(R_\kappa) R_\kappa$, which flows into the control volume due to turbulent fluctuations inside the plume, only increases the excess velocity section, marked by *A*. What equation (A7.2-41) suggests is that Section *B* of the velocity profile would also be enlarged by the entrainment process, which is obviously not correct. The same error occurs by using a cone-shaped control volume, if the coaxial mass flux through the circumferential area is not taken into account. Uniquely in the special case $u_\infty = 0$ both equations are identical.

The momentum equations developed by Schatzmann also differ from those developed previously for similar reasons: When Hirst's or Fan's momentum equations are applied to a momentum plume in a co-flowing stream they fail to conserve the excess momentum flux. Nevertheless, Hirst, Fan etc. obtained reasonable agreement between theory and development. This is explained according to Schatzmann (1978, 1979a) by the empirical nature of the entrainment hypothesis. This empirical input to the mathematical model, together with skillful data fitting in order to fix the constants, may explain why models with internal inconsistencies managed to achieve the aforementioned agreement.

The scheme that was summarized in this appendix was tested by Schatzmann and his co-workers against approximately eighty different sets of data, from both laboratory and field measurements, with very satisfactory results; some representative comparisons are reproduced here, in Figures A7.2-4 and A7.2-5 (see Schatzmann, 1979a, for details). An extension of this scheme to "moist" plumes has also been developed (Schatzmann and Policastro, 1984).

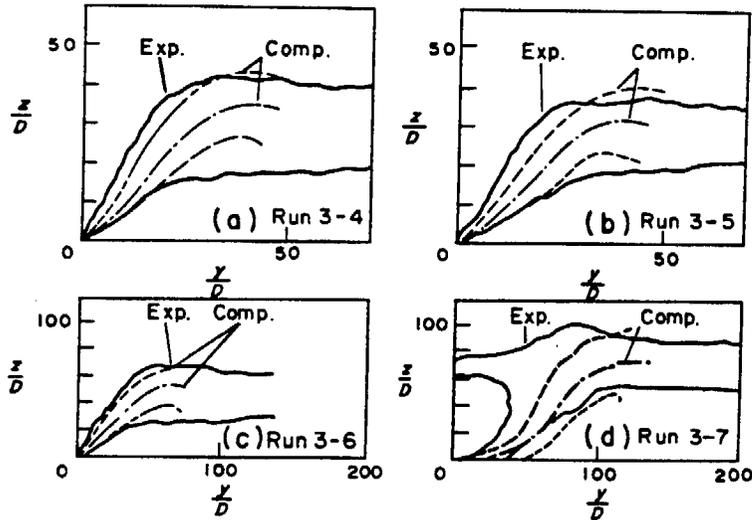


Figure A7.2-4

Buoyant Plumes Discharged at Various Angles into a Stably Stratified Ambient.

Calculations from the Model of Schatzmann

Compared with Laboratory Data of Fan (1967)

(D : plume diameter; z : height from source; y : downstream distance)

(Source: Schatzmann, 1979a)

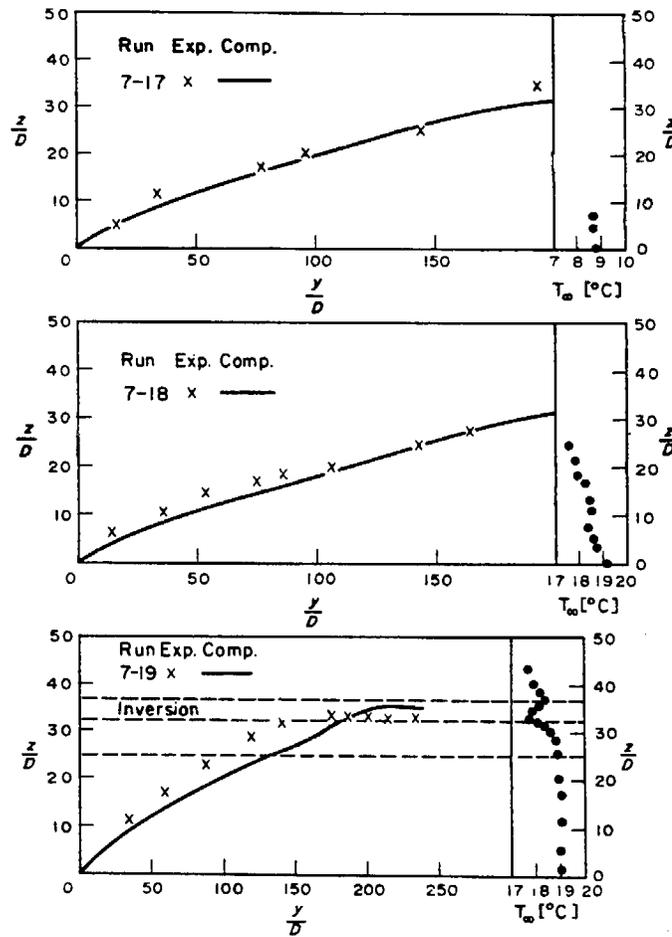


Figure A7.2-5

Trajectories of Buoyant Plumes Discharged into Stratified Ambient Cross-Winds
with and without Temperature Inversion.

Calculations from the Model of Schatzmann

Compared with Field Data of Slawson and Csanady(1971)

(D : plume diameter; z : height from source; y : downstream distance)

(Source: Schatzmann, 1979a)

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APPENDIX A7.3

**The Internal Structure
of Buoyant Plumes in the Near Field
(Briggs, 1975)**

The properties of the internal structure of a rising plume can be of great interest since they determine mixing in the early stages of plume evolution. Some of the details of structure within a rising plume have been studied through laboratory experiments on horizontal thermals, which closely resemble bent-over plumes in cross-section. Based on available data from the streamline measurements of Richards (1963), the vorticity measurements of Tsang (1971), and the concentration measurements in a bent-over laboratory plume of Fan (1967) Briggs (1975) summarized the following conclusions about bent over plume structure (see Figure A7.3-1):

First, the measurements show that almost all of the entrainment occurs across the top part of the plume. Part of the rise is due to mean vertical motion, but basically it is due to turbulent entrainment (almost by a factor of 75%). A secondary zone of entrainment exists under the middle of the plume, where induced velocities are very much higher than anywhere else around the boundary. This may be due to the low hydrostatic pressure underneath the buoyant fluid, and might not be so pronounced in a bent-over jet. Turbulence is generated here due to a strong shear of the vertical motion, evidenced by closeness of the streamlines near the center and by the flanking areas of high vorticity. This turbulence is advected upward through the middle of the plume, where it bisects the concentration maximum. The intensity it develops as it spreads across the top of the plume is partly due to horizontal divergence, which stretches vortex filaments in a direction almost tangent to the upper surface, thereby intensifying turbulent velocities perpendicular to the surface. In a buoyant plume, turbulence is also generated due to unstable internal density stratification above the concentration maxima, which are density minima. The marked decrease in turbulent entrainment around the lower flanks of the plume is probably due to the small amount of shear with the ambient at these points (it appears that the plume almost "rolls" up an imaginary inclined plane tangent to these points), and also is due to the proximity of the larger regions of high mean vorticity.

For a plume entering a fluid having ambient turbulence, Briggs (1975) suggests that it is likely that the ambient turbulence must first mix its way into the plume by means of a "frontside attack." Also, there is a strong convergence of ambient streamlines under the plume, which tends to relax

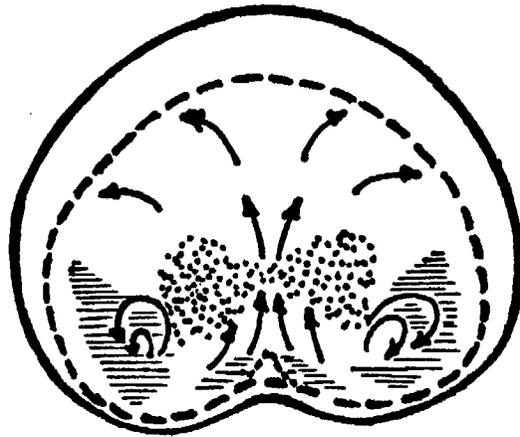


Figure A7.3-1

Structure of a Bent Over Buoyant Plume

(adapted from Briggs, 1975)

Dashed and solid lines show the shape of a plume cross section at two successive times. Arrows show streamlines of mean motion. Horizontal hatching shows high vorticity regions. Dotted areas correspond to concentration maxima.

turbulence velocities that are perpendicular to the surface.

If this analysis is true, and ambient turbulence must first break into the plume in the frontal region, then its effectiveness will be delayed due to the relatively high plume turbulence in this same region. In effect, the plume will at first advance into the ambient faster than the ambient can advance into the plume. Once the balance is reversed, as the plume motions weaken, it is quite easy to conceive that the ambient turbulence may move downward and destroy the stable double vortex structure from within, making the plume vulnerable from all sides. In other words, plume "breakup" may occur relatively quickly, as has been suggested by Csanady (1973) and others and this must be taken into account for the correct formulation of entrainment hypotheses.

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