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Some Properties of the Langevin Model for Dispersion

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SOME PROPERTIES OF THE LANGEVIN MODEL FOR DISPERSION

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LIST OF SYMBOLS

$a_n dt, b_n dt$	moments of random forcing $d\mu$ resp $d\eta$
$\tilde{c}$	instantaneous concentration
c	concentration fluctuation
C	average concentration
$d\mu, d\eta$	random velocity change
$d\omega_t$	white noise process with zero mean and variance dt
ε	viscous dissipation
$\hat{f}, \hat{g}, \hat{g}_a$	characteristic function of resp $d\mu, W$ and u_3
i	turbulence intensity
k	van Karman constant
K	eddy diffusivity
L	Monin Obukhov length
μ	random forcing
N	number of particles released
P	probability distribution function
Q	emitted mass
R_L	Lagrangian autocorrelation
r	white noise process with zero mean and variance 1
S	spectra
σ^2	second moment of u_3
T_E	Eulerian turbulence timescale
T_L	Lagrangian turbulence timescale
U	horizontal Lagrangian particle velocity
u_1	horizontal turbulence velocity fluctuation
u_3	vertical turbulence velocity fluctuation
$\bar{u}$	mean horizontal wind
$\overline{uw}$	Reynolds stress
u_*	characteristic horizontal velocity scale
W	vertical Lagrangian particle velocity
w_*	characteristic vertical velocity scale
Z	Lagrangian particle displacement
z_i	boundary layer height
$\overline{}$	ensemble average
$<>$	average over particles at height z
KME	Kramers Moyal Expansion
mcf	marginal characteristic function
mgf	moment generating function
pdf	probability density function

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FOREWORD

Our highly industrialized society releases waste products in the atmosphere, which are not all harmless. These contaminants are transported and dispersed by the mean wind and by the atmospheric turbulence. This is often a complicated process and it is difficult to predict where and in what concentration these waste products can be found back. It is e.g. hard to decide how to reduce average ground level concentrations. Only rough rules can be given. One of these is to use tall stacks to emit the pollution. However, in practice it turned out that tall stacks are usually effective in reducing ground level concentrations at night but not always during the day.

This difference in effectiveness of a tall stack can be explained by the different structure of the atmospheric turbulence during the day or the night. The part of the atmosphere, whose structure we need to know, is the layer closest to the ground in which generally releases take place. In the lowest layer of the atmosphere also called the boundary layer the motion of the air is turbulent due to two different effects: friction with the surface and heating by the sun.

First we consider friction. The air flow must obey the no-slip condition at the surface. This results in a vertical velocity gradient, which at the Reynolds numbers pertaining to the atmosphere is unstable. The consequence is turbulence which obtains its energy from the mean shear.

Secondly we turn to heat effects. During the day the sun warms the earth surface by shortwave radiation. This temperature difference between surface and air results in vertical accelerations and consequently the hot air rises, which we call convective turbulence. During the night the earth only looses heat and becomes cooler than the atmosphere. The opposite happens, that is that vertical motion in the air is suppressed.

These two effects, friction with the surface and heat effects make the boundary layer turbulent. The two causes of turbulence vary with time (day-night) and the boundary layer height changes with them, which is an important fact for dispersion. During the day, when the sun shines and feeds the turbulence, the boundary layer has a typical height of 1-2 km, while during the night it is much smaller, in the order of 200 m. This is of importance for air pollution problems, because tall stacks may emit above the boundary layer during the night. The contaminants stay there and at ground level no concentration is measured. During the day even tall stacks emit in the boundary layer and the pollutant spreads to the surface.

The relation between the turbulent state of the boundary layer, source height and ground level concentration is extremely complicated and still not well understood. Present relations to predict concentration levels e.g. the Gaussian model (to be discussed later) are based on assumptions that are most of the time incorrect. Tall stacks e.g. are not effective in minimizing the ground level concentration during the day; on the contrary, a little distance downwind the ground level concentration due to a tall stack might be larger than from a ground level source. In order to predict with more accuracy transport and dispersion of pollutants, we have to know more about the structure of the boundary layer and its turbulence and the way they effect dispersion. This thesis wants to add to this knowledge.

Three main classes of turbulence are distinguished. The type of turbulence occurring during a clear day caused by heating of the surface is called convective. During a cloudy day heat effects might play a smaller role and the boundary layer is called neutral, while in the night the surface cools down, the turbulence is suppressed and the boundary layer stable. These types of turbulence have very different characteristics. However, each class of boundary layer has its own similarity laws in the sense that parameters exist of the boundary layer in question with which all variables of the turbulence can be scaled, such that they obey a unique relationship. Also dispersion measurements scale with these parameters.

The fact that such scaling parameters exist, is of great advantage to understand dispersion. It was tried to express time or place evolution of the measured concentration distribution as function of the scaling parameters and of source height. This we call parameterization. An example is an expression found by Briggs (1983) for the maximum surface concentration as function of source height in convenctive boundary layers (see Ch. 4, Eq. (14)). However, it is not always possible to find parameterizations describing all characteristics of the concentration distribution like plume height or concentration fluctuations. When the measurements cannot be caught in such analytical expressions, we can build physical models, like windtunnels or water tanks that show how the turbulence and the mean wind transport and disperse contaminants.

To understand the results of physical dispersion models in relation to the turbulence we have to rely on knowledge of the last, which can be gained from measurements. This konwledge can in turn also be obtained from models describing the motion of the air in a turbulent boundary layer. These turbulence or boundary layer models are based on the equations of motion, which are nonlinear and very complicated. Even with the large computers of today a solution cannot be calculated. The flow in the boundary layer cannot be known in all its details. We have to relax on our requirements and be satisfied with boundary layer models that describe mean quantities of the flow, like e.g. profiles of the variance of the turbulent velocities. These boundary layer models are satisfactory, because we are seldom interested in more than the statistics of the turbulence motions.

In case the contaminants are released in an atmosphere with a mean horizontal wind u, the dispersion models can make use of the following fact. If the advection by the mean wind is dominant over the downwind dispersion material found at a distance x has travelled during a time t = u/x. Via this relation model results for 1D vertical dispersion from an instantaneous source (release at a specific time) in an atmosphere at rest can be used for similar dispersion from continuous sources in an atmosphere with a mean wind that does not depend on height. The concentration field at a downwind distance x from this continuous point source is equal to the concentration field from the instantaneous source measured at time u/x. Continuous single point sources that emit in the convective boundary layer (CBL), where the mean wind does not depend on height, have our main interest.

Atmospheric dispersion measured by air pollution control agencies is usually observed at fixed points, the so-called Eulerian frame. The dispersion so measured, is called absolute dispersion in contrast with relative dispersion, where the dispersion relative to the center of gravity of the plume is observed. Relative dispersion is difficult to describe in an Eulerian frame, while much easier in a Langrangian frame, where the observer moves with the particles released. Actually, both processes, absolute and relative dispersion, can be described in such a Lagrangian frame.

The most well-known models for absolute dispersion are the Eulerian K-models. They are based on the Eulerian conservation of mass equation. From this equation a time rate equation for the concentration C is derived in which the concentration flux $\overline{wc}$ appears: $\frac{\partial C}{\partial t} = - \frac{\partial \overline{wc}}{\partial z}$. This flux is related to the concentration gradient by an eddy diffusivity K as $\overline{wc} = - K \frac{\partial C}{\partial z}$ (see also Ch.1). In a model where the eddy diffusivity K is not a function of the coordinates the concentration distribution is Gaussian, the Gaussian plume models. In these Gaussian absolute dispersion models the mean concentration is described as function of downwind distance x. The spread is determined by spread parameters $\sigma_y(x)$ and $\sigma_z(x)$ that are, besides a function of x, also a function of atmospheric stability.Pasquill (1961) made plume spread functions for different turbulence classes (Fig. 0.1). The plume behaviour in these models is not dependent on source height, the plume axis is horizontal if no boundary effects occur and no varying mean height is taken into account. These models are shown to be incorrect in strongly inhomogeneous turbulence where the height of the plume axis is seen to change rapidly with x. The exact change is strongly dependent on source height. Note that the plume axis is the averaged height of the concentration plume and this changing of the axis height with distance should not be confused with meandering, which is the slow bodily motion of the plume.

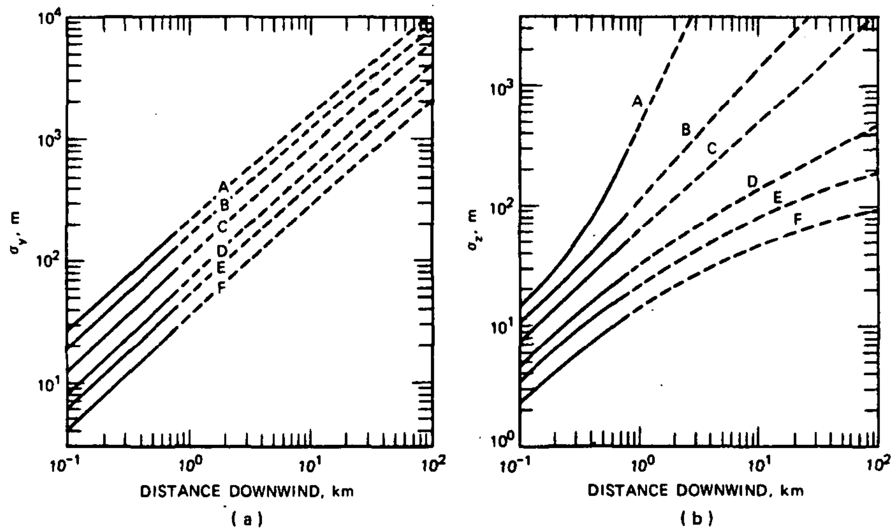

Fig. 0.1 Curves of σ_y and σ_z as reported by Pasquill (1961) for the turbulence types

A: very unstable; B: moderately unstable;

C: slightly unstable; D: neutral; E: slightly stable;

F: moderately stable.

The first Lagrangian model we mention is the puff-model. We distinguish material emitted at different timesteps from each other and call this a puff. Puff-models describe how these puffs are advected by the mean wind, while a relation is given for the concentration distribution evolution. These models assume again that the concentration distribution is Gaussian which is not always true. We turn therefore to more sophisticated models and refer for further details to a review of Eliassen (1984).

In many Lagrangian dispersion models the velocity of each released particle is regarded to be a stochastic process. The dispersion is modelled by the displacement statistics of an ensemble of released particles. The turbulent flow, in which the particles are released, is specified by averaged quantities. Many realisations of such a turbulent flow exist that all meet these averaged values. Each particle of the ensemble is thought to be released in such a different flow realisation. However, the dispersion models do not give flow realisations but can suffice with specifying flow properties at the place of the particle. Together these particles form an ensemble whose average values give us the dispersion characteristics. The concentration is e.g. known from how many particles on the average are present in a certain volume at a certain time.

We will mainly be concerned with absolute Lagrangian dispersion models. Many different Lagrangian absolute dispersion models exist. These stochastic dispersion models are also called Monte Carlo models. They differ in how they formulate the effect of the turbulence on the motion of the particles. Recently, simple and powerful models have been built based on a specific stochastic equation, the Langevin equation. In this equation the effect of the turbulence is modelled as a random force that changes the velocity of the particles. These models are able to describe mean concentration, concentration fluctuations, and if necessary more involved statistical variables (relative dispersion). The most recent models can describe plume behaviour in all turbulence situations. Even dispersion in very inhomogeneous circumstances is stisfactorily described (see Ch. 4).

In this thesis we fill in the frame of ideas set up in this introduction. The first chapter is a discussion of the atmospheric boundary layer. Our interest is in dispersion of passive contaminants (that is non-buoyant) in inhomogeneous boundary layers like the convective boundary layer. We discuss the measured dispersion characteristics in such situations and we also discuss preliminaries for Lagrangian models to describe these phenomena. The theoretical basis for stochastic Lagrangian models is built up in Ch. 2, where we name especially the theoretical investigations we made, for a large time analysis of the Langevin model. Most Langevin models describe vertical dispersion or vertical and lateral dispersion of non-buoyant material. After we have given a review and interpretation of these models in Ch. 3, we build up our own model. In our model the lateral dispersion is left out because the lateral dispersion in a convective boundary layer is well-known and easy to predict because it is proven to be almost Gaussian (Willis and Deardorff, 1978). Downwind dispersion can be neglected compared to advection, so that our model is 1-D describing vertical dispersion. Our model was published in an article in Quart. J. Roy. Met. Soc. (1986) which is integrally included in Ch. 4. Our study shows that the Langevin model is very powerful and can describe the involved dispersion characteristics in very inhomogeneous situations, like in the convective boundary layer. However, it turned out that the steady state of the concentration distribution in our Langevin model was not uniform, which made us interested in comparing our model to another Langevin model. This comparison is carried out in Ch. 5.

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Chapter 1

INTRODUCTION TO DISPERSION

Ch. 1. Introduction to dispersion

Introduction

In this thesis we are concerned with dispersion in the atmospheric boundary layer. Three main classes of boundary layers are distinguished: neutral, stable and unstable (convective). The turbulence in these classes is quite different and depending on this, dispersion in these layers show different behaviour. However, the layer close to the ground, the surface layer shows strong similarity and will be discussed first.

1.1 Surface layer

A concept very often used to organise experimental turbulence data is scaling. Scaling parameters are sought so that turbulence variables, made dimensionless with these parameters, show similarity, that is they collapse on to universal relationships. These parameters can generally be interpreted in terms of a characteristic height, velocity and temperature of the turbulence process.

Near the ground there exists a surface layer where mechanical turbulence is dominant and in which the so-called Monin-Obukhov similarity is valid. This similarity theory says that all turbulence variables scale with z, τ_o and $\overline{w\theta_o}$, where z is height, $\tau_o = -\overline{uw_o}$, the kinematic surface stress and $\overline{w\theta_o}$ the kinematic surface heat flux. The characteristic scaling parameters become for lenght L, the Monin Obukhov length, $u_* = \tau_o^{1/2}$ for velocity and $T_* = -\overline{w\theta_o}/u_*$ for temperature. The

length L is defined as the height where the production of turbulence by buoyancy effects and windshear is equal. This length can be calculated by equating buoyancy and mechanical production terms in the turbulent kinetic energy equation (Businger, 1984). The kinetic energy equation in case of horizontal homogeneity may be written in the form

$$\frac{1}{2}\frac{\partial q^2}{\partial t} = -\overline{uw}\frac{\partial \bar{u}}{\partial z} + \frac{g}{\theta}\overline{w\theta} - \frac{\partial}{\partial z}\overline{w(\frac{1}{2}u_i^2 + \frac{p}{\rho_o})} - \varepsilon , \qquad (1.1)$$

where $\frac{1}{2}q^2 = \frac{1}{2}\overline{u_i u_i}$ is the kinetic energy per unit of mass, $\overline{uw}$ the kinematic Reynolds stress, $\bar{u}$ the horizontal mean wind, θ the potential temperature, p the pressure, ρ_o the density and ε the viscous dissipation. This equation is derived from the equations of motion splitting all quantities in an average value and a fluctuation (Reynolds decomposition). The first term on the righthand side is the shear production term, which represents the rate at which the mean flow contributes to the turbulent kinetic energy. The second term is the buoyancy production term. The third term is a combined transport and pressure term, which does not produce or dissipate energy.

We assume that the wind in the lowest layer up to the height -L, the surface layer, is given by a logarithmic wind profile $\frac{\partial \bar{u}}{\partial z} = u_*/kz$. Here k is the von Karman constant. Then, equating the buoyancy and mechanical production terms at the height z = -L we get

$$\frac{g/\theta \ \overline{w\theta_o}}{- \overline{uw} \ \frac{\partial \bar{u}}{\partial z}} = - \frac{g}{\theta} \frac{\overline{w\theta_o}}{u_*^3} kL = 1,$$

which yields indeed

$$L = \frac{- \theta \ u_*^3}{g \ \overline{w\theta_o} \ k} . \tag{1.2}$$

1.2 Stable boundary layer

Above the surface layer the boundary layer might have different stability. In a stable boundary layer (SBL) the air is cooled at the earth surface due to outgoing radiation, subsequent conduction into the overlying air leads to a stable temperature gradient. This usually occurs during the night. The vertical motion of the air is suppressed and the only source of turbulence is wind shear (mechanical production). This mechanism can sustain turbulence only in a relatively thin boundary layer and that is why a stable boundary layer is only around 200 m deep. Profiles characteristic for the windspeed, wind direction and potential temperature in the SBL are depicted in Fig. 1.1.

The structure of the SBL is not only determined by turbulence, but also by other processes like gravity waves (see e.g. De Baas and Driedonks, 1985) and long wave radiation. Also due to the fact that this layer is usually non-stationary. Generally valid expressions of profiles of the Reynolds stresses, heat flux and velocity variances are difficult to find. Still, to get an impression of these quantities we give the profiles found in a well behaved SBL by Nieuwstadt (1984a) (Fig. 1.2) and refer further to observations of the SBL structure which have been reported by e.g. Mahrt et. al. (1979) and in articles of Nieuwstadt (1984a, 1984b).

In the stable boundary layer above the surface layer we can not find a constant characteristic velocity, temperature and height scale. However, here the turbulence variables scale with local values (Nieuwstadt 1984). The characteristic length is Λ, the local Monin-Obukhov length, defined as

$$\Lambda = - \frac{\tau^{3/2}}{k(g/T)\overline{w\theta}_o} ,$$

where $\tau = [\overline{uw}^2 + \overline{vw}^2]^{1/2}$, k the von Karman constant and, g/T the buoyancy parameter. The characteristic velocity is $u_* = (-\overline{uw(z)})^{1/2}$ and the characteristic temperature is $T_* = -\overline{w\theta(z)}/u_*(z)$.

In the limit $\frac{z}{\Lambda} \to \infty$ the dimensionless combinations of turbulence variables approach a constant value. This region is called the <u>z-less stratification layer</u> (Wyngaard, 1984). Here the scaling parameters are $\tau = - \overline{uw}$ and $\overline{w\theta}$. The characteristic velocity is $u_*(z)$ and the temperature can be formed from these scaling parameters analogous to the surface layer values.

These scaling regions are summarized by Holtslag and Nieuwstadt (1986), whose graphical representation we give in Fig. 1.3. The regions are depicted as function of the nondimensional height z/z_i and the stability parameter z_i/L. Here z_i is the boundary layer height.

Stacks that emit non-buoyant material into the SBL have been observed to have very thin plumes that do not spread over very long distances due to the fact that vertical motions are suppressed by the stable stratification and dispersion becomes a relatively slow process (Fig. 1.4).

The characteristic timescale of turbulence T is not the only timescale involved. Also the buoyancy frequency $N = (\frac{g}{\rho}\frac{\partial \rho}{\partial z})^{\frac{1}{2}}$, where ρ is the mean air density, plays a role. The behaviour of dispersion then depends on the interplay of timescales T and N^{-1}. Pearson et al. (1983) report that for large dispersion times molecular diffusion becomes important involving a third timescale. Their argument is that a fluid element in a SBL which has a density that is different from its environment changes its density due to molecular processes. For large times they expect the spread of a plume to continue to grow due to molecular diffusion. However, data discussed by Britter et al. (1983) and Venkatram et al. (1984) do not show this.

The fact that the density difference between fluid elements and their environment changes in time makes a Lagrangian consideration more involved (see section 1.5.2). An equation for the particle velocity is needed that include the buoyancy effects due to this density difference and in addition we need an equation for the density difference. In case molecular diffusion indeed plays a role it is even more difficult. The fluid elements then loose their identity. In the Lagrangian study of Pearson et al. (1983) control volumes are considered that might indeed loose the original fluid elements.

For further details on dispersion in the SBL we refer to the afore mentioned articles and to the review of Hunt (1984).

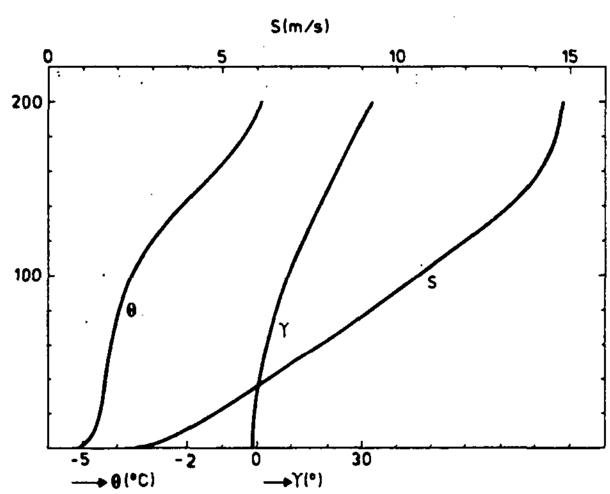

Fig. 1.1 Characteristic profiles of the windspeed S, wind direction Υ and potential temperature θ in a stable boundary layer (from Nieuwstadt, 1984a).

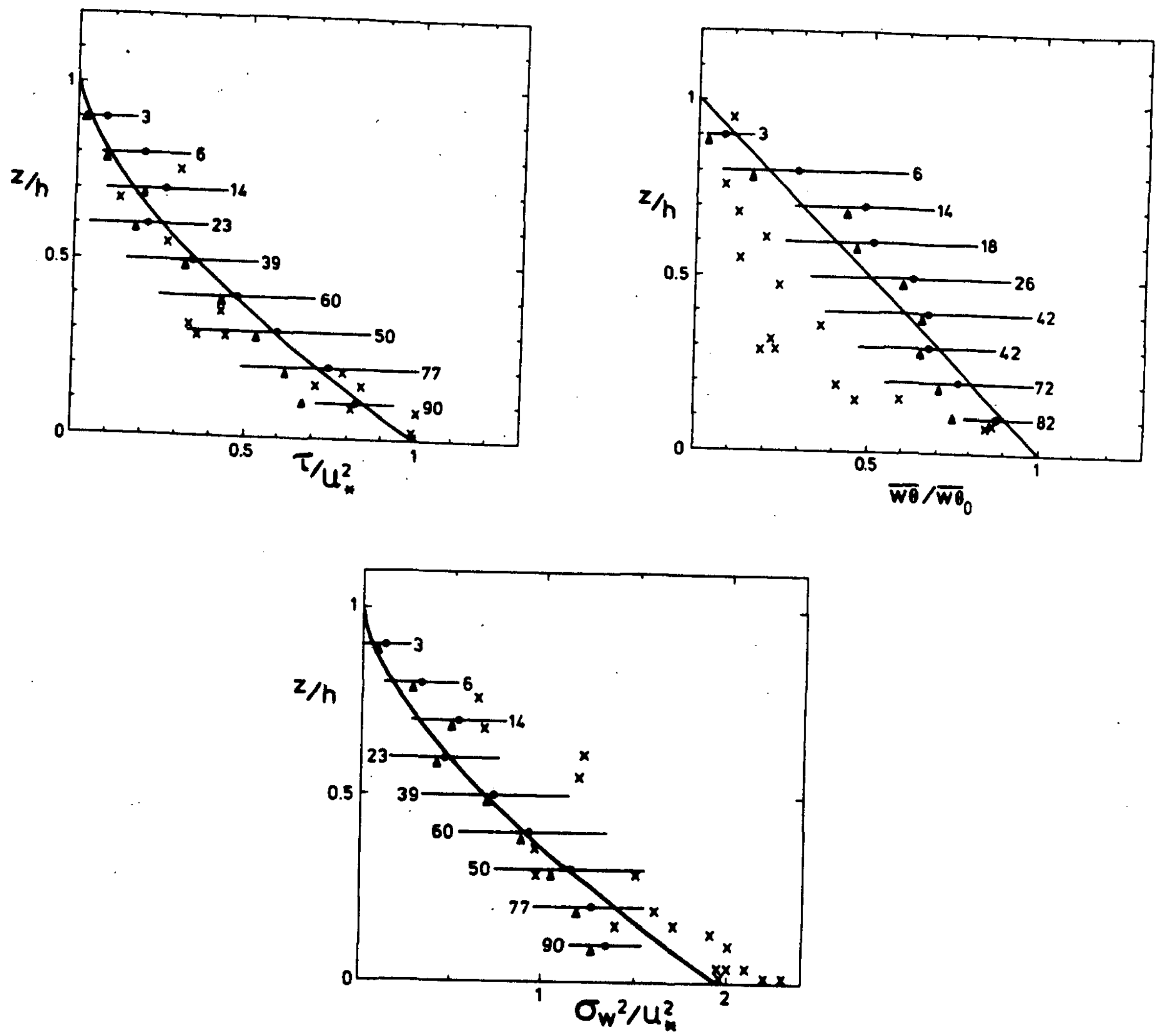

Fig. 1.2 (a) The vertical profile of the moment flux τ, nondimensionalized with its surface value u_*^2 as a function of z/h. The solid curve is the function $(1-z/h)^{3/2}$, where h is the boundary layer height.

(b) The vertical profile of the temperature flux $\overline{w\theta}$, nondimensionalized with its surface value $\overline{w\theta_o}$ as a function of z/h. The solid curve is the function (1 - z/h).

(c) The vertical velocity variance σ_w^2, nondimensionalized with u_*^2 as a function of z/h. The solid curve is the function of $1.96\ (1 - z/h)^{3/2}$.

The data are grouped in intervals of z/h. At the midpoint of each range the average of the nonfiltered observations is shown by solid circles, together with the standard deviation and the number of data. The solid triangles indicate the average of the filtered data. The observations of Caughey et al. (1984) are shown by crosses. (From Nieuwstadt, 1984a).

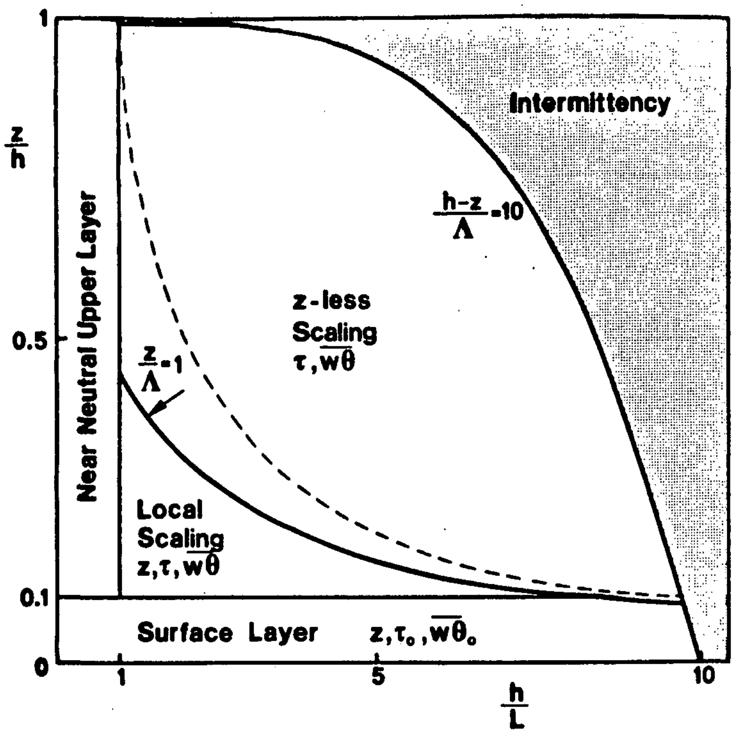

Fig. 1.3 Definition of scaling regions in the SBL (L > 0) as a function of the nondimensionalised height z/h and the stability parameter h/L, where h is the boundary layer height and L the constant Monin-Obukhov length (Eq.1.2). The dashed line is given by z/L = 1. Basic scaling parameters for the turbulence are indicated.
(From Holtslag and Nieuwstadt, 1986).

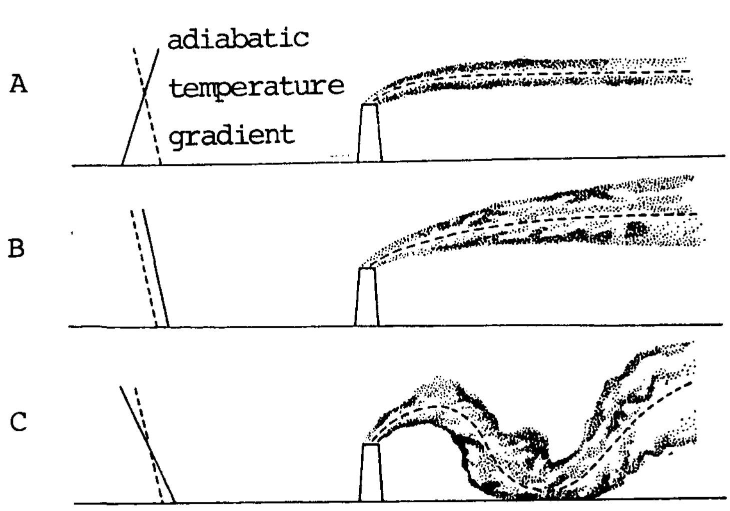

Fig. 1.4 Shape of a plume released from a stack in (a) stable, (b) neutral and (c) unstable circumstances. To the left the temperature profile is indicated, where the dashed line is the adiabatic profile.
(From "Luchtverontreiniging en weer", KNMI, 1979).

1.3 Neutral boundary layer

Neutral turbulence occurs when there are no buoyuancy effects. The only turbulence generating mechanism is then windshear. This might happen when there is cloudcover and strong winds. However, as already very small temperature differences have strong effects, the flow in the atmosphere seldomly occurs to be exactly neutral (unlike in windtunnels, where it is the most easy to realize flow). Venkatram and Paine (1985) described dispersion in a shear dominated boundary layer, usually called neutral, although as they say also it is in fact a stable boundary layer. We will not discuss this type of turbulence further.

1.4 Convective boundary layer

1.4.1 Sublayers and scaling

During clear periods the sun heats the surface, which in turn heats the air by convection. Strong upward air motions and large turbulence fluxes result and the atmosphere effectively mixes released material in the vertical. In this section we give a description of the convective boundary layer and characteristics of dispersion in such conditions. Dispersion models that describe these phenomena are extensively discussed in Chapter 2 and 4.

We consider the horizontally homogeneous convective boundary layer (CBL), where no clouds occur. The turbulence extends to a certain height, which we call the boundary layer height z_i. In the CBL convective turbulence production (due to buoyancy effects) is dominant over mechanical turbulence production (due to windshear), except close to the ground and the height, where the production of turbulence by the two mechanisms is equal.

Except the surface layer below $z = -L$ there can be distinguished two other small layers, the free convection layer, where the adaption of the surface layer to the bulk of the CBL the mixed layer takes place and the entrainment layer at the top where interaction with the stable layer aloft occurs (Caughey, 1984). Each region has its own scaling parameters. With the basic scaling parameters a characteristic velocity, temperature and a length can be formed.

In the free- convection layer u_* plays no role any more, but the scaling height is still z. A characteristic velocity and temperature are defined as function of the height z, kinematic surface flux $\overline{w\theta_0}$ and the buoyancy parameter g/θ. The characteristic velocity is $w_f = (\frac{g}{T}\,\overline{w\theta}\,z)^{1/3}$, the temperature is $\theta_f = (T/g\,(w\theta)^2/z)^{1/3}$. This free convection layer might reach a height of about 0.1 z_i.

At the top, from roughly 0.8 z_i, till 1.2 z_i in the entrainment layer warm air from above entrains the boundary layer. The processes in this layer are not yet well understood. We refer to a review of Driedonks and Tennekes (1984).

We are most interested in the well mixed layer, that covers the largest part of the convective boundary layer. In this layer all quantities are well mixed (Deardorff, 1974a,b; Willis & Deardorff, 1974; Deardorff & Willis, 1985; Driedonks, 1981). The mean wind and potential temperature e.g. are practically constant with height (see Fig. 1.5). We note here that recent "top-down and bottom-up" theory on mixing in the CBL states that the profiles might differ from uniform depending on the ratio of the fluxes at the bottom and the top of the CBL (Wyngaard and Brost, 1984).

Deardorff (1974a,b) found that the relevant scaling parameters in the mixed layer are the boundary layer height z_i, a characteristic velocity scale w_* defined by

$$w_* = \left(\frac{g}{T} z_i \overline{w\theta_o}\right)^{1/3} \tag{1.3}$$

and the characteristic temperature $\theta_* = -\overline{w\theta_o}/w_*$. All turbulence variables should scale with these two variables w_* and θ_* to give dimensionless groups that are only functions of z/z_i (mixed layer scaling). Deardorff found that this is indeed the case for $-z_i/L > 10$ and $\bar{u} < 6\, w_*$. The requirement limiting the windspeed is usually satisfied, as w_* is often larger than 1 m/s, while a typical $\bar{u}$ is 5 m/s.

The scaling regions in the CBL are summarized by Holtslag and Nieuwstadt (1986), whose graphical representation is given in Fig. 1.6.

With these scaling parameters turbulence and dispersion measurements in the CBL can be analysed. Ground level concentrations are often measured. However, measurements in the atmosphere aloft are more difficult to obtain. The CBL has a typical height of 1-2 km, while present measuring masts have at most a height of about 300 m. The structure of the larger part of the CBL can only be measured with aircrafts or floating balloons. The first method with aircrafts has the disadvantage of being very expensive, while with the balloon method large distances can not be covered in a short time and no instantaneous view on the whole CBL can be obtained. For a survey on turbulence measurements we refer to Caughey (1984) and for a literature survey on dispersion measurements we refer to Vanderborght and Kretzschmar (1984). Laboratory models are build to simulate turbulence and dispersion in the CBL. These laboratory models revealed the more detailed structure. A description of this structure and of plume behaviour in the CBL follow.

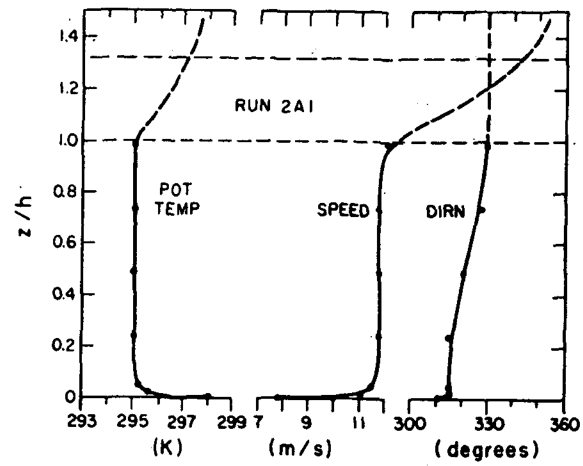

Fig. 1.5 Profiles of wind speed, wind direction and potential temperature. The near-adiabatic lapse rate and the negligible mean wind shear in the mixed layer are typical of strongly convective conditions. (From Kaimal et al., 1967).

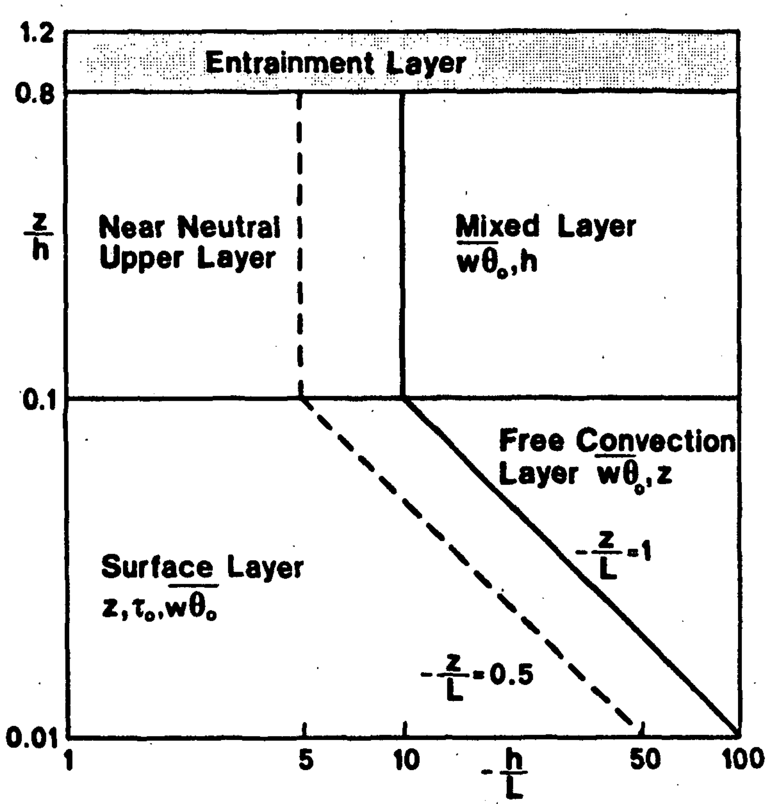

Fig. 1.6 Definition of scaling regions in the unstable ABL (L < 0). Basic scaling parameters for the turbulence are indicated.
(From Holtslag and Nieuwstadt, 1986).

1.4.2 Turbulence structure in the CBL

The CBL can be simulated in a windtunnel or a watertank. In such a physical model attempts are made to duplicate the boundary layer at a reduced scale. But we have to be satisfied with an approximation of the atmospheric situation. Atmospheric flows are e.g. much more intermittent than laboratory flows and we can also not expect to find the full velocity probability distributon function of the turbulence as the higher moments of this p.d.f. are difficult to represent in a laboratory model (Plate, 1982). But for the purpose of finding the general structure of turbulence the boundary layer can accurately enough be simulated. In that respect the experiments in a watertank by Willis and Deardorff (1974) gave new insight in the vertical structure of the CBL.

We may also start from the fluid dynamic equations. Solutions to the full equations of motion that describe the overall behaviour of turbulence are not known as the equations are strongly nonlinear. However, numerically they can be solved. Computer models are build that solve the equation of motion for the CBL and results are obtained, that can not analytically be derived. Computer models have the advantage that they can be limited to a description of only those dispersion characteristics that we are interested in, e.g. surface concentrations. We mention the numerical models of Deardorff (1974a), simulating the CBL, which added to the knowledge obtained in the watertank.

We now describe the insight in the CBL we gained from both laboratory models and numerical models. In the CBL a highly organized structure of upward motions, so-called updrafts, occur. They are accompanied by regions of downward motion, the downdrafts. The air in updrafts moves much faster than in downdrafts. Continuity requires that over a flat surface the average vertical velocity is equal to zero. Therefore the updrafts occupy a smaller area in the horizontal plane.

Due to the asymmetry in up- and downward motions the probability density function of the vertical velocity at a certain height is found to be skewed (see Fig. 1.7). The most frequent value of the velocity is not equal to the zero mean velocity, but is found in downdrafts and the distribution has a negative mode. The area under the probability curve at the positive half of the velocity axis is smaller than at the negative half representing that rising air occupies a smaller area in a horizontal plane than sinking air. The probability curve has a long tail for positive velocities, which is due to the above discussed fact that rising air has relatively large velocities. The most frequent velocity (the mode) becomes smaller with height, so that the velocity distribution becomes more Gaussian. An example of such a distribution function is given in Fig. 1.7.

Baerentsen and Berkowicz (1984) reviewed measurements that have been carried out in the convective boundary layer in the atmosphere or in the laboratory. They determined the profiles of $\overline{u_3^2}$ and $\overline{u_3^3}$, the second and third moment of the vertical velocity fluctuations. The profiles that fitted the data best are given by

$$\overline{u_3^2}/w_*^2 = 1.54(z/z_i)^{2/3} \exp(-2\, z/z_i)$$
$$\overline{u_3^3}/w_*^3 = 0.8\, z/z_i\, (1 - z/z_i)(1 + 0.667\, z/z_i)^{-1} \qquad (1.4)$$

We show in Ch. 2 that these profiles are needed as input for the Langevin models. In the limit $z/z_i \rightarrow 0$ (reaching the free convection layer) these profiles approach $\overline{u_3^2} \sim z^{2/3}$ and and $\overline{u_3^3} \sim z$. This is consistent with free convection layer scaling. In the free convection layer the variables $\overline{u_3^2}$ and $\overline{u_3^3}$ should scale with resp. w_f^2 and w_f^3, where the characteristic velocity w_f is given by $w_f = (\frac{g}{T}\, \overline{w\theta}\, z)^{1/3}$.
The profiles Eq. (1.4) are depicted in Fig 1.8.

Another very important parameter of convective turbulence is T_L, the Lagrangian timescale. The Lagrangian timescale is a measure for the lifetime of eddies as experienced by a particle that travels with these eddies and defined as the integral over the velocity autocorrelation. We will review measurements that have been carried out to determine T_L later, as they are based on theory we did not yet discuss. We will see that $T_L \sim z_i/w_*$, which is in the order of 20 min.

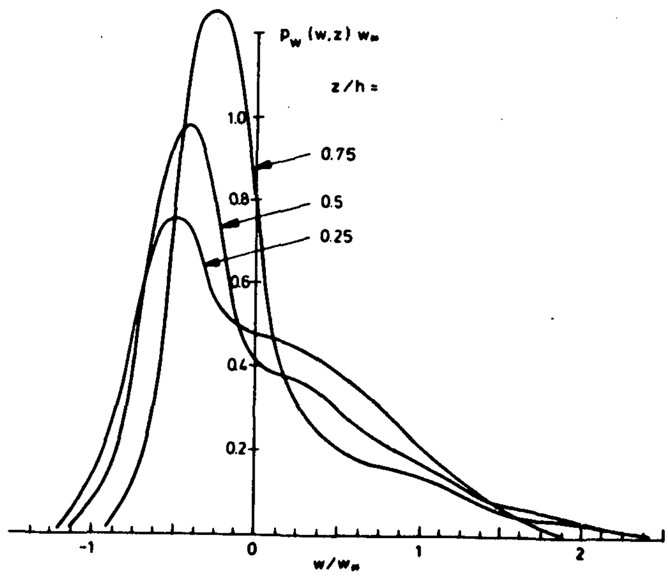

Fig. 1.7 Probability density of vertical velocity at three levels of a convective mixed layer. (From Lamb, 1984)

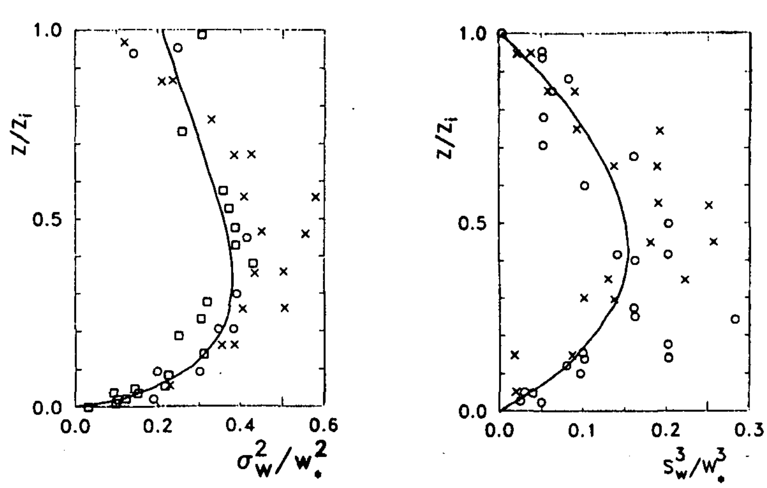

Fig. 1.8 a) The normalized variance of the vertical velocity fluctuations in the CBL. Solid line: Eq. 1.4 Squares: Minnesodata data (Izumi and Caughey, 1976). Circles: Aircraft measurements (Willis and Deardorff, 1974). Stars: Water tank data (Willis and Deardorff, 1974).

b) The normalized skewness of the vertical velocity in the CBL. Solid line: Eq. 1.4 Circles: Lenschow et al. (1980). Crosses: Water tank data (Willis, priv. comm.).

From Baerentsen and Berkowicz (1984).

1.4.3 Dispersion characteristics

A picture of the turbulence structure in the CBL has now become more clear. Our main interest is in the behaviour of particles that follow this turbulent motion. Insight in the dispersion characteristics was given by experiments, carried out by Willis and Deardorff (1976, 1978, 1981) and which gave quite surprising results. They performed experiments with a ground level source and with several elevated sources and found that the dispersion characteristics of a plume are strongly dependent on source height. This is explained by the fact that the vertical structure of the turbulence is strongly height dependent. The vertical spread for small times ($t < 0.1\ z_i/w_*$) of particles released from elevated sources is larger than from a ground source as the turbulence velocity fluctuations ($\overline{u_3^2}$) increase with height. But for larger times the spread of the ground level source plume increases even such that it becomes larger than for an elevated source at times $t \sim 2/3\ z_i/w_*$. (see Fig. 1.9).

Particles released from a ground level source almost all move horizontally untill they are swept upwards by an updraft. The lifetime of updrafts is very large (larger than $2\ z_i/w_*$) and particles in an updraft remain in there for a long time. By the time most particles from the surface source are picked up in an updraft the few particles that started immediately in an updraft still move upwards. This causes the plume axis (the average height of the particles) to rise after a time in the order of z_i/w_*. Particles released from an elevated source have by contrast a larger probability to be emitted in a downdraft than in an updraft. Because the downdrafts too have a very long lifetime, the plume axis moves downward for small times (Fig. 1.10).

When particles released from an elevated source approach the ground they begin to move horizontally and it takes a while before they get picked up by an updraft. This results in a accumulation of particles near the ground and a maximum ground level concentration occurs (Fig. 1.10). The times for which this occurs become larger with source height. Particles from sources above the middle of the CBL are already well mixed before they can reach the ground. For further details we refer to the review of Lamb (1984).

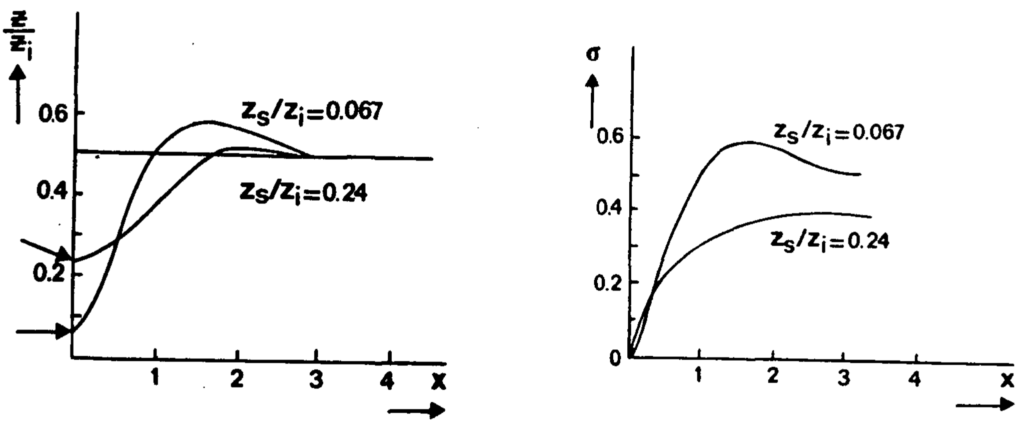

Fig. 1.9 Mean particle height $\bar{Z}/z_i$, and mean variance $\sigma = \overline{(Z - z_s)^2}^{1/2}/z_i$, as a function of downwind distance $X = \frac{x}{\bar{u}}\frac{w_*}{z_i} = t\frac{w_*}{z_i}$ for source heights

$z_s/z_i = 0.067$, and $z_s/z_i = 0.24$ and $z_s/z_i = 0.49$
(From Willis and Deardorff, 1976, 1978).

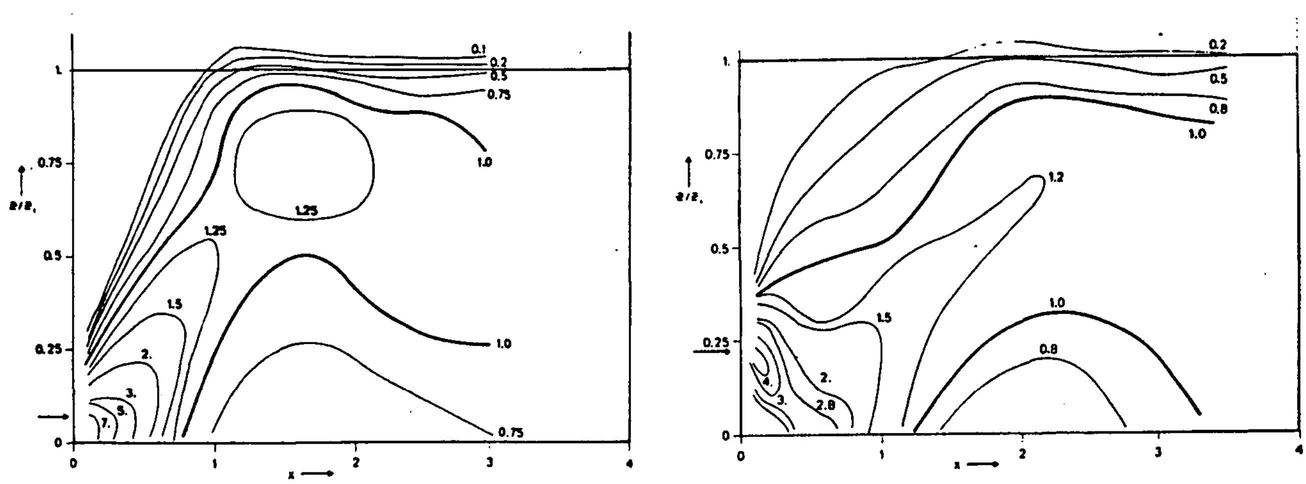

Fig. 1.10 Contours in the vertical x, z plane of the dimensionless concentration for the source heights: (a) $z_s/z_i = 0.067$ and (b) $z_s/z_i = 0.24$. Source height is indicated by arrow on ordinate.
(From Willis and Deardorff, 1976, 1978). (See also Ch. 5).

1.5 Numerical models for dispersion

We now arrive at the numerical models used to describe dispersion in the convective boundary layer. Mathematical models vary with the point of view taken by the modeller. Two basically different descriptions of dispersion exist, the Eulerian and the Lagrangian description. A Eulerian description gives values at a fixed point, usually points at rest relative to the earth. Lagrangian models follow a particle moving with the air. Of the Eulerian dispersion models we will only give the underlying ideas, while the Lagrangian dispersion models are the subject of this thesis.

1.5.1 Eulerian models

In Eulerian models the dispersion process is formulated in terms of the equation of conservation of dispersed material. This is a differential equation for the (instantaneous) concentration $\underset{\sim}{c}$ reads

$$\frac{\partial \underset{\sim}{c}}{\partial t} + \frac{\partial \underset{\sim}{u}_i \underset{\sim}{c}}{\partial x_i} = 0.$$

In this equation the instantaneous velocity $\underset{\sim}{u}$ of the turbulent flow appears, with all its details about random fluctuations. This fluctuating velocity $\underset{\sim}{u}$ is not exactly known and the equation can not be used in this form. From this conservation equation, equations can be derived in which only averaged values occur (Businger, 1984). These statistical values, e.g. the mean wind, the averaged concentration and flux, can be measured and the equations can be used in applications. We derive these equations for one dimension (the z-direction) decomposing $\underset{\sim}{u}$ and $\underset{\sim}{c}$ according to the Reynolds convention in a mean value $\overline{u_3}$ resp. C and a fluctuating component w resp. c. Substituting $\underset{\sim}{w} = \overline{u_3} + w$ and $\underset{\sim}{c} = C + c$ in the conservation of mass equation and averaging gives us the time rate equation for C:

$$\frac{\partial C}{\partial t} = - \overline{u_3} \frac{\partial C}{\partial z} - \frac{\partial \overline{wc}}{\partial z} . \qquad (1.5)$$

Substracting this equation from the original equation for $\underset{\sim}{c}$, we get an equation for c. Analogously an equation for w can be derived from the equation of motion. Multiplying the equation for c with w and the one for w with c, adding and averaging gives an equation for the flux $\overline{wc}$. An infinite series of time rate equations for the moments $\overline{w^n c}$ can be generated in this way. The next problem is that an infinite series of differential equations can not be solved. Therefore, usually this series is broken off after the first or second equation. The last equation kept is closed by assuming that the highest moment still appearing in this equation is simply related to lower moments. These are the so-called "K-models" resp. "second-order closure models"

The K-models close Eq. (1.5) by the assumption that $\overline{wc} = - K \frac{\partial C}{\partial z}$, the "gradient transfer hypothesis". A basic requirement for this hypothesis is that the eddies working on the plume are smaller than the plume itself. In case the eddy diffusivity K is assumed to be constant the resulting concentration distribution is Gaussian. These are the "Gaussian plume models" (Sutton, 1953, Monin and Yaglom, 1977, Ch. 10.3), which are often used.

We show that dispersion of a ground source can be described with a K-model. Generally, the eddy diffusivity should scale with the characteristic velocity and length scales. In the surface layer the characteristic length of the eddies is linear in height and the eddies that act on a ground source plume are of the size of, or smaller than the mean height of the plume. Thus a basic requirement for the gradient hypothesis is satisfied and the dispersion of the ground source plume in the surface layer can be described by a K-model (Tennekes and Lumley, 1972). The evolution of the plume might also be described by a time dependent eddy diffusivity. When the plume grows, the K to be used becomes larger and this can instead be described by K being a function of time. Controversy exists about whether it is physically correct that K is a function of time $K(t-t_0)$ (Deardorff, 1974c, Yaglom, 1976, Pasquill and Smith, 1974).

For an elevated source it is not obvious what K we should use. The K-theory can only succesfully be applied for large times when the length scales of the turbulence are sufficiently small compared with the width of the plume.

More details about K-models can be found in the literature (e.g. Pasquill and Smith, 1974 and Wyngaard, 1984).

The second order closure models carry along the equation describing the time evolution of the concentration flux. These models are more involved and we refer to the review of Wyngaard (1984) and Monin and Yaglom (1977, Ch. 19). From now on we will only be concerned with Lagrangian models.

1.5.2 Lagrangian models

Lagrangian models describe the motion of particles that passively follow the flow. The particles are moved around by the various turbulence eddies so that their trajectories are very random. To model this behaviour the particle velocity is subjected to a random forcing (see Ch. 2). The model is then a stochastic model as opposed to Eulerian models which are usually deterministic. We describe concepts on which Lagrangian models are based.

Stochastic processes like the velocity in these stochastic Lagrangian models are specified by their probability function. A probability distribution function (pdf) $P(z,t\|z',t')$ defines the probability that a particle which was at z' at time t' arrives at z at time t. (We consider 1-D problems). From Lagrangian models this pdf can be obtained by releasing an ensemble of particles at z_s and tracing their trajectories. The number of particles that arrive at time t in a small interval around z, gives the probability $P(z,t|z_s,0)$. This ensemble must consist of a sufficiently large number of dispersing particles to guarantee that the mean is taken over all possible trajectories. For an extensive discussion of ensembles we refer to Lamb (1984).

This probability function for z is related to the mean concentration C by the fundamental theorem. This fundamental theorem for an instantaneous source at $z = z_s$, that emitted a mass Q at $t=0$ reads (Csanady, 1980,p. 23-25, Monin and Yaglom, 1977, Ch. 10.2).

$$C(z,t) = Q\, P(z,t\|z_s,0). \qquad (1.6)$$

This ensemble averaged concentration is not equal to an instantaneously observable one. The last is only one realisation out of the ensemble of possible concentrations. Each time we measure we will find another realisation and the instantaneous concentration deviates from the ensemble averaged oncentration. This deviation from the mean is called the concentration fluctuation. In testing the model results against measurements we should keep this in mind.

We are only concerned with Lagrangian models describing averaged concentration and concentration flux. In Ch. 2 we show that these quantities can be calculated from stochastic Lagrangian models that describe the motion of particles that move independently from each other. One particle is released at a time. These models are called single particle models and describe absolute dispersion. Other Lagrangian models that, besides the mean concentration and flux also want to describe concentration fluctuations, release at least two particles at the same time. The movement of the two particles is made interdependent to model the fact that the turbulence is correlated in space. An ensemble of such pairs of particles is released. These more particle models are called relative dispersion models or puff-models (Csanady, 1980, p. 85). The last name is confusing as it is also used for a totally different class of models, the first Lagrangian models we discussed in the foreword. If even higher moments of the concentration need to be described more than two particles, whose motions are interdependent have to be released at the same time. Models that simulate an ensemble of such groups of particles are called multiple particle models. In Ch. 2 we will extend on the value of absolute and relative dispersion models. In this chapter we will restrict ourselves to absolute dispersion.

The concept of an ensemble-mean used in Lagrangian models corresponds to a large number of measurements in a long series of similar experiments. We are not often able to perform so many similar experiments in practice as atmospheric conditions differ from hour to hour. On the contrary, concentrations and fluxes in the atmosphere are measured as time averages during one single experiment. In stationary conditions the following hypothesis is usually adopted. When the averaging time is made sufficiently large it is assumed that the time-averaged value converges to the ensemble mean. This highly likely hypothesis is called the ergodic theorem (Monin and Yaglom, Ch. 3.3). It enables us to test models describing ensemble average quantities against time averaged measurements.

1.5.3 Taylor's theorem

An important relation for particle spread in homogeneous stationary turbulence is derived by G.I. Taylor (1921). In one dimension (the vertical) for an atmosphere at rest Taylor's theorem reads

$$\overline{Z^2(t)} = 2\,\overline{W^2} \int_0^t (t-\tau)\, R_L(\tau)\,dt \,, \tag{1.7}$$

where $\overline{Z^2(t)}$ is the spread of the particles, $\overline{W^2}$ the second moment of the Lagrangian velocities usually taken to be equal to the standard deviation of the vertical velocity fluctuations u_3^2 R_L and is the Lagrangian velocity autocorrelation. This autocorrelation is a measure of persistence of the Lagrangian particle velocity W defined by

$$R_L(t,\tau) \equiv \overline{W(t)W(t+\tau)} \;/\; W^2(t). \tag{1.8}$$

The ensemble averaging in this definition is carried out over velocities at two different times of the same particle out of the ensemble at two different times, so that R_L gives indeed the persistence of the velocity of one particle. In stationary turbulence the average is independent of t and $R_L(t,\tau) = R_L(\tau)$. Measurements of the autocorrelation function in homogeneous turbulence show that $R_L(t)$ can be approximated by an exponential, $R(\tau) = \exp(-\tau/T_L)$, although the exponential function drops off too quickly at longer timelags. This can also be assumed for convective turbulence but in stable stratification R_W shows negative loops (Pasquill, 1984).

For small lag-times τ the velocity has not yet changed much, the persistence is still maximal, expressed by an autocorrelation $R_L(\tau)$ equal to 1 and Taylor's theorem gives for the small time behaviour of the spread:

$$\overline{Z^2(t)} = \overline{u_3^2}\, t^2 \qquad \text{for } t \to 0 \,. \tag{1.9a}$$

For large lag-times the two velocities W(t) and W(t + τ) in Eq. (1.8) of a specific particle out of the ensemble become uncorrelated and the autocorrelation R_L goes to zero. Taylor's theorem gives for large time behaviour of the spread:

$$\overline{Z^2(t)} = 2\, \overline{u_3^2}\, T_L (t - t_1) \qquad \text{for } t \to \infty \,, \tag{1.9b}$$

where T_L and t_1 are Lagrangian timescales defined by

$$T_L \equiv \int_0^\infty R_L(\tau)d\tau \text{ and } t_1 \equiv \frac{1}{T_L} \int_0^\infty \tau\, R_L(\tau)d\tau \,. \tag{1.10}$$

In a convective boundary layer T_L is in the order of 20 min. Consistent with the restriction of vertical dispersion the integral timescale T_L in stable boundary layers is very small or zero. Because T_L is almost zero it may be convenient to use other integral timescales more characteristic of dispersion in the SBL like the one based on the first moment of R_L that is $T = \left| \int_0^\infty \tau R_L(\tau)d\tau \right|^{1/2}$ (Pearson et al., 1983 and Venkatram et al., 1984). For intermediate times the spread depends on the shape of $R_L(\tau)$. Taylor's theorem for the exponential autocorrelation in homogeneous turbulence reads

$$\overline{Z^2(t)} = 2\,\overline{u_3^2}\,[t\,T_L - T_L^2\,(1 - \exp(-t/T_L)]\ . \qquad (1.11)$$

Taylor's theorem is only valid in stationary homogeneous turbulence. For inhomogeneous turbulence no analytical results exist against which the models can be tested. Lagrangian models can be tested against both time asymptotes in stationary homogeneous turbulence. In Ch. 2 we will describe the Lagrangian Langevin equation which shows the correct behaviour for small and large time. Eulerian K-models have the disadvantage that they only describe dispersion accurately when the length scales of the turbulence are small compared to the width of the plume. They only give the large time asymptote.

1.5.4 Lagrangian timescale T_L

We see that the Lagrangian timescale T_L is an important turbulence parameter appearing in the description of dispersion. This Lagrangian characteristic was not yet discussed. In stationary, homogeneous turbulence T_L can be derived from Taylor's theorem using Eulerian measurements for the particle spread and the turbulence quantity $\overline{u_3^2}$. (Note that this is based on the usual assumption that the Eulerian spread $\overline{u_3^2}$ is equal to the Lagrangian spread $\overline{W^2}$ appearing in the Taylor's theorem). This is an advantage as Eulerian measurements, which are taken at a fixed point are much easier to perform than Lagrangian ones. For inhomogeneous turbulence a considerable number of theoretical and practical investigations have tried to relate Eulerian and Lagrangian timescales. Once such a relation is established, no Lagrangian measurements are required for application of e.g. the Lagrangian Langevin models (see Ch. 2 and 4). These investigations and the resulting parameterization of T_L will be discussed.

Taylor's theorem can be used to deduce the autocorrelation R_L from Eulerian spread measurements in stationary, homogeneous situations. Integrating this autocorrelation gives T_L, without having to make Lagrangian measurements. Unfortunately turbulence in the atmospheric boundary layer can be considered only horizontally homogeneous. Taylor's theorem can only be used to derive the horizontal integral timescale (defined as the integral over the horizontal velocity autocorrelation). Li and Meroney (1982) give an review of different studies, measuring the horizontal T_L based on this method. These studies postulate that the observed Eulerian spread can also be described by a universal non-dimensional function f such that

$$\sigma_y(t) = 2\, \overline{v^2}^{\frac{1}{2}} \int_0^t (t - \tau) R_L(\tau) d\tau = \overline{v^2}^{\frac{1}{2}}\, t\, f(t/T_i) \;, \qquad (1.12)$$

where $\overline{v^2}$ is the variance of the cross-wind horizontal velocity fluctuations. The function f is fitted to the data of σ_y and the time scale T_i is a (stability dependent) timescale, determined by $f(t/T_i = 1) = 0.5$. Different functional forms for f were found that all fit the lateral spread data. From this function $R_L(\tau)$ and then T_L can be derived. Results of these experiments gave values of T_L as function of stability and it turned out that T_L's derived from different functions f, varied as much as a factor 5. This method is therefore very inaccurate. In addition, the vertical integral time scale (defined as the integral over the vertical velocity autocorrelation) can not be deduced this way, because the atmosphere is not homogeneous in the vertical.

For horizontal timescales in inhomogeneous conditions and for vertical integral timescales a theoretical relation between T_L and the Eulerian integral timescale T_E was sought. In Eulerian measurements the fluctuations appear to be faster, because turbulent eddies are advected along a fixed point by the mean wind. This is expressed by T_E being smaller than T_L. The lifetime of an eddy T_L is equal to the ratio of the integral length L and its velocity, statistically represented by σ so that $T_L = L/\sigma$. We assume Taylor's frozen turbulence hypothesis to be valid i.e. that the mean wind $\overline{u}$ is sufficiently strong to blow eddies along the measuring point in such a small time that the eddies do not change. This can be assumed if the turbulence intensity $i = \sigma_L/\overline{u}$ is much smaller than 1. Then the Eulerian timescale is represented by $L/\overline{u}$ and the ratio of the two timescale T_L/T_E is proportional to the inverse of the turbulence intensity

$$T_L/T_E = \beta = B/i. \tag{1.13}$$

The turbulence intensity i is a measure for the stability and B is a proportionality coefficient.

Corrsin (1963) derived Eq. (1.13) differently, relating T_L and T_E by considering spectra. He assumed that the peak frequency n_E and n_L in the inertial subranges of the Eulerian and Lagrangian spectra are proportional to the timescales T_E resp. T_L. Gryning in his thesis (1981) extended on this by not only considering the inertial subrange. Het assumed that for $n < n_E$ resp. $n < n_L$ the spectra are constant and equal to the peak value. Corssin's assumption about a relation between peak frequencies and timescales is not needed, now we can use the fact that the spectrum at zero frequency is proportional to the integral of the autocorrelation which in turn is equal to the timescale:

$$S_{E,L}(0) = 4\ \sigma^2_{E,L} \int_0^\infty R_{E,L}(\tau)d\tau = 4\ T_{E,L}\ \sigma^2_{E,L}. \tag{1.14}$$

The spectra, as function of the frequency n, are described by

$$\begin{aligned} S_E(n) &= C\ \bar{u}^{-2/3}\ \varepsilon^{2/3}\ n^{-5/3} && n \geqq n_E \\ &= C\ \bar{u}^{-2/3}\ \varepsilon^{2/3}\ n_E^{-5/3} && n < n_E \\ S_L(n) &= A\ \varepsilon\ n^{-2} && n \geqq n_L \\ &= A\ \varepsilon\ n_E^{-2} && n < n_L\ , \end{aligned} \tag{1.15}$$

where ε is the dissipation and A and C constants.
The timescales follow as

$$T_E = \tfrac{1}{4}\ C\ \bar{u}^{-2/3}\ \varepsilon^{2/3}\ n_E^{-5/3}\ \sigma_E^{-2} \text{ and}$$

$$T_L = \tfrac{1}{4}\ A\ \varepsilon\ n_L^{-2}\ \sigma_L^{-2}\ .$$

Assuming that in homogeneous, stationary turbulence the total turbulent energy $\int_0^\infty S_E(n)dn = \sigma_E^2$ is equal to $\int_0^\infty S_L(n)dn = \sigma_L^2$ and eliminating N_L and N_E leads to Eq. (1.13) with for B the expression $B = 2.5\ C^{3/2}/A$.

Now a theoretical relation between T_L and T_E is established, we will discuss methods to measure β or B. The first method makes use of the fact that T_L and T_E are the integrals of R_L resp. R_E and β can therefore be obtained by measuring both autocorrelations at the same time. We will give examples after discussing the ideas behind a second method. This second method assumes that the Lagrangian and Eulerian autocorrelations are similar in shape but displaced over a scale factor $T_L/T_E = \beta$:

$$n\ S_L(n) = \beta\ n\ S_E(\beta n) \text{ and } R_L(\beta\tau) = R_E(\tau). \qquad (1.16)$$

Slowing down the fluctuation rate in Eulerian measurements by an appropriate factor β should give the Lagrangian values. This implies that the spectra should also have the same shape but Eqs. (1.15) shows, however, that that is not the case. Empirically, a certain resemblance is noted though (Snyder and Lumley, 1971). The insensitivity of T_L for the exact shape of the autocorrelation implies that this method can give reasonable results. We discuss examples of methods to find the relation between T_L and T_E. The first example is a laboratory experiment for (neutral or stable) grid turbulence and not based on either of the above methods. The second example is an experiment in the convective boundary layer where both methods were compared.

The first example a laboratory study by Snijder and Lumley (1971) was made to derive autocorrelations in grid turbulence. It was essentially a study where particles with different terminal velocities were used. For each kind of particle T_L was measured via the autocorrelation function $R_L(\tau)$. Extrapolating the results to particles that are identical to fluid elements (no terminal velocity) one value for the turbulence T_L was obtained. Snijder and Lumley also measured L/σ where L is the integral length scale and σ^2 is the variance of the turbulence velocities. They found that T_L is exactly equal to L/σ. Unfortunately they did not measure T_E directly at the same time and a value for B is not derived. Only if we assume that T_E is exactly equal to $L/\bar{u}$, we find B = 1 (as used by Hunt, 1984). Assuming that the lighter particles represent Lagrangian measurements and the velocities of the heavy particles can be interpreted as Eulerian, Snijder and Lumley calculate that $T_L/T_E = \beta = 3$. These results are very indirectly derived and are based on broad assumptions.

The second example an experiment in the atmosphere to calculate β and B was done by Hanna (1981). He released neutral balloons in the daytime boundary layer with which he made Lagrangian measurements. At the same time Eulerian measurements were made at a tower and by aircraft. Deriving T_L and T_E directly from measured autocorrelations he finds an average $\beta \approx 1.6$. Assuming that the peak frequencies T_M in the Eulerian and Lagrangian spectra are related to T_L resp. T_E by $T_{M_{E,L}} = 6T_{E,L}$ he finds that $\beta \sim 1.8$. Plotting the β measured from the spectra against turbulence stability given by the turbulence intensity i he finds that here is a large scatter (for vertical measurements $i = \sigma_w/\overline{u}$ and for horizontal measurements $i = \sigma_{v,u}/\overline{u}$). In neutral conditions with strong winds (large 1/i) the relation is best represented by $\beta = 0.4/i$. For convective conditions with low winds (small 1/i) the relation is $\beta \approx 0.7/i$. (Fig. 1.11)

The conclusion is that the value T_L is not easy to specify. In trying to parameterize T_L as a function of more easily measurable variables we meet the following difficulties. The factor β between T_L and T_E depends on the turbulence intensity i, a measure for stability. But also the proportionality coefficient B in the relation $\beta = B/i$ varies with stability. Pasquill and Smith (1984) quote a variation in B from 0.35 till 0.8.

Once the relation between T_L and T_E is established we encounter the problem of parameterizing T_E. Different parameterizations for different stabilities exist. Hanna (1981) states that the Eulerian timescale for horizontal fluctuations can be given by

$$T_E = 0.25\, z_i/\overline{u}. \qquad (1.17)$$

Mixed layer scaling gives that the vertical timescale T_E^w is proportional to z_i/w_* expressed as $T_E^w = c\, z_i/w_*$. In our model applied to a CBL (Ch. 4) we will use

$$T_L = z_i/w_* \qquad (1.18)$$

corresponding to c = 1 and $\beta = 1$. This in turn corresponds to B = 0.7 and i = 1.4, which are values for strongly convective circumstances. For further details about measurements in the atmosphere we refer to Hanna (1984).

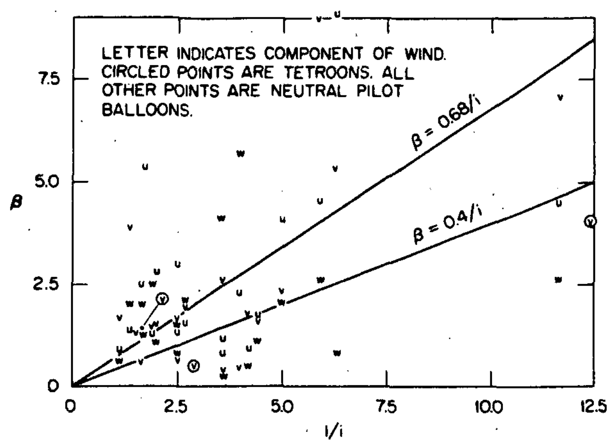

Fig. 1.11 Observed ratios $\beta = T_L/T_E$ plotted versus inverse turbulence intensity $1/i = \overline{u}/\sigma_w$ or $\overline{u}/\sigma_u$. Lagrangian timescales were obtained from the autocorrelations. The letter at each point represents the velocity component. A circled letter indicates a tetroon. (From Hanna, 1981)

1.5.5 Discussion of Eulerian and Lagrangian models

As a conclusion we want to summarize the advantages of Lagrangian dispersion models over Eulerian models. In the simplest Eulerian models vertical dispersion of contaminants is characterised by an eddy diffusivity K, usually modelled as $K = \sigma^2 T_L$. These models assume that the turbulence is Gaussian. Lagrangian models are numerically easier and can take into account more aspects of the turbulence (e.g. skewness) without becoming more complicated. In Ch. 2 we describe how this is done in our Lagrangian model based on the Langevin equation. An advantage of this Lagrangian model is that it combines the numerical advantages of Lagrangian models with the advantage of an Eulerian input. The only Lagrangian parameter that is needed, is the Lagrangian time scale of the turbulence T_L. Another advantage of Lagrangian models is that, with the position of the velocity of each particle known at all times, it is possible to alter parameters at every timestep. In doing so, dispersion in complex situations can be modeled without significantly increasing the sophistication of the model. The effect of windshear on the vertical dispersion can easily be included in Langevin models as a height-dependent advection term with further possibilities of extension to 3-D dispersion. Although it is still debated whether buoyant plumes (releases that are hotter than the air) can also be described, we will show that Langevin models are very successful for non-buoyant plumes even in very inhomogeneous turbulence.

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Chapter 2

THEORY OF STOCHASTIC LAGRANGIAN DISPERSION MODELS

Ch. 2 Theory of stochastic Lagrangian dispersion models

Introduction

The dispersion models we are concerned with are all Lagrangian models. In this chapter we discuss both old and new theory useful in analysing these Lagrangian dispersion models.

These Lagrangian models describe dispersion by following particles as they wander around in the atmosphere. Most of these models describe the velocity of the particles and well as a random or stochastic process. In the models dispersion statistics are calculated by releasing many particles and averaging over the stochastic values. The concentration distribution is calculated from the trajectories of a large number of particles. The first two sections 2.1 and 2.2 are a general introduction to the theory of stochastic process. We discuss the notations used in the models and we also give an extensive explanation on what is understood by the concepts "particle" and "concentration".

We make a distinction between instantaneous concentrations as occur in the real atmosphere, specified in single particle models or in multiple particle models. We show that these instantaneous concentrations contain progressively more information on dispersion when "more particle" models are used. Based on the explanation of what we understand by instantaneous concentration we give a different and more elaborate derivation of a relation between Lagrangian and Eulerian quantities involving concentration values derived by van Dop et al (1985).

Lagrangian dispersion models describe the velocity of released particles by equations which are autoregressive. Different autoregressive models are used. For one of those we use the word diffusion as this Lagrangian autoregressive process can also be described by the Eulerian diffusion equation. The general dispersion process need not be equivalent to diffusion. Brownian motion e.g. looked upon at coarse timesteps is real diffusion, while dispersion in turbulence is only in the far time limit a process which can be described by the diffusion equation.

Recently there is much interest in Lagrangian dispersion models based on the Langevin equation. This equation describes the velocity history by a damping term and a term for the effect of turbulence eddies, the random forcing term. The third section 2.3 is a discussion of two recent theoretical researches into modelling this random forcing function. We will show that although these researches seemed different, they use the same techniques: one research is done in phase space, the other in fourier space. The requirements put on the dispersion process in the models are different, however, in stationary turbulence they give the same prescription of the random forcing.

The fourth section is a paragraph on a rule how to integrate and differentiate stochastic processes, the so-called Itô calculus. This we need in the fifth section which deals with large time behaviour of Langevin models. Large time limits existed for homogeneous situations. We expand their derivation to weakly inhomogeneous Gaussian turbulence and show how this can be done by rescaling the turbulence. We discuss the implications of this large time behaviour.

2.1 Lagrangian models for dispersion

2.1.1 Lagrangian concepts

Notations

In a Lagrangian dispersion description particles are followed starting from a source. The desired insight in the dispersion process is obtained from the statistics of a large number of such particles. Before we describe the theory of these Lagrangian models we first explain some of our notations to avoid confusion.

We use capitals for Lagrangian variables and lower case symbols for Eulerian variables. The Lagrangian variable Z(t) denotes a trajectory of a particle. The lower case z is used for the spatial coordinate, which is an independent variable. The 1D-models, in which we consider the motion of a particle only along one coordinate direction, say the vertical, describe the Lagrangian vertical velocity W(t) and the Lagrangian displacement (height) Z(t) of a marked particle wandering through a turbulent flow .

The probability, that a particle is found in the Eulerian height interval $\varepsilon[z,z+dz]$ and that its velocity W at the same time ranges between the Eulerian values w and w + dw is defined as P(z,w;t)dzdw, where P(z,w;t) is the joint probability density function (pdf) of the two stochastic variables Z and W at time t. The bivariate pdf P(z,w;t) is related to the monovariate pdf P(z;t) by

$$\int_{\text{all } w} P(z,w;t)dw = P(z;t) \tag{2.1}$$

The average over an ensemble of released particles at time t will be denoted by an overbar. This is an average regardless of the position of the particles in space. We have for instance

$$\overline{W(t)} = \frac{\iint w\ P(z,w;t)dzdw}{\iint P(z,w;t)dzdw}\ . \tag{2.2a}$$

The number of particles this ensemble is taken over might be described by a superscript e.g. $\overline{W(t)}^N$. On the other hand the average denoted by brackets is a conditional average over all released particles, which are located in a interval [z,z + dz] at time t. We have

$$\langle W \rangle = \frac{\int w \ P(z,w;t)dw}{\int P(z,w;t)dw} \ . \qquad (2.2b)$$

Close to the source these two averages are about equal, because all particles can still be found in the same small height interval. As we will see they become very different in inhomogeneous turbulence when time proceeds.

The average (time average or average over relaisations) of Eulerian variables, e.g. the fluctuating turbulence vertical velocity $u_3(z,t)$ will be denoted by an overbar. The average of the n-th power of u_3 is $\overline{u_3^n(z,t)}$. Note that this average is, like the bracketed average over Lagrangian variables a local average.

Particles and concentration

Lagrangian descriptions make use of the concept of particles. Because different views on particles exist, we specify what we mean by a particle.

We consider particles that are small enough to follow all turbulent eddies. In the atmosphere the smallest turbulence length scale, the Kolmogorov scale, is in the order of 1mm. At these small scales velocity gradients still exist, but we assume that the particle does not get distorted by them. The motion of the particle can than be described as that of a single point. On the other hand we assume that the particle is so large that it contains many molecules. The particle can then be said to have a concentration and as we neglect molecular processes this particle concentration is conserved.

Compared to the dimensions of the flow the particles are still infinitely small and the concentration due to a particle must be described in terms of a delta function. However we would like the concentration to be a smooth function. To obtain such a description and to remain consistent at the same time with this delta function description we could define the instantaneous concentration $\tilde{c}$ as the total mass of particles in a height interval Δz divided by Δz. This interval should be small compared to the dimensions of the flow, but still so large that it can contain many particles. If the i-th particle contains a mass g_i of the contaminant the definition of $\tilde{c}$ reads

$$\tilde{c}(z,\Delta z,t) \equiv \frac{1}{\Delta z} \int_{z}^{z+\Delta z} \sum_{i} g_i \ \delta(Z_i(t)-z')dz' \ . \qquad (2.3)$$

This concept gives smooth functions of z for the concentration. However, the fact that we should consider length intervals Δz to define concentrations makes the notation rather involved and does not lead to new insights. We therefore simply write

$$\tilde{c}(z,t) \doteq \sum_i g_i \delta(Z_i(t)-z) \tag{2.4}$$

and remember that instead of a point z we should consider a small interval around it. The dispersion of contaminants in the atmosphere is then described by the motion of fluid particles containing a certain mass of contaminants. We will call these marked particles. It is assumed that the marked particles have the same dynamics as surrounding fluid elements.

"Instantaneous concentration"

Consider a dispersion problem in the atmosphere. Concentration measurements made at a certain time are called instantaneous concentrations $\tilde{c}$. From a time series of these concentrations and of turbulence velocity $\tilde{u}_3$, quantities like the average concentration, the flux $\overline{\tilde{u}_3\tilde{c}}$ and fluctuation correlations can be calculated. The last quantity, the spatial fluctuation correlations $\tilde{c}(z)\tilde{c}(z')$ measured in such an air dispersion problem, are non-zero, as the turbulence is correlated in space.

Two kind of dispersion descriptions exist, single and multiple particle models, which are both able to describe averaged concentrations and fluxes, but only the latter can describe the nonzero concentration fluctuations. This is because the instantaneous concentrations in the single particle model do not contain information on correlations in space (as we will show in the next section). Atmospheric dispersion can not fully be described by single particle models. A single particle model can only fully describe an experiment in the atmosphere, where one particle at the time is emitted, with such time intervals that their initial velocities are uncorrelated. Then instantaneous concentrations of the single particle model contain the same information as the measured ones. However, single particle models are very useful when we are only interested in the averaged concentration and flux, because they are simpler than multiple particle models. We elaborate this in the next sections by first discussing single and multiple particle models and then comparing them.

2.1.2 Single particle models versus multiple particle models

In single particle models one particle at a time is released. An ensemble is build up by repeating this process over many different realisations of the same flow, while the initial velocities of the particles are independent of each other. The random forcings different particles experience due to the turbulence eddies, are also uncorrelated resulting in the fact that the motion of different particles is completely uncorrelated.

Multiple particle models take into account that the turbulence is correlated in space. M particles are released at the same time with initial velocities and the random forcings that are interdependent in order to model this aspect of the turbulence. An ensemble is build up of a large number of such groups of particles. This latter model is usually also and therefore confusingly, referred to as a puff model (see General introduction where the first Lagrangian model we discuss is the puff model).

In the following we will explain the difference between instantaneous concentrations in single and multiple particle models and the restrictions this puts on the use of these models.

Single particle releases

First consider a 1D experiment where N particles are released at one point all marked with the same mass g. The particles are released one by one, setting time equal to zero for each particle when it starts. The path of particle i is given by $Z^i(t)$ and we define an instantaneous particle "concentration" due to (only) one particle by

$$\tilde{c}_s(z,t) = g\delta(Z^i(t)-z) \quad , \tag{2.5}$$

where δ denotes Dirac's delta function. The sub- and superscript s stands the realisation in the single particle model and is used to distinguish it later from a realisation (release) in multiple particle model values. We write concentration between quotes as this variable has the dimensions of mass. (As stated earlier we should consider mass per interval).

A definition of an ensemble average consistent with this particle and concentration concept is simply the sum over all particles. The ensemble average of the discrete quantity $\tilde{c}_s$, the concentration C_s, is e.g. defined by

$$C_s(z,t) \equiv \overline{\tilde{c}_s(z,t)}^N = \sum_{i=1}^{N} g\delta(Z^i(t)-z) \ . \qquad (2.6)$$

This is consistent with the fact that the integral of the ensemble average concentration over height is equal to the total amount of mass released Q: $\int C(z,t)dz = Ng = Q$.

The fundamental theorem Eq. (1.2) links Eq. (2.6) to the probability function P(z;t) by C(z,t) = Q P(z;t) . We then get

$$C_s(z,t) = \sum_{i=1}^{N} g\delta(Z^i(t)-z) = Q\ P(z;t) = Q \int P(z,w;t)dw \ . \qquad (2.7a)$$

We see that in discrete notation the pdf P(z;t) is given by

$$P(z,t) = \frac{1}{N} \sum_{i=1}^{N} \delta(Z^i(t)-z),$$

where N should be large.

We also want to discuss the flux in a single particle model. Therefore we need the bracketed moment of the particle velocity W. Moments of W in continuous notation are given by Eq. (2.2b). Using the above discrete rotation of the pdf P(z;t) the conditional average reads

$$\langle W^n \rangle_s = \frac{\frac{1}{N} \sum_{i=1}^{N} (W^i(t))^n \delta(Z^i(t)-z)}{\frac{1}{N} \sum_{i=1}^{N} \delta(Z^i(t)-z)} \ .$$

The concentration flux is defined as $\overline{\tilde{u}_3\tilde{c}}$, where $\tilde{u}_3$ is the Eulerian turbulence velocity that transport the particle. The flux in the single particle model is given by

$$\overline{\tilde{u}_3\tilde{c}} = \sum_{i=1}^{N} \tilde{u}_3(Z^i,t)\ \delta(Z^i(t)-z)g = \langle W\rangle gNP(z,t) = (\langle W\rangle C)_s \ , \qquad (2.7b)$$

where the one before last equality uses that the particles are passive: the "Lagrangian" particle velocity W(t) is identical to the value of the

"Eulerian" velocity field $\tilde{u}_3(z,t)$ at the location of the particle.

For products that involve higher powers of velocity we get by the same method

$$\overline{\tilde{u}_3^n\tilde{c}} = \sum_{i=1}^{N} \tilde{u}_3^n(Z^i,t)\delta(Z^i(t)-z)g = (\langle W^n\rangle C)_s \qquad (2.7c)$$

Splitting the instantaneous concentration $\tilde{c}$ in an ensemble mean C and a fluctuation c and using $\tilde{u}_3 = u_3$ we get

$$\overline{\tilde{u}_3^n\tilde{c}} = (\langle W^n\rangle C)_s = \overline{u_3^n}C + \overline{u_3^n c} \qquad (2.8)$$

This formula, a relation between Lagrangian en Eulerian quantities involving concentration values, was also given by v. Dop et al. (1985) in their appendix A. Here we have shown that it is valid when concentration values are used that result from a single particle model. To avoid confusion about when this relation is valid we have been very careful in our derivation about what information the concentration values carry. We will show that concentration values resulting from multiple particle models contain more information e.g. about concentration fluctuations and carrying out the same analysis we show that Eq. (2.8) is also valid in multiple particle models.

Multiple particle releases

Now consider an experiment where at each time M particles are simultaneously released (M = 2,3...). In total an ensemble of N particles is used. In these models the initial velocities of the particles in one release $j(j = 1, \ldots, \frac{N}{M})$ are correlated and also the random forcing different particles experience in one release are interdependent. The path of particle i in the j-th multiple particle release is given by $Z_i^j(t)$. The instantaneous concentration for each release is defined as

$$\tilde{c}_m(z,t) = \sum_{i=1}^{M} g\delta(Z_i^j(t)-z) \ , \qquad (2.9)$$

This instantaneous concentration $\tilde{c}_m$ Eq. (2.9) contains more information about concentrations in the atmosphere than the one $\tilde{c}_s$ in a single particle release (Eq. (2.5.)). We will show that apart from being able to derive the average concentration and the flux from this quantity $\tilde{c}_m$ we can also use it to derive the concentration fluctuations. This information is contained in $\tilde{c}_m$ because concentration fluctuations originate from the relative movement of particles with respect to each other. This relative movement occurs because of the fact that the turbulence velocities are correlated in space and is modeled in multiple particle models as the paths of particles released at the same time are dependent.

We will show that averages of values linear in instantaneous concentration in both single and multiple particle models are the same, while averaged values of quantities nonlinear in instantaneous concentration are not.

The average concentration in a multiple particle release is given by considering the ensemble of N/M releases:

$$C_m = \overline{\tilde{c}_m(z,t)}^{N/M} = \sum_{j=1}^{N/M} \tilde{c}_j(z,t) = \sum_{j=1}^{N/M} \sum_{i=1}^{M} g\delta(Z_i^j(t)-z) \qquad (2.10)$$

Let us investigate the RHS of this equation. The fact that the displacements Z_i of the M particles in one release j are correlated does not affect the ensemble averages of quantities that only involve values of one single particle i. The ensemble average of such a quantity is the same as it would be in a single particle release. This means that we can drop the index j and write the RHS of Eq. (2.10)

as $\sum_{i=1}^{N} g\delta(Z^{i}(t)-z) = \overline{\tilde{c}_s}^{N}$. Eq. (2.10) becomes

$$C_m(z,t) = \overline{\tilde{c}_m(z,t)}^{N/M} = \overline{\tilde{c}_s}^{N} = Q\,P(z;t)\ . \qquad (2.11a)$$

The conclusion is that both single and multiple particle models give the averaged concentration. Other quantities linear in $\tilde{c}$ can also both be expressed in values obtained both in a single or in a multiple particle experiment. E.g. the fluxes $\overline{\tilde{u}_3^n\tilde{c}}$ are given by

$$\overline{\tilde{u}_3^n\tilde{c}} = \overline{(\tilde{u}_3^n\tilde{c})_m}^{N/M} = \overline{(\tilde{u}_3^n\tilde{c})_s}^{N} = \langle W^n\rangle C(z,t) \qquad (2.11b)$$

and Van Dop et al.'s relation is proven to be also valid for multiple particle releases.

Quantities nonlinear in instantaneous concentration can only be expressed in multiple particle results. For example the instantaneous concentration fluctuations in the m-th release can be defined as

$$\tilde{c}_m(z,t)\tilde{c}_m(z',t) = \sum_{i=1}^{M}\sum_{i'\neq i}^{M} g^2\ \delta(Z_i^j(t)-z)\delta(Z_{i'}^j(t)-z'), \qquad (2.11c)$$

which contains all cross products of the M particles in the j-th release. The ensemble averaged concentration fluctuation is defined as

$$\overline{\tilde{c}_m(z,t)\tilde{c}_m(z',t)}^{N/M} = \sum_{j=1}^{N/M} \tilde{c}_m(z,t)\tilde{c}_m(z',t) \sim P_2(z,z';t)\ .$$

As the variables Z_i and Z_j are dependent, $P_2(z,z';t)$ cannot be split into two single probability distributions. This is equivalent to stating that quantities that are products of properties of different particles can not be obtained from single particle releases. Quantities that involve products of two particle values, like concentration fluctuations, can be described in a two-particle model. To obtain higher order products more information is needed than the instantaneous concentrations in single and two particle models contain.

We conclude that the number of particles to be released simultaneously depends on how detailed we want to describe dispersion. If only the mean concentration is required a single particle model is sufficient. Concentration fluctuations follow from a two particle model and if higher products (of order M) of different particles are needed, a M-particle release model should be used.

We are interested in the quantities such as mean concentration C, the mean height $\overline{Z}$, width of the plume $\overline{Z^2}$ and fluxes $\overline{\bar{u}_3^n \bar{c}}$ which are all quantities that can be given by a single particle model. In the following we will only deal with <u>single particle models.</u>

2.1.3 Autoregressive models

The displacement and velocity of particles released into a turbulent atmosphere is a stochastic process. In an unbounded area the average distance to the source will grow in time and the displacement process is a non-stationary stochastic process.

In a bounded area the dispersion always reaches a steady state, where the velocity moments of the particles are equal to those of the turbulence at that height. These turbulence moments are constant in time and the velocity process is stationary.

This is also true for the velocity of particles dispersing in an unbounded volume, if the turbulence is stationary and homogeneous. In stationary homogeneous turbulence the particles will on the average experience the same velocity changes, irrespective of where the particles are. The moments of the velocity of the particles will remain equal to those of the turbulence (which do not change in time) and the velocity process is stationary.

In inhomogeneous turbulence the velocity process is not stationary, because the velocity changes depend on the position of the particles. While the particles spread more and more the ensemble of particles will see a larger part of the inhomogeneous turbulence and averaged quantities like the velocity moments become a function of time. These averaged quantities are not stationary anymore. However, the velocity process in an unbounded atmosphere with inhomogeneous turbulence may still be considered approximately stationary, when the dispersion process is considered over timesteps for which the average particle displacement is much smaller than the lengthscale associated with the turbulence inhomogeneity.

The class of models we want to use are applicable to stationary processes (Box and Jenkins, 1971, Ch. 4). The fact that the velocity of particles dispersing in an unbounded inhomogeneous turbulent atmosphere is a (weakly in-stationary process, whereas the displacement is not, implies that dispersion can easiest be modelled by a model for the velocity). We will therefore be concerned with dispersion models describing the velocity.

The velocity process of particles dispersing in a turbulent medium can be modelled by the class of autoregressive models. An autoregressive model is a discrete stochastic model that describes the value of the process at a certain time as a linear combination of values of the process at previous times together with a random forcing. So if the velocity at a time t_n is denoted by W_n and the random forcing at this time by μ_n then

$$W_n = \alpha_1 W_{n-1} + \alpha_2 W_{n-2} + \dots + \alpha_p W_{n-p} + \mu_n \tag{2.12}$$

is called an autoregressive process of order p (AR(p)). The rationale behind this name is that W_n is expressed as a function of other variables, or in other words W_n is said to regress on these other variables. When W_n is regressed on previous values of itself, the model is said to be autoregressive.

The order of the AR, that we use to model dispersion problems with, is dependent on the properties of the dispersion process. The autoregressive process that we use should e.g. exhibit the same autocorrelation function and spectrum as the dispersion process. In the next sections we will show that each order of AR(p) exhibits a different class of auto correlations and spectra, where the exact shape depends on the coefficients α_p of the AR(p). Zero order models, the well known random walks, are e.g. used to describe Brownian motion seen on coarse timesteps. The Langevin equation, a first order process, was originally used to describe Brownian motion seen at finer timesteps. Later this equation was also used for homogeneous turbulence dispersion and recently it is applied to inhomogeneous turbulence. Second order AR process have certain disadvantages, that make that they are not used for dispersion modelling. The theory of all these models is discussed in the next subsections.

2.1.4 Zero-order autoregressive model

The first type of dispersion we want to discuss is dispersion of particles due to collisions of molecules, which is called Brownian motion. This type of dispersion, seen at coarse timesteps, can be described by a zero-order autoregressive model.

The physical picture of this dispersion process is as follows. The particles are considered to be so small, that collisions with the surrounding molecules result in random changes of the particles velocity. On the other hand the particles are considered to be much larger than the molecules and the particles feel a friction in the fluid, due to which their velocity gets damped. The time scale, at which the particle velocity has become totally independent of its initial velocity due to this friction, is called β^{-1}. This Brownian motion is sometimes also called molecular diffusion. However, it does not describe the mixing of two chemically different compounds, nor does it describe the diffusion of molecules just like turbulence dispersion does not describe the dispersion of turbulence. On the contrary, the particles considered here, are much larger than the molecules and experience collisions with many molecules in one timestep. The total effect of these collisions is modelled as one random velocity change (random forcing).

The equation used to describe Brownian motion depends on the coarseness of our description. The timescale β^{-1} of this molecular process is very small (order of a second) and when this process is described by a model in which $\Delta t >> \beta^{-1}$, the velocity changes with uncorrelated jumps so that it can be modeled by a zero-order autoregressive process. In this subsection we will analyse this coarser description of Brownian motion and leave the discussion of descriptions on a finer time scale to the next subsection.

We describe Brownian motion in one direction, say the z-direction. The zero-order AR model we use describes the velocity W of the particle at each timestep Δt. The time passed after release is $t = n\Delta t$ and the velocity at this timestep is given by the equation

$$W_{n\Delta t} = \gamma \, r_{n\Delta t}. \qquad (2.13a)$$

Here r is a white noise process with normalised variance

$$\overline{r_{n\Delta t}} = 0 \; ; \; \overline{r_{n\Delta t}\, r_{n'\Delta t}} = \delta(n-n'),$$

where $\delta nn'$ is the Kronecker delta defined by

$$\delta nn' = 0 \qquad \text{for } n \neq n' \qquad (2.13b)$$
$$= 1 \qquad \text{for } n = n' \, .$$

In the following this interpretation will be given to all δ's unless otherwise specified. The factor γ is the variance of the velocity $\langle W^2(t)\rangle^{1/2}$ and a measure for the intensity of the collisions. In homogeneous situations γ is a constant, while in inhomogeneous situations γ is a function of height z.

We discussed before that each type of dispersion should be modelled by an autoregressive process, that has the same auto correlation and spectra. We investigate how these functions look for a zero-order AR model. By showing that they are the same as the measured autocorrelation and spectra in Brownian motion an coarse timestep we show that zero-order AR models are good descriptions of Brownian motion.

The autocorrelation function R_W for a process W is defined by

$$R_W(k\Delta t, n\Delta t) \equiv \frac{\overline{W_{(k+n)\Delta t}\, W_{k\Delta t}}}{\overline{W^2_{k\Delta t}}} \qquad (2.14)$$

and is a measure of "persistence" of the velocity. If the velocity is very persistent, it has the same value at the next time step and the autocorrelation is equal to unity. A process, where the velocity is completely independent on the former value, has an autocorrelation which is equal to zero. If W is a stationary process, R_W is independent of the time $k\Delta t$ and only depends on the time lag $n\Delta t$. For the zero-order process Eq. (2.13) in stationary homogeneous conditions (γ = constant) R_W becomes

$$R_W(n\Delta t) = \frac{\gamma^2\, \overline{r_{(k+n)\Delta t}\, r_{k\Delta t}}}{\gamma^2\, \overline{r^2_{k\Delta t}}} = \delta_{no}, \qquad (2.15)$$

where k is arbitrary.

We see, as expected for a zero-order model, that the correlation between velocities at different times ($n \neq 0$) is zero, which means that persistency of the velocity is absent.

The <u>spectrum</u> of a stochastic process is defined as the Fourier transform of the autocorrelation. In discrete form the definition reads

$$S(\theta_n) = \sum_{n=0}^{\infty} R(n\Delta t)e^{i\theta_n n\Delta t} .$$

The spectrum for the zero-order process W Eq. (2.13) reads

$$S_W(\Theta_n) = \sum_{n=0}^{\infty} R_W(n\Delta t)e^{i\theta_n n\Delta t} = 1 . \quad (2.16)$$

We conclude that any stationary dispersion process with a deltafunction-like autocorrelation (Eq. (2.15)) and (thus) a constant spectrum (Eq. (2.16)) can be modelled by a zero-order AR process.

We now should show, that the zero-order AR process for the velocity has the same velocity autocorrelation and spectrum as the one in Brownian motion, measured at coarse timesteps. This can indeed be shown. However, we will instead investigate the <u>displacement</u> characteristics of this zero-order model, because they give us the concentration in which we are mainly interested. We show that the displacement characteristics of the zero-order AR-model are a good description of Brownian motion measurements.

The displacement can be investigated as follows. Each timestep Δt the particle makes a displacement step $\Delta Z_{n\Delta t}$ equal to $W_{n\Delta t}\Delta t$. The sum of these displacements gives the trajectory of a particle as function of time. The resulting process $Z_{N\Delta t} = \sum_{0}^{N} \Delta Z_{n\Delta t}$ is called the <u>discrete random walk</u> and is a standard problem in textbooks on probability theory (e.g. Chandrasekhar, 1943). We will discuss how we can calculate the pdf of this randomwalk Z. Once we have this pdf P(z,t) we can calculate variables that can be tested against measurements, to se whether the zero-order AR is a good description of Brownian motion.

The displacement $Z_{n\Delta t}$ follows from the difference equation Eq. (2.13)

$$\Delta Z_{n\Delta t} = Z_{(n+1)\Delta t} - Z_{n\Delta t} = W_{n\Delta t}\,\Delta t = 2D^{1/2}\,\omega_{n\Delta t} . \quad (2.17)$$

with $\overline{\omega_{n\Delta t}} = 0$, $\overline{\omega_{n\Delta t}\omega_{n'\Delta t}} = \delta_{nn'}$, Δt and $2D = \Upsilon^2\Delta t$.
We see that the fact that the velocity changes with uncorrelated jumps (Eq. (2.13)), results in displacement steps $\Delta Z_{n\Delta t}$ that are also uncorrelated, $\Delta Z_{n\Delta t}$ is a white noise process with variance $2D\Delta t$. Why we use the factor 2D

will be explained in subsection 2.2.2.

To calculate the trajectory $Z_{n\Delta t}$ of the particles we should be more specific about the random term $r_{n\Delta t}$. Textbooks deal with two special white noise processes. The first assumes a Gaussian white noise (Durbin, 1983, p. 6, Eq. (1.4)), the other a dichotome process (Chandrasekhar, 1943). In the second white noise process, the dichotome process, $\omega_{n\Delta t}$ has an equal probability of ½ to be positive or negative. The displacement is a constant step length ℓ (note lower case) to the right or to the left $\Delta Z_{n\Delta t} = +/- \ell$(In the first case $\Delta Z_{n\Delta t}$ could have all possible lengths, as the probability of these lengths was Gaussian). As $\overline{(\Delta Z_{n\Delta t})^2} = 2\,D\Delta t$ Eq. (2.17) we see that ℓ and Δt are related by $\ell^2 = 2\,D\Delta t$. The pdf of ΔZ reads

$$P(\Delta z_{n\Delta t}) = \tfrac{1}{2}\,\delta(\Delta Z_{n\Delta t}-\ell)+\tfrac{1}{2}\,\delta(\Delta Z_{n\Delta t}+\ell), \tag{2.18}$$

(Chandrasekhar, 1943).

From the Central Limit Theorem we know that both processes lead to a Gaussian distribution of the sum Z because this theorem states that the sum of independent random variables, regardless of their distribution function, is Gaussian. In other words this theorem it follows that the probability of the trajectories Z is rather unsensitive to the exact description of the white noise ω_t. So these two cases of zero-order models, one with a Gaussian white noise process and the other with a dichotome white noise process, both give the same random walk process Z. We derive the exact randomwalk pdf in the first case.

In the first case $\omega_{n\Delta t}$ is Gaussian and the probability for ΔZ is consequently also Gaussian. A Gaussian pdf is specified by its first and second moment. The first and second moment of ΔZ read

$$\overline{\Delta Z} = 0 \qquad \text{and} \qquad \overline{(\Delta Z_{n\Delta t})^2} = 2D\Delta t.$$

The pdf for ΔZ reads

$$P\,(\Delta z_{n\Delta t}) = (4\pi D\Delta t)^{-\frac{1}{2}}\exp\{-\frac{(\Delta z_{n\Delta t})^2}{4D\Delta t}\}. \tag{2.19}$$

Note that we notate the probability of a stochastic variable Z to be equal to z as P(z).

Our goal is to specify the characteristics of the particles trajectory, so we ask for the probability that the trajectory $Z_{n\Delta t} = \sum_{n=0}^{N} \Delta Z_{n\Delta t}$ reaches a certain point z. The steps ΔZ are Gaussian distributed and uncorrelated in time and it follows that the sum of these steps $Z_{N\Delta t}$ is also Gaussian distributed (This can be explicitly proven, see v. Kampen, 1983, p. 27). Its pdf is specified by the first and second moment that read

$$\overline{Z}_{N\Delta t} = 0 \qquad \text{and} \qquad \overline{(Z_{N\Delta t})^2} = 2DN\Delta t$$

and the probability function of the random walk we looked for reads

$$P(z_{N\Delta t}) = (4\pi DN\Delta t)^{-\frac{1}{2}} \exp -*\frac{(z_{N\Delta t})^2}{4DN\Delta t}*. \tag{2.20}$$

Chandrasekhar proved that $P(z_{n\Delta t})$ in the dichotome case is also given by Eq. (2.20) by considering all possible random walks of N steps and determining how many of these end in point $Z_{N\Delta t}$ (path integral method). We will not repeat this lengthy derivation here, but use the central limit theorem as discussed above, that states that also in this case the pdf of the trajectories $Z_{N\Delta t}$ is given by Eq. (2.20).

Continuous form

Autoregressive processes are defined as discrete process, while we want to test the zero-order AR for Brownian motion against the continuous Taylor formula Eq. (1.). To do this the discrete random walk is replaced by a continuous random process. We can construct this continuous process by putting $t = N\Delta t$ and $Z = N\Delta Z$ and letting $N \to \infty$ while $\Delta t \to 0$. At the same time the steps must become infinitesimal $\Delta Z \to dZ$. The probability function of the continuous random or drunkard's walk $Z(t) = \int_0^t dZ$ becomes the continuous equivalent of Eq. (2.19)

$$P(z,t) = (4\pi Dt)^{-\frac{1}{2}} \exp(-z^2/4Dt) . \tag{2.21}$$

From this probability function it follows that the particle spread is given by $\overline{Z^2} = 2Dt$. It is clear that Z as discussed in section 2.1.3 is indeed a non-stationary process, because the spread of the particles is a function of time. We see that this zero-order model gives the large time limit as predicted by Taylor's theorem Eq (1.7).

We proved that zero-order processes are satisfactory descriptions of Brownian motion seen at coarse timesteps. For $t < \beta^{-1}$, this zero-order model is not an adequate description since we expect from Taylors theorem for small times that $\overline{Z^2} \sim t^2$. Besides to Brownian motion at coarse timesteps this model also applies to turbulence dispersion seen at timesteps which are much larger than the Lagrangian timescale T_L.

In the next paragraph we discuss first-order models, which will turn out to be a good description of Brownian motion and turbulence dispersion for both small and large times.

2.1.5 First- order autoregressive models

We described the Brownian motion on a coarse time scale, where $\Delta t > \beta^{-1}$. This is a natural description as the timescale β^{-1} in this process is small. In turbulence the timescale at which velocities become uncorrelated (the Lagrangian timescale T_L) is of order of 100s. Here a zero-order model would be restricted to coarse timesteps, which are larger than 100s. In such a description all small time details would be lost. If we look at finer timesteps, turbulence dispersion and also Brownian motion has to be described by a different model. At such finer timesteps the velocities of the particles are correlated in time, the particles remember their previous velocity. That the next velocity depends on the current value, means that we have to describe the velocity process by an AR process of higher order. Here we investigate the first-order process.

Brownian motion and turbulent dispersion

For the description of Brownian motion at small timescale, we return to the physical description we gave of this process. Due to the friction, exerted by the fluid on the particle the particle looses its velocity. This can be modelled by including a damping term in the governing equation. In continuous form the equation governing for Brownian motion becomes

$$\frac{dW}{dt} = -\beta W + \eta \quad \text{and} \quad \frac{dZ}{dt} = W, \tag{2.22}$$

where μ is the random forcing due to collisions. This equation is called the Langevin equation and for the description of turbulent dispersion in homogeneous stituations the same equation is used, substituting the Lagrangian timescale T_L for β^{-1}. However, in turbulent dispersion we don't consider hard particles but particles as described in section 2.1.1.

We investigate this first-order dispersion model. This Langevin model involves a white noise process for η assuming that accelerations of the particles happen in an infinitely small time and are uncorrelated in time. In Brownian motion but also in turbulence this is a fair assumption; the accelerations in turbulence occur at the Kolmogorov timescale t_k, which is in the order of a second. We also know that $t_k/T_L \sim (Re)^{-\frac{1}{2}}$. This means that in highly turbulent flow ($Re \gg 1$) t_k and T_L are wide apart, so that a range of times t exists $t_k << t < T_L$, for which the accelerations of fluid particles can be indeed be considered to take place in an infinitely small time and can be considered to be uncorrelated. The moments of this white noise can be argued for as follows.

When the temperature and composition of the medium are constant throughout the volume considered, Brownian motion is a homogeneous process. The random forcing and the timescale β do not depend on z. This process can then be modelled by a random force with zero mean $\overline{\eta} = 0$ and variance $\overline{\eta(t')\eta(t'')} = 2\sigma^2\beta(dt)^{-1}\delta_{t't''}$. Here σ^2 is the variance of the particle velocity, when the particle is in thermal equilibrium with the surrounding molecules: $\sigma^2 = \frac{kT}{M}$, with k the Bolzmann constant, T temperature and M the molecular mass. This expression for $\overline{\eta^2}$ reflects that the variance of a white noise process goes to infinity for $dt \to 0$. Because of this we prefer to write the Langevin equation in incremental form, using $\eta dt = d\mu$

$$dW = -\frac{W}{T_L}dt + d\mu \text{ and } dZ = Wdt. \tag{2.23}$$

Here $d\mu$ is a Gaussian white noise process with $\overline{d\mu} = 0$ and $\overline{d\mu(t')d\mu(t'')} = 2\sigma^2\beta\, dt\, \delta_{t't''}$. For turbulent dispersion we substitute T_L for β^{-1} and then σ^2 is the second moment of the turbulence velocities $\sigma^2 = \overline{u_3^2}$.

To interprete this all the discrete form

$$W_{n+1} = (1 - \frac{\Delta t}{T_L})W_n + \Delta\mu$$

is probably the most clear. This in connection with defining integrals of stochastic variables as will be discussed in section 2.4. Although we prefer this last discrete notation, we will not rigorously avoid the continuous incremental form Eq. (2.23).

We will show that by the above specifications of $d\mu$ it is ensured that in Brownian motion the particles are continuously in thermal equilibrium if the initial velocities are in thermal equilibrium. In turbulence dispersion we consider particles that have the same mass as an equally large fluid element. "Thermal equilibrium" here means simply that the variance of the particle velocities is equal to that of the turbulence velocities ($\overline{W}(t) = 0$ and $\overline{W^2(t)} = \sigma^2 = \overline{u_3^2}$). Before we show that this is ensured, we discuss the first-order model and its autocorrelation and spectrum. Then we will show that the models are fair descriptions for both small and large time behaviour. This can be shown for both the velocity and the displacement characteristics.

We investigate the first-order dispersion model Eq. (2.23) in discrete form, the form in which autoregressive processes are usually modelled. In discrete form the Langevin equation reads

$$W_{(n+1)\Delta t} = \alpha W_{n\Delta t} + \Delta\mu_{n\Delta t} \quad \text{and}$$
$$Z_{(n+1)\Delta t} = Z_{n\Delta t} + W_{n\Delta t}\Delta t \, , \tag{2.24}$$

with $\alpha = 1 - \Delta t/T_L$. We investigate its autocorrelation and spectrum.

The <u>autocorrelation</u> $R_W(k\Delta t)$ of a first order velocity process Eq. (2.24) can be calculated by multiplying the equation by $W_{(n+1-k)\Delta t}$ and ensemble averaging. We obtain, if the correlation between the velocity and the random forcing is zero, which we will show later (section 2.4):

$$\overline{W_{(n+1)\Delta t}W_{((n+1)-k)\Delta t}} = \alpha \, \overline{W_{n\Delta t}W_{(n-(k-1)\Delta t}} \, .$$

If the velocity process is stationary then we can divide this equation on both sides by $\overline{W^2_{n+1}} = \overline{W^2_n}$. Then from the autocorrelation function definition Eq. (2.14) we see that R_W satisfies the relation $R(k\Delta t) = \alpha R((k-1)\Delta t)$ for $k \geq 1$. With $R(0) = 1$ we get $R(k\Delta t) = \alpha^k$. For a general first-order process Eq. (2.24) to be stationary we have to require that $-1 < \alpha < 1$. The negative α's correspond to an autocorrelation function that for large k's decays exponentially to zero and oscillates in sign. This case is not of our interest as we have $0 < \alpha = 1 - \frac{\Delta t}{T_L} < 1$. For positive α's and for large k's the velocity autocorrelation becomes

$$R(\tau) = \lim_{\substack{k\to\infty \\ k\Delta t = \text{constant}}} \left(1 - \frac{\Delta t}{T_L}\right)^k = e^{-\frac{\tau}{T_L}} \, , \tag{2.25}$$

where $\tau = k\Delta t$. Note that the requirement that k is large or the requirement Δt is small give both the same τ. So the shape of the autocorrelation function of our first order process Eq. (2.24) is exponential and scales with T_L. This is consistent with the definition of T_L Eq. (1.10) as the integral over the autocorrelation from $\tau = 0$ till $\tau = \infty$. Analogously the velocity autocorrelation of the Brownian motion process is an exponential function that scales with β^{-1}.

From measurements it is indeed found that turbulent dispersion and also molecular diffusion at a finer timescale can be described by exponential autocorrelations. However, other autocorrelations like $R(\tau) = (1+\tau/T_L)^{-2}$ describe the measurements equally well and it is concluded that dispersion does not depend very strongly on the exact shape of R (Pasquill, 1983, pp. 123-125).

A shortcoming of our Langevin model is that the autocorrelation Eq. (2.15) has an undefined tangent at the origin. Near the origin the shape of the autocorrelation function of turbulence dispersion should be determined by the microscale t_m, where t_m is defined as

$$t_m^{-2} = - \tfrac{1}{2} \left. \frac{d^2R_L(\tau)}{d\tau^2} \right]_{t=o} ,$$

and the expansion of $R(\tau)$ near the origin should read

$$R(\tau) = 1 - \frac{\tau^2}{t_m^2} + \ldots$$

Our Langevin model for turbulence dispersion does not show this behaviour for times in the order of t_m (order of second). However, this shortcoming is not serious.

The <u>spectrum</u> of the Langevin equation can be calculated as follows. Decompose the velocity and the random forcing function in a Fourier series $A(\theta)$ resp. $B(\theta)$ defined by

$$W_{n\Delta t} = \sum_{o}^{\infty} A(\theta)\, e^{i\theta n\Delta t} \quad \text{and}$$

$$\Delta\mu_n = \sum_{o}^{\infty} B(\theta) e^{i\theta n\Delta t} . \qquad (2.26)$$

As $\Delta\mu_n$ is a white noise process B is not a function of the frequency θ; $d\mu$ has a constant spectrum.
Substitution of Eq. (2.26) in Eq. (2.24) gives

$$A(\theta) = \frac{B}{e^{i\theta\Delta t} - \alpha} .$$

Multiplying with its complex conjugate gives

$$\|A(\theta)\|^2 = \frac{\|B\|^2}{1 + \alpha^2 - 2\alpha \cos \theta\Delta t} .$$

Then expanding this in Δt neglecting terms of order $O(\Delta t^3)$ results in

$$\|A(\theta)\|^2 = \frac{\|B\|^2}{1 + \alpha^2 - 2\alpha + \alpha (\theta\Delta t)^2} ,$$

which by substituting $\alpha = 1 - \frac{\Delta t}{T_L}$ and $\|B\|^2 \equiv \overline{(\Delta\mu)^2} = 2 \frac{\sigma^2}{T_L} \Delta t$ gives

$$S(\theta) \equiv \|A(\theta)\|^2 = 2 \frac{\sigma^2 \; T_L}{(1 + T_L^2\theta^2)} \frac{1}{\Delta t} . \qquad (2.27)$$

This velocity spectrum has a θ^{-2} behaviour at frequencies large compared to T_L^{-1}. Monin and Yaglom (1977, Ch. 5.8) show that a Lagrangian spectrum of turbulence velocities should have a minus-two power law in the inertial subrange. Therefore the first-order process known as the Langevin equation is a good description for homogeneous turbulent dispersion on a finer time scale.

We showed that the Langevin model is a good description of turbulence dispersion and of Brownian motion on coarse timesteps. Now we investigate the velocity variance and spread of the particles as given by this model to show that the random forcing function in this homogeneous model ensures that the particles are always in thermal equilibrium with the environment if they are released in thermal equilibrium. The Langevin equations in continuous incremental form Eq. (2.23) has constant coefficients in a homogeneous medium and can be solved to give

$$W(t) = W_o \, e^{-t/T_L} + e^{-t/T_L} \int_{\mu(o)}^{\mu(t)} e^{t'/T_L} d\mu(t') \quad \text{and}$$

$$(2.28)$$

$$Z(t) = W_o T_L \, (1 - e^{-t/T_L}) - T_L \, e^{-t/T_L} \int_o^t e^{t'/T_L} \, d\mu(t') + T_L \int_o^t d\mu(t') ,$$

where T_L may be interchanged with β^{-1} (Lin and Reid, 1962, Ch. 4). It follows immediately with the above specified random forcing function and initial conditions, that $\overline{W}(t) = 0$ and $\overline{Z}(t) = 0$. This conclusion is only valid in homogeneous conditions. In nonhomogeneous conditions $d\mu$ becomes a function of displacement. Then we have to know the place of the particle from t'=0 till t to calculate the integrals in which $d\mu$ is involved.

Squaring Eq. (2.28) and ensemble averaging we get

$$\overline{W^2(t)} = \overline{W_o^2}\, e^{-t/T_L} + e^{-t/T_L} \int_0^t \int_0^t e^{(t'+t'')/T_L}\, \overline{d\mu(t')d\mu(t'')}$$

$$+ 2e^{-2t/T_L} \int_0^t e^{t'/T_L}\, \overline{W_o d\mu(t')} \, .$$

The initial velocity W_o is uncorrelated with $d\mu(t)$ and $\overline{d\mu(t')d\mu(t'')} = 2\sigma^2\beta\, dt\, \delta_{t't''}$. So we get

$$\overline{W^2(t)} = \sigma^2 \tag{2.29a}$$

We showed that the particles are always in thermal equilibrium with the environment: $\overline{W(t)} = 0$ and $\overline{W^2}(t) = \sigma^2$. Analogously we find

$$\overline{Z^2(t)} = 2\sigma^2\, [t\, T_L - T_L^2\, (1 - e^{-t/T_L})] \tag{2.29b}$$

We see that the velocity process is indeed a stationary process, whereas the displacement is not.

Eq. (2.29b) is for both short and large times identical to Taylor's classical formula (Eq. 1.10)

$$\overline{Z^2}(t) = \sigma^2 t^2 \qquad \text{for} \qquad t \ll T_L \text{ and}$$

$$= 2\sigma^2 t\, T_L \qquad \text{for} \qquad t \gg T_L .$$

This first-order model (Eq. 2.22) or Eq. (2.23) with the proper initial conditons appears to be particularly suited for the description of Brownian and turbulent dispersion in homogeneous and stationary situations. This homogeneous Langevin equation is not directly applicable to turbulent dispersion in inhomogeneous conditions. In that case the random forcing function has to be modelled differently. This analysis will be pursued later in section 2.3, after we have prepared the necessary theory in section 2.2.

2.1.6 Higher order autoregressive models

The measured autocorrelation and spectrum of dispersion processes that we want to model, may be more complex than the ones described in the previous paragraphs. This might lead to the idea of describing the velocity process by a higher order AR process, which has more degrees of freedom. However, we show that these processes lack an important property.

We introduce the concept Markov process. A Markov process is a stochastic process in which the next value only depends on the current value and not on the previous values. Only zero-order and first-order AR processes possess this Markov property by definition. In the zero-order model Eq. (2.13) $W_{n\Delta t}$ does not even depend on the current velocity $W_{(n-1)\Delta t}$. The velocity is therefore a Markov process. The displacement Z in this model Eq. (2.17), also a zero-order AR process, is therefore also a Markov process. In the Langevin model for W (Eq. 2.24), a first-order model for the velocity, the current velocity depends on the velocity one timestep back and the velocity is thus also a Markov process. From this Langevin equation an equation for the displacement can be derived, which can be shown not to possess the Markov property, the individual displacement steps depend on former values. The equation for $Z_{n\Delta t}$ from Eq. (2.24)

$$
\begin{aligned}
Z_{(n+1)\Delta t} &= Z_{n\Delta t} + W_{n\Delta t}\Delta t \\
&= Z_{n\Delta t} + (\alpha\, W_{(n-1)\Delta t} + \Delta\mu_{(n-1)\Delta t})\Delta t \\
&= Z_{n\Delta t}(1 + \alpha) - \alpha\, Z_{(n-1)\Delta t} + d\mu_{(n-1)\Delta t}\Delta t\ .
\end{aligned}
$$

This Z process is not a Markov process as values two timesteps back are involved. It is a second-order AR process.

If a process is not Markovian, like our process for Z, we can change to a description in which we include more variables and it can be shown that such a multivariate process might be Markovian. In turbulence dispersion e.g. the process (Z,W) is Markovian as (Z_n, W_n) determines (Z_{n+1}, W_{n+1}). Sometimes, reasons other than possessing the Markov property or not, make it even necessary to include more variables. E.g. in case of spatial inhomogeneity, we cannot describe its effect on dispersion by only looking at the Markovian velocity process. We have to know where the particles are, to know the effect of the inhomogeneity. In other words we have to consider the bivariate process (W,Z).

Higher order AR processes do not possess the Markov property. In the next chapter we will show that this is a serious disadvantage as we can no longer derive its Eulerian equivalent the Kramers Moyal Expansion, that describes the time evolution of the probability distribution. A second order model for the velocity can be written as a Markov process for the acceleration and velocity. However, little measurements exist for the acceleration and for these reasons we think the Langevin model is the best AR process to describe dispersion with.

2.2 Kramers Moyal expansions

2.2.1 Derivation of Kramers Moyal expansions

The Langevin equation in homogeneous situations can analytically be solved. Expressions for the mean and variance of displacement and velocity can be derived (see Eq. (2.28) and (2.29)). From these equations it followed that in homogeneous turbulence the particles are always in thermal equilibrium. In inhomogeneous turbulence this is not true, except for the release time (if the initial conditions are so specified) and the steady state. In inhomogeneous situations the resulting (nonlinear) Langevin equation cannot be integrated and no analytical results can be obtained. To prepare for an analysis of the Langevin model in inhomogeneous conditions we derive an Eulerian equivalent of the Lagrangian Langevin equation. With these Eulerian equivalents we show that except for the zero-order model the dispersion models are not equivalent with the diffusion equation. The higher-order processes can not be called diffusion.

In inhomogeneous turbulence we distinguish ensemble averages over all particles from averages over particles at a certain height z, because only in homogeneous turbulence these two averages are equal.

Dispersion in inhomogeneous turbulence is described in the vertical by an equation for the velocity W and the place Z of a particle. We consider a general bivariate Markov process (Z,W) in continuous notation, where Z and W are related by dZ = Wdt. By definition the evolution of a Markov process is determined by its present state only. This is expressed in the general Markov property for the probability density function P(z,w;t):

$$P(z,w;t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} P(z-\Phi,w-\psi;t-dt)P_{tr}(\Phi\|\psi|z-\Phi,w-\psi)d\Phi d\psi \ , \qquad (2.30)$$

where $P_{tr}(\Phi,\psi\|z-\Phi,w-\psi)$ is the stationary transition probability that a particle at $(Z-\Phi,W-\psi)$ makes a jump (Φ,ψ) to (Z,W) in a time dt. Note that $\Phi = dZ$ and $\psi = dW$ are Lagrangian variables, denoted by capitals, while z and w are Eulerian coordinates. Since W and Z are related through dZ(t) = W(t)dt we have

$$P_{tr}(\Phi,\psi|z-\Phi,w-\psi) = \hat{P}_{tr}(\psi|z-\Phi,w-\psi)\delta(\Phi-wdt).$$

Subsituted in Eq. (2.30) this gives

$$P(z,w;t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} P(z-\Phi,w-\psi;t-dt)\hat{P}_{tr}(\psi\|z-\Phi,w-\psi)\delta(\Phi-wdt)d\Phi d\psi$$

$$= \int_{-\infty}^{\infty} P(z-wdt,w-\psi;t-dt)\hat{P}_{tr}(\psi\|z-wdt,w-\psi)d\psi. \qquad (2.31)$$

Expansion of the integrand of Eq. (2.31) in a Taylor series, while neglecting terms of higher order in dt, gives

$$P(z-wdt,w-\psi;t-dt)\hat{P}_{tr}(\psi\|z-wdt,w-\psi) =$$

$$P(z,w;t)\hat{P}_{tr}(\psi\|z,w) - wdt\frac{\partial}{\partial z}(P\hat{P}_{tr}) + \sum_{n=1}^{\infty}\frac{(-1)^n\ \psi^n}{n!}\frac{\partial^n(P\hat{P}_{tr})}{\partial w^n} - dt\ \hat{P}_{tr}\frac{\partial P}{\partial t}$$

(2.32)

In the following we will use

$$\int_{\text{all }\psi} \hat{P}_{tr}(\psi|z,w)d\psi = 1 \quad , \qquad (2.33a)$$

$$\int \psi^n\ \hat{P}_{tr}\ (\psi\|z,w)d\psi = \langle\psi^n\rangle_w \quad , \qquad (2.33b)$$

$$\int \psi^n\ \frac{\partial^n\hat{P}_{tr}}{\partial w^n}\ (\psi|z,w)d\psi = \frac{\partial^n}{\partial w^n}\ \langle\psi^n\rangle_w \ , \qquad (2.33c)$$

where the subscript w means that the conditional average is taken over particles with velocity W. The identity (2.33a) is a general property of pdf. The second identity (2.33b) can be rewritten as

$$\int (dW)^n\ \hat{P}_{tr}(dW|z,w)d(dW) = \langle(dW)^n\rangle_w \ ,$$

that is Eq. (2.33b) is equivalent to the average of $(dW)^n$ over all marked particles at height Z = z and with velocity W = w. It calculates the average velocity change of particles at a certain point (z,w) in phase space. Eq. (2.33c) estimates the change of this average when the Eulerian velocity w change. As the velocity changes dW (integration variable) are not dependent on the Eulerian velocity w (with respect to which we make the derivation) we can take the derivation outside the integral sign.

Substituting Eq. (2.33) into Eq. (2.32) we get

$$P(z,w;t) = \int P(z,w;t)\hat{P}_{tr}(\psi\|z,w)d\psi - dt\int w\,\frac{\partial(P\hat{P}_{tr})}{\partial z}\,d\psi$$

$$+\int\sum_{n=1}^{\infty}(-1)^n\,\frac{\psi^n}{n!}\,\frac{\partial^n(P\hat{P}_{tr})}{\partial w^n}\,d\psi - dt\int\hat{P}_{tr}\,\frac{\partial P}{\partial t}\,d\psi. \qquad (2.34)$$

Using the Eq. (2.33) we get for the first term on the RHS of Eq. (2.34):

$$\int P(z,w;t)\hat{P}_{tr}(\psi\|z,w)d\psi = P(z,w;t)\int\hat{P}_{tr}\,d\psi = P(z,w;t)\ .$$

Analogously, the last term of Eq. (2.34) gives

$$\int\hat{P}_{tr}\,\frac{\partial P}{\partial t}\,d\psi = \frac{\partial P}{\partial t}\ .$$

In the second term we use, that we only consider particles with Z=z and W=w. It becomes

$$\int w\,\frac{\partial(P\hat{P}_{tr})}{\partial z}\,d\psi = w\,\frac{\partial P}{\partial z}\int\hat{P}_{tr}\,d\psi + w\,P\,\frac{\partial}{\partial z}\int\hat{P}_{tr}\,d\psi = w\,\frac{\partial P}{\partial z}\ .$$

The third term yields

$$\int\psi^n\,\frac{\partial^n(P\hat{P}_{tr})}{\partial w^n}\,d\psi = \frac{\partial^n}{\partial w^n}\int\psi^n\,P\hat{P}_{tr}d\psi$$

$$= \frac{\partial^n}{\partial w^n}\,P\int\psi^n\,\hat{P}_{tr}d\psi = \frac{\partial^n}{\partial w^n}\,P\langle\psi^n\rangle_w\ .$$

Substitution of the above equations in Eq. (2.34) gives

$$P(z,w,t) = P(z,w,t) - w\,dt\,\frac{\partial P}{\partial z} + \sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\,\frac{\partial^n}{\partial w^n}\,(P\langle\psi^n\rangle_w) - dt\,\frac{\partial P}{\partial t}\ .$$

Thus, we get the <u>general KME for a bivariate Markov process</u> (van Kampen, 1983, p. 215)

$$\frac{\partial P(z,w;t)}{\partial t} + w\,\frac{\partial P}{\partial z} = \sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\,\frac{\partial^n}{\partial w^n}\left\{\frac{P\langle\psi^n\rangle_w}{dt}\right\}\ . \qquad (2.35)$$

Analogously, we can derive the KME for a monovariate process Z. This KME for P(z;t) reads

$$\frac{\partial P}{\partial t}(z;t) = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n}{\partial z^n} \{P \frac{\langle\phi^n\rangle}{dt}\} \quad , \qquad (2.36)$$

where $\langle\phi^n\rangle$ is the average of $(dZ)^n$ taken over particles at the height z.

We derived KME's, a tool to investigate Langevin models in inhomogenous turbulence. In the next section we apply the general KME to the zero-order and first-order autoregressive processes derived before for homogeneous turbulence. This will show us that only the zero-order model is equivalent with the diffusion equation. The treatment of dispersion for inhomogeneous models based on the here derived general KME is presented in section 2.3.

2.2.2 KME for zero order process in a homogeneous medium

We apply the KME derived in the proceeding section to the simple random walk model, Eq. (2.17). This continous homogeneous random walk is the monovariate Markov process $dZ = 2D^{\frac{1}{2}}\omega_t$, where ω_t is a (e.g. Gaussian) white noise process with $\overline{\omega_t} = 0$ and $\overline{\omega_t^2} = dt$. From this equation the moments $\langle (dZ)^n \rangle$ can be derived. We have $\langle dZ \rangle = \overline{dZ} = 0$ and $\langle (dZ)^2 \rangle = \overline{(dZ)^2} = 2Ddt$, while all higher moments are zero in order dt. The KME for a general monovariate process Eq. (2.36) applied to this random walk is a diffusion equation:

$$\frac{\partial P(z;t)}{\partial t} = D\,\frac{\partial^2 P}{\partial z^2}\ . \qquad (2.37)$$

This is the reason why this special dispersion process is called a diffusion process.

Here we also see why we choose the constant in the random walk process Eq. (2.13) equal to 2D. It turns out that this gives the classical formulation of a diffusion equation with diffusivity D. The pdf describing the probability of the random walk trajectory $P(z,t) = (4\pi Dt)^{-\frac{1}{2}}\exp(-z^2/4Dt)$ (Eq. (2.2.1)), is indeed the solution of this KME Eq. (2.37).

2.2.3 KME for first-order process in a homogeneous medium

Brownian motion on a finer timescale and also homogeneous turbulence dispersion is described by a bivariate Markov Process (Z,W). The displacement Z and the velocity W is described by Eq. (2.23)

$$dW = -\frac{Wdt}{T_L} + d\mu \qquad \text{and} \qquad dZ = Wdt \ ,$$

with for $d\mu$ a Gaussian distribution specified by
$\langle d\mu\rangle = \overline{d\mu} = 0$ and $\langle (d\mu)^2\rangle = \overline{(d\mu)^2} = 2\sigma^2/T_L\, dt$. From this equation we derive the moments of dW needed in the general KME:

$$\langle dW\rangle_w = -\frac{wdt}{T_L} + O(dt^2) \ ,$$

$$\langle (dW)^2\rangle_w = \frac{2\sigma^2}{T_L} dt + O(dt^2) \qquad \text{and}$$

$$\langle (dW)^n\rangle_w = O(dt^2) \text{ for } n \geqq 3.$$

Substituting this in the general KME Eq. (2.35) we see that the bivariate Markov process for (Z,W) corresponds with the KME

$$\frac{\partial P(z,w;t)}{\partial t} + w\frac{\partial P}{\partial z} = \frac{\partial}{\partial w}\left(\frac{wP}{T_L}\right) + \sigma^2\, T_L \frac{\partial^2 P}{\partial w^2} \ . \qquad (2.38)$$

In this first order AR model a timescale T_L is involved which causes its KME not to be equal to the diffusion equation; we reserve with the general name dispersion for these processes. We limited the discussion to homogeneous first-order processes; inhomogeneous Langevin models will be discussed in section 2.3. They will be shown to have KME's which are differential equations of infinite order. Only in Gaussian inhomogeneous turbulence they reduce to a third-order differential equation.

2.2.4 KME for second order processes

A second order process for W is not a Markov process anymore. The probability density function does not obey the Eq. (2.35) and no KME can be derived. Our theoretical analyses break down as the derivation of the moments of the random forcing is based on the KME's of our Lagrangian model.

Another idea would be to make a model for the acceleration. This procedure of describing a higher derivative is useful in case the variable is not stationary. Differences of the variable might turn out to be stationary (Box & Jenkins, Ch. 4). Such a model would imply very small timesteps while little knowledge of accelerations at this scale in the atmosphere exists. We leave this idea therefore.

2.3 Random forcing function in an inhomogeneous Langevin model

2.3.1 Introduction of two studies paper I and II

Until recently dispersion in inhomogeneous circumstances was still problematic to model. Applying the homogeneous Langevin equation to these circumstances lead to erroneous results. This equation could not for example describe the complicated behaviour of plumes in the convective boundary layer as discussed in Ch. 1. Recently two theoretical studies have been performed on how to model the random forcing function in a Langevin model, so that we can apply it to inhomogeneous turbulence. These studies resulted in formulas for the moments of the random forcing function. In Ch. 4 we apply these formulas to the convective boundary layer and herewith show the success of these studies. The first research was done by Thomson (1984) to which we further will refer as paper I. The second research by v. Dop et al. (1985) (paper II) is an approach which for stationary circumstances leads to the same results found in I.

We found that both papers use the same mathematics. They do not directly analyse the Langevin equation, but analyse its KME (paper II) or the fourier transform of the KME (paper I). We will show that the result of both mathematical exercises is a set of moment rate equations for the velocity W of the particle. Paper II gives them in real space, while paper I gives them in fourier space.

The physics involved in the analyses is different though. The physics differ in that paper I requires certain properties of the model for large times whereas paper II specifies requirements for all times. Paper I's requirements lead to the moments of $d\mu$ in stationary turbulence, while the advantage of paper II is that it results in expressions for the moments of $d\mu$ that include instationary turbulence.

In the next three subsections the mathematics used in both researches is given and intercompared to show that they are identical. Subsection 2.3.5 and 2.3.6 give the physics of both models and the resulting equations for the moments $\langle (d\mu)^n \rangle$. The last chapter is a discussion of the physics used in both papers and of the expressions for $\langle (d\mu)^n \rangle$.

2.3.2 Mathematics used in paper II: the KME and its moment rate equations

The mathematical analysis of the Langevin equation is made to investigate what the moments of $d\mu$ should be, in order that the Langevin equation can describe dispersion in inhomogeneous circumstances. In this chapter we discuss the mathematics used in paper II. The Langevin equation considered, has the form $dW = \frac{W}{T_L}\,dt + d\mu$. The moments of $d\mu$ are formally put equal to

$$\langle (d\mu)^n \rangle = a_n\, dt\ . \tag{2.39}$$

We start the analysis from the KME of the Langevin equation. The general KME for a bivariate Markov process is given in Eq. (2.35):

$$\frac{\partial P(z,w;t)}{\partial t} + w\,\frac{\partial P}{\partial z} = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!}\,\frac{\partial^n}{\partial w^n}\left(\frac{P\langle \psi^n \rangle_w}{dt}\right),$$

where the average $\langle \psi^n(z) \rangle_w = \langle (dW)^n \rangle_w$ is a conditional average over particles with a velocity $W(t) = w$, passing through z at time t.
We can calculate $\langle \psi^n \rangle_w$ from the Langevin equation. The Langevin model gives in first order of dt

$$\begin{aligned} \langle \psi \rangle_w &= \langle dW \rangle_w = \left[-\frac{w}{T_L(z)} + a_1(z)\right]dt \quad \text{and} \\ \langle \psi^n \rangle_w &= \langle (dW)^n \rangle_w = a_n(z)dt \quad \text{for} \quad n \geqq 2\ . \end{aligned} \tag{2.40}$$

Substituting Eq. (2.40) in Eq. (2.35) we get the KME of the Langevin equation

$$\frac{\partial P(z,w;t)}{\partial t} + w\,\frac{\partial P}{\partial z} = \frac{\partial}{\partial w}\left\{\frac{w\,P}{T_L(z)}\right\} + \sum_{\nu=1}^{\infty} \frac{(-1)^\nu}{\nu!}\, a_\nu(z)\,\frac{\partial^\nu P}{\partial w^\nu}\ . \tag{2.41}$$

From this KME we can derive moment rate equations for $\langle W^n \rangle$ by multiplying Eq. (2.41) with w^n and integrating over w. They read

$$\frac{\partial C}{\partial t} = -\frac{\partial \langle W \rangle C}{\partial z}, \tag{2.42a}$$

$$\frac{\partial \langle W \rangle C}{\partial t} = -\frac{\partial \langle W^2 \rangle C}{\partial z} + \left(a_1 - \frac{\langle W \rangle}{T_L}\right)C, \tag{2.42b}$$

$$\frac{\partial\langle W^2\rangle C}{\partial t} = - \frac{\partial\langle W^3\rangle C}{\partial z} - 2\,\frac{\langle W^2\rangle C}{T_L} + (a_2 + 2a_1\langle W\rangle)C. \qquad (2.42c)$$

These are the moment rate equations used in paper II.

In the next paragraph we turn to the mathematics of paper I and in subsection 2.3.3 we will compare them.

2.3.3 Mathematics used in paper I, the equation for characteristic function

In this section we discuss the mathematics used in paper I to arrive at an expression for the random forcing function in the Langevin model applicable to dispersion in inhomogeneous turbulence. Paper I made use of moment generating functions (mgf) $\hat{g}$ of the probability function $P(z,w;t)$. We will first explain this concept. The mgf $\hat{g}(\underset{\sim}{\theta})$ of a multivariate stochastic process $\underset{\sim}{X} = (X_1, X_2, \ldots, X_k)$ is defined as a transform of $P(\underset{\sim}{X})$:

$$\hat{g}(\underset{\sim}{\theta}) \equiv \int e^{\underset{\sim}{\theta}\cdot\underset{\sim}{x}} P(\underset{\sim}{x})d\underset{\sim}{x} .$$

Expanding the integrand in a Taylor series we get

$$\hat{g}(\theta) = \sum_{m_j=0}^{\infty} \frac{\theta_1^{m_1}\theta_2^{m_2}\ldots\theta_k^{m_k}}{m_1!m_2!\ldots m_k!} \overline{X_1^{m_1} X_2^{m_2} \ldots\ldots X_k^{m_k}} . \qquad (2.43)$$

with $j = 1, 2, \ldots k$.

We see that the coefficients in the Taylor expansions of $\hat{g}(\underset{\sim}{\theta})$ are the moments of $P(\underset{\sim}{x})$. From this fact $\hat{g}$ gets its name of moment generating function.

We will only make use of a slightly different concept namely the characteristic function also denoted by $\hat{g}$. This is the fourier transform of $P(\underset{\sim}{x})$. This function has the advantage that it converges for all pdf's. It is defined by

$$\hat{g}(\underset{\sim}{\theta}) \equiv \int e^{i\underset{\sim}{\theta}\cdot\underset{\sim}{x}} P(\underset{\sim}{x})d\underset{\sim}{x} .$$

Expanding the integrand in a Taylor series we get

$$\hat{g}(\theta) = \sum_{m_j=0}^{\infty} \frac{(i\theta_1)^{m_1}(i\theta_2)^{m_2}\ldots(i\theta_k)^{m_k}}{m_1!m_2!\ldots m_k!} \overline{X_1^{m_1}X_2^{m_2}\ldots\ldots X_k^{m_k}} .$$

with $j = 1, 2, \ldots, k$.

In our first-order dispersion models we are concerned with a bivariate process (Z,W). We will not consider its general characteristic function, but we will make use of the marginal characteristic function (mcf) of $P(z,w;t)$, which is defined as the Fourier transform in only one variable, here a transform of the velocity:

$$\hat{g}(z,\theta;t) \equiv \int e^{iw\theta}\, P(z,w;t)dw \;.$$

Expanding the integral in a Taylor series yields

$$\hat{g}(z,\theta;t) = \sum_{n=0}^{\infty} \frac{(i\theta)^n}{n!} \int w^n\, P(z,w;t)dw \;.$$

We have to be careful, as two kind of moments are in use (see Eq. 2.2):

$$\overline{W^n} \equiv \frac{\int w^n\, P(z,w;t)dwdz}{\int P(z,w;t)dwdz} \quad \text{and}$$

$$\langle W^n \rangle \equiv \frac{\int w^n\, P(w,z;t)dw}{\int P(z,w;t)dw} = \int \frac{w^n\, P(z,w;t)}{P(z;t)}\, dw = \frac{\int w^n\, P(z,w;t)dw}{C(z,t)} \;.$$

We see that the mcf gives us the bracketed moments $\langle W^n \rangle$ times the averaged concentration $C(z,t)$:

$$\hat{g}(z,\theta;t) = \sum_{n=0}^{\infty} \frac{(i\theta)^n}{n!} \langle W^n \rangle C(z,t) \;. \qquad (2.44)$$

For the mathematical analysis of the Langevin model we also need the characteristic function of the random forcing function at a height z. It reads, using $\langle (d\mu)^n \rangle = a_n dt$ for $n \geq 1$ Eq. (2.39) and $a_o = 1$:

$$\hat{f}_z(\theta) \equiv \int e^{i\theta d\mu} P(d\mu)d\mu = \sum_{n=0}^{\infty} \frac{i^n \theta^n}{n!} a_n(z)\, dt = 1 + \sum_{n=1}^{\infty} \frac{i^n \theta^n}{n!} a_n(z)dt \;, \qquad (2.45)$$

Paper I derived from the Langevin equation a time rate equation for the mfg of W. After a slight modification we get a time rate equation for mcf of W, which reads

$$\frac{\partial \hat{g}}{\partial t} + \frac{\partial^2 \hat{g}}{\partial \theta \partial z} = - \frac{\theta}{T_L} \frac{\partial \hat{g}}{\partial \theta} + \hat{g} \sum_{n=1}^{\infty} \frac{i^n \theta^n}{n!} a_n(z) + O(dt^2). \qquad (2.46)$$

For the exact derivation of this equation we refer to paper I. For future discussions we note that subsituting the mcf of W (Eq. (2.44)) into the time rate equation for this function Eq. (2.46) and equating powers of θ, gives us moment rate equations for the moments of W. This we will use in the next subsection in the comparison of the mathematics used in paper I with the mathematics used in paper II.

2.3.4 Comparison of the mathematics used in paper I and II

Paper I and II derived moment rate equations for the moments of W. It can easily be shown that the equations derived in paper I given by Eq. (2.46) are equal to those derived in paper II (Eq. (2.42)). They are equal because the mathematical analysis in both papers is the same although one analysis is made in fase space and the other in fourier space. Altough this can easily be seen, we will explain it.

The mcf used in paper I is the fourier transform of the pdf P(z,w;t). From this we expect that the time rate equation for the mcf Eq. (2.46) is the fourier transform of the time rate equation for P(z,w;t) the KME Eq. (2.41). This can indeed easily be proven by multiplying the KME Eq. (2.41) by $e^{iw\theta}$ and integrating over w. This fourier transform is then exactly equal to Eq. (2.46).

It can also be put in different words, by saying that paper II also derived the time rate equation for the cf Eq. (2.46), although not explicitly. They multiplied the KME with w^n and integrated over w to get the time rate equations for $\langle W^n \rangle$. These operations for each single n can be combined. Instead of multiplying the KME by w^n we can multiply KME by $\sum_{n=0}^{\infty} \frac{i^n w^n}{n!} = e^{iw\theta}$ and then integrate over w. This is the same as fourier transforming the KME.

We showed that both papers use the same mathematics and arrive at the same moment rate equations for the velocity W.

2.3.5 Paper I's derivation of the moments of the random forcing function

We discussed the mathematics that resulted in Eqs. (2.42) for the moments of W in both studies. We now turn to the physics of the analyses. These consist of requirements on the velocity statistics of the particles. The physical requirements differ in both papers. Paper I proceeded by considering the steady state $\frac{\partial \hat{g}}{\partial t} = 0$. It was argued, that in this circumstance the released particles must have the same velocity characteristics as the surrounding fluid particles; so $\hat{g} = \hat{g}_a$ where $\hat{g}_a$ is the mcf of the turbulence velocity fluctuations u_3:

$$\hat{g}_a = \sum_{n=0}^{\infty} \frac{(i\theta)^n}{n!} \overline{u_3^n} \rho(z,t) ,$$

where $\rho(z)$ is the density of the air $\rho(z) = \int P(z,u_3)du_3$.

We note that paper I required that the mgf of the particle velocities $\hat{g}$ and the mgf of the turbulence velocities $\hat{g}_a$ are equal. From the equations for these mgf's Eq. (2.44) and (2.47) it follows that this is equivalent to requiring that $\langle W^n\rangle C(z) = \overline{u_3^n}\, \rho(z)$. This is not equivalent as paper I claims to $\langle W^n\rangle = \overline{u_3^n}$ because $C(z) \neq \rho(z)$, but only proportional to $\rho(z)$, because the absolute value of the concentration $C(z)$ varies of course with the total mass released. The proportionality constant in $C(z) = \text{const}\ \rho(z)$ is determined by this total mass and the volume in which this mass is dispersed. From now on we only consider situations where ρ does not vary in height so that ρ divides out in Eq. (2.46) and this slight inaccuracy becomes unimportant.

Substituting the requirement $\langle W^n\rangle = \overline{u_3^n}$ in the steady state of Eq. (2.46) we get

$$\hat{g}_a \sum_{n=1}^{\infty} \frac{i^n\theta^n}{n!} a_n(z) = \frac{\partial^2 \hat{g}_a}{\partial\theta\partial z} + \frac{\theta}{T_L}\frac{\partial \hat{g}_a}{\partial\theta} \qquad \text{for } t \to \infty .$$

We can write this equation, using the definition of the mcf for $d\mu$ (Eq. (2.45)), as

$$\hat{f}_z(\theta) = 1 + \frac{dt}{T_L}\frac{\theta}{\hat{g}_a}\frac{\partial \hat{g}_a}{\partial\theta} + \frac{dt}{\hat{g}_a}\frac{\partial^2 \hat{g}_a}{\partial\theta\partial z} + O(dt^2) . \qquad (2.47)$$

This analysis was made to derive equations for the function $a_n(z)$ in the moments of $d\mu$. By substituting $\hat{g}_a$ and $\hat{f}_z$ (Eq. (2.45)) in Eq. (2.47) and equating powers of θ, there follow equations for $a_n(z)$ that we summarize by

$$a_n(z) = \frac{d\overline{u_3^{n+1}}}{dz} + n\,\frac{\overline{u_3^n}}{T_L} - \sum_{k=1}^{n-1} \binom{n}{k} \overline{u_3^{n-k}}\, a_k(z) \; . \qquad (2.48)$$

With these moments of the random forcing function $\langle (d\mu)^n \rangle$ the Langevin model should give a good description of dispersion in inhomogeneous circumstances.

2.3.6 Paper II's derivation of the moments of the random forcing function

Paper II derived the Langevin model for inhomogeneous turbulence by comparing the Langevin model to the Eulerian conservation of mass. This comparison is not made directly between the Langevin equation and the conservation of mass, but made between the moment rate equations for the velocity derived from either one. The moment rate equations for the velocity as implied by the Langevin model were derived from its KME and are given in Eqs. (2.42). We will also derive the moment rate equations for the velocity from the Eulerian equations.

The Eulerian moment rate equations, for the velocity are deduced from the Eulerian equation of conservation of motion and of mass. They can be derived by decomposing the instantaneous concentration $\tilde{c}$ into a mean and fluctuating part $\tilde{c} = C + c$ and analogous for other quantities involved (see e.g. Businger, 1984). These moment rate equation form an infinite hierarchy. The first three Eulerian moment rate equations in a horizontally homogeneous case, and with no mean flow read

$$\frac{\partial C}{\partial t} = - \frac{\partial \overline{u_3 c}}{\partial z} \quad , \tag{2.49a}$$

$$\frac{\partial \overline{u_3 c}}{\partial t} = - \frac{\partial \overline{u_3^2 c}}{\partial z} - \overline{u_3^2} \frac{\partial C}{\partial z} + \overline{c \frac{du_3}{dt}} \quad \text{and} \tag{2.49b}$$

$$\frac{\partial \overline{u_3^2 c}}{\partial t} = - \frac{\partial \overline{u_3^3 c}}{\partial z} - \overline{u_3^3} \frac{\partial C}{\partial z} + \overline{u_3^2} \frac{\partial \overline{u_3 c}}{\partial z} + 2 \overline{u_3 c} \frac{\partial \overline{u_3^2}}{\partial z} + 2 \overline{(u_3 c)' \left(\frac{du_3}{dt}\right)'} \quad . \tag{2.49c}$$

(The notation $(\ )' = (\ ) - \overline{(\ )}$ is used.)

Paper II derived the moments of $d\mu$ by comparing the Langevin moment rate equations Eqs. (2.42) to these Eulerian moment rate equations Eqs. (2.49) in a comparison for all time. In this comparison Eq. (2.8) is used, the equation that relates Lagrangian moments to Eulerian moments. This analysis resulted in the first three moments that are summarized by

$$a_n(z) = \overline{\frac{du_3^n}{dt}} + n \frac{\overline{u_3^n}}{T_L} - \sum_{k=1}^{n-1} \binom{n}{k} \overline{u_3^{n-k}} \, a_k(z). \tag{2.50}$$

These are the general equations as derived in paper II for the moments of the random forcing in the Langevin model that make it applicable to inhomogeneous turbulence.

To compare Eq. (2.50) with paper I's formula we deduce paper II's formula in <u>stationary turbulence</u>. In stationary turbulence

$$\frac{du_3^n}{dt} = u_i \frac{\partial u_3^n}{\partial x_i} = \frac{\partial u_3^{n+1}}{\partial x_i} \ ,$$

where in the last equality the continuity equation $\frac{\partial u_i}{\partial x_i} = 0$ is used. We want to emphasize that even in a 1-D description of dispersion we still have to take into account that the turbulence is 3-D. Also using that in horizontally homogeneous turbulence $\overline{u_3^{n+1}}$ only depends on the vertical coordinate we have

$$\frac{d\overline{u_3^n}}{dt} = \frac{d\overline{u_3^{n+1}}}{dz} \ .$$

Using this in Eq. (2.50) we find that they are identical to Eq. (2.48).

2.3.7 Discussion

Closure relations

In paper II expressions are derived for $a_n(z)$ by comparing the Langevin equation the Eulerian conservation equations. Correspondence of the Langevin equation with the Eulerian conservation equations is not guaranteed by these formulas for the moments alone, in addition closure relations are needed. The Langevin equation is equivalent to the Eulerian conservation equations for the first three velocity moments in case the moments of dμ are described by Eq. (2.50), with as extra requirement that the following closure relations must be satisfied:

$$\overline{c \frac{du_3}{dt}} = - \frac{\overline{u_3 c}}{T_L} \quad \text{and} \tag{2.51a}$$

$$\overline{(u_3 c) \left(\frac{du_3}{dt}\right)'} = - \frac{\overline{u_3^2 c}}{T_L} \ . \tag{2.51b}$$

In paper II the validity of these equations is discussed and though Eq. (2.51a) has some justification, Eq. (2.51b) is generally not true. It is found that Eq. (2.51a) is valid in case the following three assumptions are satisfied: (i) The turbulence should be stationary, (ii) The concentration distribution should not vary too much with height, so that the concentration distribution can be assumed to be locally linear and (iii) The velocity-autocorrelation is assumed to be exponential. This last assumption is also made in the Langevin model and is often validated by experiments.

We want to compare the closure relations Eq. (2.51) with those applied in the often used first order (K-) or higher order closure models and see whether that gives us an idea of their validity. These Eulerian models break off the infinite series of moment rate equations and close the last equation kept (see Ch. 1). We briefly review the closures of these Eulerian equations where we follow Deardorff (1978) for the case of homogeneous turbulence. In homogeneous turbulence the concentration distribution is approximately Gaussian. Deardorff stated that when the first equation for $\frac{\partial C}{\partial t}$ Eq. (2.49a) is closed with $\overline{u_3 c} = - K \frac{\partial C}{\partial z}$, the Gaussian solution with the correct spreading is reproduced for a single source, when the diffusivity K is given by

$$K(t;t_o) = \overline{u_3^2}\, T_L \{1 - \exp(-(t-t_o)/T_L)\}, \tag{2.52}$$

where t_o is the release time.

To obtain the Gaussian solution for a single source in the second order closure models the closures should read

$$\overline{u_3^2 c} = - K \frac{\partial}{\partial z} \overline{u_3 c} \ , \tag{2.53a}$$

$$\frac{1}{\rho} \overline{c \frac{\partial p}{\partial z}} = \frac{\overline{u_3 c}}{T_L} \tag{2.53b}$$

and K given by the above formula Eq. (2.52).

The same Gaussian solution will result in third order closure models when the closure relations read

$$\overline{u_3^3 c} = 3\, \overline{u_3^2}\, \overline{u_3 c} - K \frac{\partial}{\partial z} \overline{u_3^2 c} \ , \tag{2.54a}$$

$$\frac{1}{\rho} \overline{u_3 c \frac{\partial p}{\partial z}} = \frac{\overline{u_3^2 c}}{T_L} \tag{2.54b}$$

and K again given by Eq. (2.52).

Problems with these Eulerian model closures do arise though, because when the model is thus closed K should be a function of time, whereas K is an intrinsic function of the fluid. In the general case of multiple, non-simultaneous sources (different t_o's) K is different for each source and K can no longer be specified as one overall function of time t. Deardorff then points out that depending on what approximation is assigned to K, other closure relations for the pressure terms might give better results.

Although, the closure relations can not be exact, they give us an idea of how well the Langevin equation describes a dispersion process. In a situation where buoyancy, viscosity and the coriolis force can be neglected the closures Eq. (2.53b) and (2.54b) become equal to the closures that guarantee that the Langevin model is equal to the Eulerian conservation equation Eqs. (2.51). This fact will later be used in Ch. 4 where we intercompare different Langevin models.

The question arises why in paper II closure equations occur, while in paper I not. We show that this is so because the closure relations of paper II are always satisfied in the steady state. Analogously to the general derivation of the closure equations in section 2.3.6 we derive the first three Lagrangian moment rate equations for the steady state using $\langle W^n \rangle = \overline{u_3^n}$ (paper I's requirement). We get a first equation which is identically zero and then

$$\left(\frac{\partial \overline{u^2}}{\partial z} - a_1\right)C = 0$$

$$\left(a_2 - \frac{2\overline{u_3^2}}{T_L} - \frac{\partial \overline{u_3^3}}{\partial z}\right)C = 0 \qquad (2.55)$$

The first three Eulerian moment rate equation are identically zero in the steady state so that if the Langevin model has to correspond to this Eulerian description, the first and second Lagrangian moment rate equations should also be identically zero. From this, the steady state equations for $\langle (d\mu)^n \rangle$ follow without the need for closure relations and that is the reason why they do not occur in paper I. Or in other words the closure relations found in paper II are always satisfied in the steady state.

As a consequence the approach in paper I is not able to deal with nonstationary turbulence, where no steady state exist. Furthermore this approach does not give us an idea of how good a description a certain Langevin model is in the course of time, as no comparison with the Eulerian conservation equations is made. In Ch. 5 we will use Paper II's method to make an intercomparison for different Langevin models.

Moments of random forcing

We discussed the mathematics and physics of the analysis of the Langevin equation in paper I and II which in both cases lead to the same formulation of the random forcing applicable in inhomogeneous turbulence. We want to discuss the result, the relations Eq. (2.50) found for the moments of the random forcing function $d\mu$. In stationary inhomogeneous but horizontally homogeneous turbulence the first three moments are given by Eq. (2.48)

$$a_1(z) = \frac{d\overline{u_3^2}}{dz} \quad ,$$

$$a_2(z) = 2\,\frac{\overline{u_3^2}}{T_L} + \frac{d\overline{u_3^3}}{dz} \text{ and}$$

$$a_3(z) = 3\,\frac{\overline{u_3^3}}{T_L} + \frac{d\overline{u_3^4}}{dz} - 3\,\overline{u_3^2}\,\frac{d\overline{u_3^2}}{dz} \; .$$

In Ch. 5 we show that the Langevin model where the random forcing function is modelled by Eq. (2.48) is indeed a good description of dispersion in inhomogeneous circumstances.

We want to discuss the form of the first moment $\langle d\mu\rangle/dt = d\overline{u_3^2}/dz$. This first moment models the "drift acceleration" particles experience in inhomogeneous circumstances. Particles that move into a region with a larger $\overline{u_3^2}$ tend to obtain larger velocities fluctuations (not velocities!) and disperse therefore more quickly. A mean acceleration into the regions with larger $\overline{u_3^2}$ is generated. This is modelled in the first moment of $d\mu$ as can be seen by averaging the Langevin equation:

$$\frac{\langle dW\rangle}{dt} = \frac{d\overline{u_3^2}}{dz} \; .$$

We see a mean acceleration occuring.
(The fact that the mean acceleration appears in the increment notation of the Langevin equation multiplied by dt nl $\langle d\mu\rangle = d\overline{u_3^2}/dz$ should not be misinterpreted, it is not a drift velocity!)

The papers I and II modelled the Langevin equation such that it is applicable to inhomogeneous turbulence. In such circumstances not only the velocity u_3 but also T_L might vary with height. The effect of T_L varying with height is, that the velocity of particles that move into a region where T_L is larger, becomes more persistent. A mean acceleration into these regions with larger T_L appears (Durbin and Hunt, 1980). The effect of height variances in T_L does not appear in the random forcing but is automatically incorporated in the friction term $-\frac{W}{T_L(z)}$. This will be shown more explicitly in section 2.5.4, where we derive a large time limit of the Langevin equation and where this drift term will appear.

Let us consider the special case of Gaussian turbulence. The uneven moments of u_3 are then zero, while the even moments are related by

$$\overline{u_3^{2n}(z)} = \frac{(2n-1)!}{2^{n-1}(n-1)!}\,(\overline{u_3^2(z)})^n \ .$$

The first three moments of $d\mu$ given by Eq. (2.48) reduce to:

$$a_1(z) = \frac{d\overline{u_3^2}}{dz} \ , \tag{2.56a}$$

$$a_2(z) = 2\,\frac{\overline{u_3^2}}{T_L} \text{ and} \tag{2.56b}$$

$$a_3(z) = 3\,\overline{u_3^2}\,\frac{d\overline{u_3^2}}{dz} \ . \tag{2.56c}$$

We will prove that in Gaussian turbulence all higher moments of $d\mu$ are zero. We depart from the equation for the characteristic function $\hat{f}_z(\theta)$ of $d\mu$ in Gaussian turbulence. The general equation is Eq. (2.47):

$$\hat{f}_z(\theta) = 1 + \frac{dt}{T_L}\,\frac{\theta}{\hat{g}}\,\frac{\partial \hat{g}}{\partial\theta} + \frac{dt}{\hat{g}}\,\frac{\partial^2 \hat{g}}{\partial z \partial\theta} + O(dt^2) \ ,$$

where $\hat{g}$ is the mcf of u_3. In stationary Gaussian turbulence the mcf reads

$$\hat{g} = \exp(-\tfrac{1}{2}\,\theta^2\,\overline{u_3^2}(z))\rho \tag{2.57}$$

If we substitute this in Eq. (2.47) we find

$$\hat{f}_z(\theta) = 1 + \theta\ \Delta t\ \frac{d\overline{u_3^2}}{dz} + \theta^2\ \frac{\Delta t}{T_L}\ \overline{u_3^2} + \tfrac{1}{2}\ \theta^3\ \Delta t\ \overline{u^2}\ \frac{d\overline{u_3^2}}{dz} + O(\Delta t^2). \tag{2.58}$$

Since $\langle(d\mu)^n\rangle \equiv \frac{\partial^n}{\partial\theta^n}\hat{f}(\theta)\Big]_{\theta=0}$ and $\hat{f}(\theta)$ is a cubic polynomial in θ, all moments higher than the third are identically zero, which completes our prove. This concludes our investigation of the moments of the random forcing in the Langevin model, as applied to inhomogeneous Gaussian turbulence.

2.4 Itô calculus

In this chapter we discuss how to differentiate and integrate stochastic variables. For instance in the formal solution of the Langevin equation

$$W(t) = W(o) - \int_o^t \frac{W}{T_L}\, dt' + \int_o^t d\mu(t') \qquad (2.59)$$

an integral over a stochastic variable appears. This stochastic variable is not differentiable and the integral is therefore not a well-defined function, untill we have given an interpretation. An integral over a deterministic variable a is defined in the Riemann-Stieltjes sense

$$\lim_{\substack{j\to\infty \\ \Delta t\to 0}} \sum_j a(t_j^*)\Delta t_j .$$

It can be shown (Durbin, 1983, p. 8; Øksendahl, 1980, Ch. 3) that unlike in the Riemann-Stieltjes integral it makes a difference which point t_j^* in the interval $\Delta t_j = t_{j+1}-t_j$ is chosen, when we apply this definition to an integral over a stochastic variable. The choice $t_j^* = t_j$ (the left end point) is called the nonanticipating definition of the integral and the integral is called the Itô integral. This feature of not using "future" values gives the Itô integral an advantage over other interpretations. For instance an integral

$\int_{z_s}^{Z} T_L(z)d\mu(z)$ is in the non-anticipating way defined as

$$\sum_{j=0}^{m-1} T_L(z_j)[\mu(z_{j+1})-\mu(z_j)],$$

where $z_o = z_s$ and $z_m = Z$. The function $T_L(z_j)$ is independent of the increment $\mu(z_{j+1}) - \mu(z_j)$ and only depends on the "past", no "future" values are involved. Here we recall that in section 2.1.5 we stated that the discrete form of the Langevin equation is preferable because of the discrete definiton needed to interprete integrals of stochastic variables.

We have to give a differentiation rule that is consistent with the chosen integration rule. With the Itô integral comes an Itô differentiation rule, together called Itô calculus. (Øksendahl, 1980, Ch. 3).
The Itô differentiation rule states that if Z is a stochastic variable and

if $\psi(Z,t)$ is a function of Z and t, the differential ψ is given by the full Taylor series

$$d\psi = \frac{\partial\psi}{\partial t}\,dt + \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial^n\psi}{\partial Z^n} (dZ)^n \; . \tag{2.60}$$

In this series we may have to retain higher order terms of dZ. In case dZ is a random variable with higher moments of order dt.

First we give an example of the differentiation rule, which we will use in the next section. This is the calculation of the differential

$$d \int_{z_s}^{Z} \frac{dZ'}{T(Z')} \; ,$$

where Z is a stochastic variable.
We put

$$\psi = \int_{z_s}^{Z} \frac{dZ'}{T(z')}$$

Itô calculus states that because ψ is a function of the stochastic variable Z we have

$$d\psi_z = dZ \left.\frac{d\psi}{dZ}\right|_z + \tfrac{1}{2}(dZ)^2 \left.\frac{d^2\psi}{dZ^2}\right|_z + \ldots \tag{2.61}$$

We calculate the terms on the RHS:

$$\frac{d\psi}{dZ} = \frac{d}{dZ} \int_{z_s}^{Z} \frac{dZ'}{T(Z')} = \frac{1}{T(Z)} \tag{2.62a}$$

$$\frac{d^2\psi}{dZ^2} = \frac{d}{dZ}\left(\frac{1}{T(Z)}\right) = -\frac{1}{T^2(Z)}\frac{dT}{dZ} \tag{2.62b}$$

Substituting Eq. (2.62) into Eq. (2.61) we get

$$d \int_{z_s}^{Z} \frac{dZ'}{T(Z')} = \sum_{n=0}^{\infty} \frac{(dZ)^n}{n!} \frac{d^n}{dZ^n}\left(\frac{1}{T(Z)}\right) \tag{2.63}$$

This was the calculation of the differential we need in the next section.

We illustrate this rule further by an alternative derivation of the Eq. (2.50) for the moments of $d\mu$ We apply the Itô differentation rule to $\psi = W^n$. It gives

$$dW^n = \frac{\partial W^n}{\partial W} dW + \tfrac{1}{2} \frac{\partial^2 W^n}{\partial W^2} (dW)^2 + \ldots$$

$$= n\, W^{n-1}\, dW + \tfrac{1}{2}\, n(n-1) W^{n-2} (dW)^2 + \ldots$$

Taking the conditional average using that $\langle W^m (dW)^P \rangle = \langle W^m \rangle \langle (dW)^P \rangle$ and substituting the moments $\langle (dW)^n \rangle$, derived from the Langevin equation, we get

$$\frac{d\langle W^n \rangle}{dt} = -\, n \frac{\langle W^n \rangle}{T_L} - n \langle W^{n-1} \rangle a_1 + \tfrac{1}{2}\, n(n-1)\, \langle W^{n-2} \rangle a_2 + \ldots$$

Note that the moments $\langle W^n \rangle$ are per definition no stochastic functions and their derivatives with respect to t do exist. If we require that in a steady state $\langle W^n \rangle = u_3^n$, then the above equation gives us the same expressions for a_n as expressed by Eq. (2.50).

Last but not least we give an example to show the consistency of Itô differentation and integration while illustrating that "normal" differentiation and integration rules do not apply. We consider the stochastic function

$$f(\omega_t, t) = C \exp(\omega_t - t/2), \tag{2.64}$$

where ω_t is Gaussian white noise with pdf

$$P(\omega_t, t) = (2\pi t)^{-\frac{1}{2}} \exp(-\omega_t^2/2t).$$

(see also Durbin, 1983).
Itô differentiation applied to Eq. (2.64) gives

$$df = \frac{\partial f}{\partial \omega_t} d\omega_t + \tfrac{1}{2} \frac{\partial^2 f}{\partial \omega_t^2} (d\omega_t)^2 + \frac{\partial f}{\partial t} dt = f\, d\omega_t + \tfrac{1}{2} f\, dt - \tfrac{1}{2} f\, dt$$

and we find the equation

$$df = f\, d\omega_t \;. \tag{2.65}$$

This is a surprising result as from integration rules for non-stochastic variables we would have expected that the solution of Eq. (2.65) would be

$$f = C \exp(\omega_t). \tag{2.66}$$

However, to prove that Eq. (2.64) and (2.66) are not consistent, we Itô-differentiate the last to give

$$df = \frac{\partial f}{\partial \omega_t}\,\partial\omega_t + \tfrac{1}{2}\,\frac{\partial^2 f}{\partial \omega_t^2}\,dt \;+ \frac{\partial f}{\partial t}\,dt$$

$$= f\,\partial\omega_t + \tfrac{1}{2}\,f\,dt$$

and the inconsistency is proven.

We showed that we have to be careful in differentiating stochastic variables. The same goes for integration. We will show that Itô integration of Eq. (2.65) gives Eq. (2.64).

Itô integration of Eq. (2.65) gives

$$\int df = \sum_{j=0}^{m-1} f(\omega_{t_j}, t_j)\,[\omega_{t_{j+1}} - \omega_{t_j}].$$

To prove our first point we average this equation, where averages of a function $g(\omega_t, t)$ are defined as

$$\overline{g(\omega_t, t)} = \int_{-\infty}^{\infty} g(\omega_t, t) P(\omega_t, t)\,d\omega_t.$$

This gives zero on the RHS, because of the non-anticipation and we get $\overline{f} = C$, where C = constant.

Executing the averaging of Eq. (2.64) we get

$$\overline{f} = \frac{C\exp(-t/2)}{(2\pi t)^{\frac{1}{2}}} \int \exp(\omega_t - \omega_t^2/2t)\,d\omega_t = C$$

and we proved that Eq. (2.64) and (2.65) are consistent in Itô calculus.

2.5 Markov limits

2.5.1 Introduction

We are interested in the behaviour of the marked particles at large travel times. This behaviour can be decribed with the concept Markov limits. These limits are Lagrangian equations that describe the time history of the trajectories Z(t) for large times. However, we have to be careful in specifying what we mean by large times.

In homogeneous turbulence the only relevant timescale is T_L and by large times we mean times large compared to T_L that is the limit $t/T_L \rightarrow \infty$. In inhomogeneous turbulence T_L is not a well defined integral timescale anymore as the velocity is not stationary. (Durbin and Hunt, 1980). However, in practice T_L is defined as described in Ch. 1. In addition T_L is no longer the only relevant timescale. There is also another timescale T_i which is indicative for the effect of the inhomogeneity. How in detail this timescale T_i depends on the turbulence properties, will be kept open here. When the inhomogeneity timescale T_i is much larger than the Lagrangian timescale T_L the turbulence is called weakly inhomogeneous. By large times we will refer to times, that are large compared to T_L, but still small compared to T_i. Strongly inhomogeneous turbulence means that T_i is of the same order as T_L and both timescales play an equally important role.

Originally the concept "Markov limit" was used in homogeneous turbulence for the limit $T_L \rightarrow 0$ and t fixed. Under certain constraints the limit $T_L \rightarrow 0$ (t fixed) is equivalent to the limit $t \rightarrow \infty$ (T_L) fixed and the large time analysis of the Langevin equation in homogeneous turbulence was therefore made before by taking the limit $T_L \rightarrow 0$ without however explicitly naming the contraints. (Durbin, 1983). In inhomogeneous turbulence it appears that the limits $t \rightarrow \infty$ and $T_L \rightarrow 0$ are no longer equivalent. T_L is not the only timescale involved, but also the inhomogeneity timescale T_i is introduced and it can not be expected that the above limit $T_L \rightarrow 0$ will give the desired large time behaviour. We show that in both homogeneous and weakly inhomogeneous turbulence extra constraints are necessary to guarantee the equivalence between the two limits. A Markov limit derived without these contraints would give wrong results, because in the process of letting $T_L \rightarrow 0$ the turbulence is modified. What we need to do is to replace the limit $t \rightarrow \infty$ by another limit in which the turbulence retains its characteristics. This will be the limit $T_L \rightarrow 0$ under the following constraint. We rescale the turbulence by letting $T_L \to 0$ while $\overline{u_3^2} \to \infty$, in such a way that its dispersive property, specified by the diffusivity $K = \overline{u_3^2}\, T_L$, remains the same function of height. We see that in such a limit the characteristic length of the turbulence $\ell = \overline{u_3^2}\, T_L$ also goes to zero. This shows that in such a limit we rescale the turbulence process to bring out the large time behaviour. The constraint on K will appear to be of major importance.

2.5.2 Markov Limit of homogeneous Langevin equation for W

In homogeneous turbulence the velocity distribution is taken to be Gaussian. The turbulence is fully determined by T_L and $\sigma^2 = \overline{u_3^2}$ which are both independent of height. We have already seen in section 2.3.7 that dispersion in such circumstances can be described by a Langevin equation with all moments of the random forcing function $\langle(d\mu)^n\rangle$ equal to zero, except the second, which reads $\langle(d\mu)^2 = 2\,\sigma^2/T_L\,dt$. We can write $d\mu = (2\sigma^2/T_L)^{1/2}d\omega$ where $d\omega$ is the so-called Wiener process with $\overline{d\omega} = 0$ and $\overline{d\omega^2} = dt$. The Langevin equation reads

$$dW = \frac{W}{T_L}\,dt + \left(\frac{2\sigma^2}{T_L}\right)^{1/2} d\omega_t \quad \text{and}$$

$$dZ = W dt \ . \tag{2.67a}$$

Here we will summarise the derivation of the Markov limit in homogeneous situations. In homogeneous cases new dimensionless variables $\tau = t/T_L$, $\tilde{W} = W/\sigma$, $\tilde{Z} = Z/\sigma T_L$ and $d\tilde{\omega}_t = T_L^{-1/2}\,d\omega_t$ can be introduced. The Langevin equation scaled with these variables reads

$$d\tilde{W} = -\,\tilde{W}\,d\tau + \sqrt{2}\,d\tilde{\omega}t \quad \text{and}$$

$$d\tilde{Z} = \tilde{W}\,d\tau \ . \tag{2.67b}$$

We are interested in the limit $t \to \infty$. As τ is the only timescale, the limit $t \to \infty$ (T_L) fixed is equivalent to $T_L \to 0$ (t fixed). We want to stress that letting $T_L \to 0$, while keeping all other parameters fixed, means that the turbulence properties are basically modified, because the eddy diffusivity $K = \sigma^2 T_L$ goes to zero. We have to look for a way of replacing $t \to \infty$ by a limit equivalent with a rescaling of the relevant turbulence quantities (in this case the timescale T_L and the energy scale σ^2) such that the dispersive character of the turbulence remains unchanged. This means, that in the limit $T_L \to 0$ we have to change σ^2 such that the eddy diffusivity $K = \sigma^2 T_L$ remains unchanged. We will show that this constraint ensures that the Markov limit model becomes equivalent with the diffusion equation

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial z}\left(K\,\frac{\partial P}{\partial z}\right) \ . \tag{2.68}$$

First we illustrate the effects of the above defined limit on the spectrum. The limit $T_L \to 0$ in the Langevin equation implies that the velocity process W looses its memory so that the velocities become uncorrelated. The velocity W becomes a white noise process. We have derived in Eq. (2.29) that the spectrum of the Langevin equation for W in stationary homogeneous conditions reads

$$S_W(\omega) = 2 \frac{\sigma^2 T_L}{[1+(\omega T_L)^2]} \frac{1}{\Delta t}$$

For $T_L \to 0$, while $\sigma^2 T_L$ remains constant the spectrum becomes indeed the spectrum of a white noise process: S_W = constant, whereas without the constraint it would not (S_W would go to zero).

After this illustration we show how the limit $T_L \to 0$ is taken in the Langevin equation to arrive at the Markov limit. Integrating the Langevin equation Eq. (2.64a), resubstituting $(\frac{2\sigma^2}{T_L})^{\frac{1}{2}} d\omega_t = d\mu$, gives

$$\int_o^t (Wdt - T_L\, d\mu) = - T_L[W(t)-W(o)] \tag{2.69}$$

Durbin (1983) showed that W(t)-W(o) remains bounded in "mean square sense". Therefore the RHS of Eq. (2.69) goes to zero when $T_L \to 0$. On the LHS of Eq. (2.69) we also find a term in which T_L is involved namely $T_L \int_o^t d\mu = \int_o^t (2\sigma^2 T_L)^{\frac{1}{2}} d\omega_t$. This term is constant according to our constraint that $\sigma^2 T_L$ remains constant. We therefore keep this term so that

$$\int_o^t W\, dt = T_L \int_o^t d\mu. \tag{2.70}$$

Differentiation and the relation W dt = dZ give the Markov limit of the Langevin for homogeneous turbulence

$$dZ = T_L\, d\mu = (2\sigma^2 T_L)^{\frac{1}{2}} d\omega_t\ . \tag{2.71}$$

This derivation can also be found in Schuss (1980, Ch. 6), where the Markov limit is called the Smoluchowski-Kramers approximation to the Langevin equation.

2.5.3 Kramers Moyal Expansion of the homogeneous Markov limit for the W-model

We derived the large time Lagrangian equation for Z(t), the Markov limit Eq. (2.71). From this equation we can build up P(z;t) by releasing an ensemble of particles and taking the ensemble average of their height. The time evolution of P(z;t) for large times is described by a differential equation which is the KME of the Markov limit.

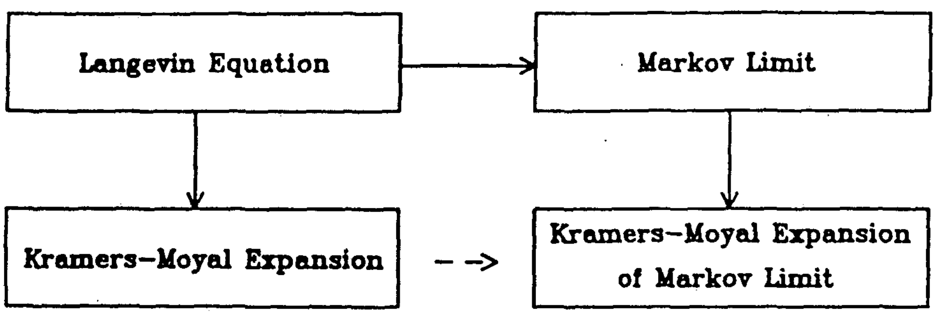

Fig. 2.1 Scheme of derivation of the equations used.

We derive this equation. In subsection 2.2.1 we derived the KME for a monovariate process Z Eq. (2.36):

$$\frac{\partial P(z;t)}{\partial t} = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \frac{\partial\left(\frac{<(dZ)^n>P}{dt}\right)}{\partial z^n} .$$

The moments $<(dZ)^n>$ can be calculated from the Markov limit Eq. (2.71). Substituting them into Eq. (2.36) leads to the equation

$$\frac{\partial P(z;t)}{\partial t} = \frac{\partial^2}{\partial z^2} (\sigma^2 T_L P) = \frac{\partial}{\partial z} (\sigma^2 T_L \frac{\partial P}{\partial z}) . \qquad (2.72)$$

This is the well-known diffusion equation which as a solution has a Gaussian distribution. This is also what we expect for large times from the Central Limit Theorem. For large times the displacement process looses its memory of the past and the increments dZ become (weakly) uncorrelated. The Central Limit Theorem states that the sum of (weakly) uncorrelated stochastic variables approaches a Gaussian probability distribution.

This Kramers Moyal Expansion of the Markov limit for homogeneous Gaussian turbulence can also directly be derived from the KME of the Langevin equation for P(z,w;t) Eq. (2.38) (Van Kampen, 1984, p. 234-236). This is done by expanding P(z,w;t) in powers of T_L. This equation can be integrated over w to give the large time limit for P(z,t) Eq. (2.72). Different derivations are summarized in Schuss (1980, Ch. 6), where also is shown that the velocity distribution also becomes Gaussian. This derivation is based on the fact that in homogeneous turbulence the expansion of P(z,w;t) in powers of T_L converges. This direct derivation can not be applied in inhomogeneous turbulence where more timescales play a role. For this reason we do not discuss this derivation further.

2.5.4 Markov Limit of inhomogeneous Langevin equation for W

Now we consider the Langevin equation in inhomogeneous turbulence, where T_L but also T_i plays a role.The Langevin equation can no longer be made nondimensional with either T_L or T_i because the moments of the random forcing function are involved functions of T_L and the inhomogeneous turbulence properties (see Eq. (2.48) or (2.50)). We can no longer express $d\mu$ as a function of the turbulence variables T_L and σ, like in homogeneous turbulence we had $d\mu = (2\sigma^2/T_L)^{1/2} d\omega_t$, but we know only its moments $\langle (d\mu)^n \rangle$. The Langevin equation can not be scaled because no nondimensionalized time can be found and the limit $t \to \infty$ is no longer equivalent to the limit $T_L \to 0$. We have to be careful in specifying what we mean by a Markov limit.

The case we will treat is the weakly inhomogeneous case where T_L is smaller than T_i. We consider a Markov Limit that describes the behaviour of the Langevin equation for times larger than T_L but still small compared to T_i.

We will deal with inhomogeneous Gaussian turbulence, specified by the Lagrangian timescale $T_L(z)$ and relevant velocity scale $\sigma(z)$. We will formally deal with the inhomogeneity by splitting T_L and σ in a shape factor $T(z)$ resp. $S(z)$ and an amplitude α resp. β so that $T_L(z) = \alpha\, T(z)$ and $\sigma(z) = \beta\, S(z)$. We replace the limit $t \to \infty$ by a rescaling of the turbulence. This means that we rescale T_L and σ^2 such that the shape of T_L and σ^2 remains the same (which means that the gradients are invariant), while we change their amplitudes α and β. We take the limit $\alpha \to 0$ and $\beta^2 \to \infty$ while $\alpha\beta^2$ = constant. This is done to guarantee that the eddy diffusivity $K(z) = T_L(z)\sigma^2(z)$ remains an invariant function of z.

We proceed to find this Markov limit. The Langevin equation reads

$$dW = -\frac{W}{T_L(Z)}\, dt + d\mu(Z)\ .$$

Multiplying by α gives

$$\alpha dW = -\frac{W}{T(Z)}\, dt \ t\ \alpha\, d\mu(Z)\ . \qquad (2.73)$$

Integrating this Langevin equation over time leads to

$$\int_0^t \frac{W(t')}{T(Z(t'))}\,dt - \alpha\, d\mu_{t'}) = \int_{z_s}^{Z} (\frac{dZ'}{T(Z')} - \alpha\, d\mu(Z')) = -\alpha[W(t)-w(0)], \qquad (2.74)$$

where z_s is the release point. We take the limit $\alpha \to 0$, while $\alpha\beta^2$ is kept constant. The factor [W(t)-W(0)] on the RHS remains bounded for all time in "mean square" sense. This can be seen from the physical insight that because the velocity is an almost stationary process, the velocity remains bounded in statistical sense. The RHS goes to zero when $\alpha \to 0$. The term on the LHS that contains α might also contain terms that involve $\alpha\beta^2$ which remain constant in the limit and we keep this term therefore. We get

$$\int_{z_s}^{Z} \frac{dZ'}{T(Z')} = \int_{z_s}^{z} \alpha\, d\mu(Z') \,. \qquad (2.75)$$

To differentiate this Eq. (2.75) we have to apply Itô calculus. (See section 2.4). Application of the Itô differentiation rule to the RHS of Eq. (2.75) gives

$$d \int_{z_s}^{Z} \alpha\, d\mu(Z') = \alpha\, d\mu(Z) \,.$$

Differentiation of the LHS gives (see examples of Itô calculus in section 2.4)

$$d \int_{z_s}^{Z} \frac{dZ'}{T(Z)} = \frac{dZ}{T}\Big]_z - \tfrac{1}{2}\frac{T'}{T^2}\Big]_z (dZ)^2 + \frac{1}{6}\,(\frac{2T'^2}{T^3} - \frac{T''}{T^2})\Big]_z (dZ)^3 + \ldots,$$

where a prime on the RHS denotes derivation with respect to z.
The higher moments of dZ in this equation can not automatically be neglected not even in order dt, because they are no longer given by $\langle (dZ)^n \rangle = \langle W^n \rangle dt^n$. In the integrated Langevin equation Eq. (2.74) we left out the RHS and so changed the original Langevin equation to a different (large time) equation. This means that the displacement Z of the large time equation is no longer so simply related to the velocity in the original Langevin equation.

Equating the LHS and RHS of Eq. (2.75) we have

$$\frac{1}{T}(dZ) - \tfrac{1}{2}\frac{T'}{T^2}(dZ)^2 + \frac{1}{6}\,(\frac{2T'^2}{T^3} - \frac{T''}{T^2})\,(dZ)^3 + \ldots = \alpha\, d\mu. \qquad (2.76)$$

For turbulence with an integral timescale T_L independent of height, the Eq. (2.76) becomes much simpler. This equation will be treated as an intermezzo in the next section as an illustration. The general case with T_L a function of z will be treated afterwards.

Intermezzo: The Markov limit for turbulence with constant T_L

In this chapter we illustrate the concept Markov Limit by discussing the one for turbulence with constant T_L. Substituting dT/dz = 0 in Eq. (2.76) gives the Markov Limit

$$dZ = T_L \, d\mu(z) \; . \tag{2.77}$$

The behaviour of this equation for large times can easiest be shown from the KME of this Markov limit. The moments $\langle (dZ)^n \rangle$ that we need in the general KME Eq. (2.36) can be derived as follows. We have $\langle (dZ)^n \rangle = T_L^n \langle (d\mu)^n \rangle$.
In turbulence where the velocity fluctuations are Gaussianly distributed the moments of dμ are given by Eq. (2.56), where $\langle (d\mu)^n \rangle = a_n dt$. Imposing that $\sigma^2(z) T_L$ should be kept a constant function of z, while taking $T_L \to 0$ we get

$$T_L a_1(z) = \frac{d(\sigma^2 T_L)}{dz} = \frac{dK(z)}{dz} \; , \tag{2.78a}$$

$$T_L^2 a_2(z) = 2\, T_L \sigma^2 = 2\, K(z) \; , \tag{2.78b}$$

$$T_L^3 a_3(z) = 3\, T_L^3\, \sigma^2 \frac{d\sigma^2}{dz} = 3\, T_L\, K(z) \frac{dK(z)}{dz} \to 0 \tag{2.78c}$$

and we have that the function $a_n(z)$ are always equal to zero for $n \geqq 4$.

$$a_n(z) = 0 \qquad \text{for} \qquad n \geqq 4 \; . \tag{2.78d}$$

It follows that only the first two moments of dZ are nonzero and we can write

$$dZ = \langle dZ \rangle + \left(\langle \frac{(dZ)^2}{dt} \rangle\right)^{1/2} d\omega_t = \frac{d(\sigma^2 T_L)}{dz} dt + (2\sigma^2\, T_L)^{1/2}\, d\omega_t ,$$

which is the Markov limit Durbin (1980) and Durbin and Hunt (1980) used, although they did not give a (correct) derivation (see Ch. 3).

Substitution of Eq. (2.78) in the general KME Eq. (2.36) shows that the KME in this case becomes the diffusion equation Eq. (2.72):

$$\frac{\partial P(z;t)}{\partial t} = \frac{\partial}{\partial z} (\sigma^2 T_L \frac{\partial P}{\partial z})$$

Monin and Yaglom (1977, Ch. 10.3) state that this equation indeed describes dispersion correctly in inhomogeneous turbulence for diffusion times larger than T_L.

Markov limit for general inhomogeneous turbulence

We start with multiplying the general Eq. (2.76) by T/2 to get

$$dZ - \tfrac{1}{2} \frac{1}{T_L} \frac{dT_L}{dz} (dZ)^2 + \frac{1}{6} (2 \frac{T'^2}{T^2} - \frac{T''}{T})(dZ)^3 + \ldots = T_L \, d\mu \; . \qquad (2.79)$$

For inhomogeneous Gaussian turbulence we can proceed as follows. We take Eq. (2.79) to higher powers and take the conditional average. On the RHS then appears the term $\langle T_L^n (d\mu)^n \rangle$. This quantity is defined in the non-anticipating sense so that T_L and $d\mu$ are independent (see section 2.4). The RHS becomes $T_L^n(z) \langle (d\mu)^n \rangle = T_L^n \, a_n(z) dt$ and are given in order dt (see Eq. (2.56) for a_n) by

$$T_L \, a_1(z) = T_L(z) \frac{d\sigma^2}{dz} = \alpha\beta^2 \, T(z) \frac{dS^2}{dz} \quad \rightarrow \text{invariant function of } z,$$

$$T_L^2 \, a_2(z) = 2 \, T_L \sigma^2 = 2 \, K(z) \quad \rightarrow \text{invariant function of } z,$$

$$T_L^3 \, a_3(z) = 3 \, T_L^3 \, \sigma^2 \frac{d\sigma^2}{dz} = 3 \, \alpha \, \alpha^2 \beta^4 \, T^3 \, S^2 \frac{dS^2}{dz} \rightarrow 0$$

and

$$T_L^n \, a_n(z) = 0 \qquad \text{for } n \geq 4 \text{ as } a_n(z) = 0 \text{ for } n \geq 4. \qquad (2.80)$$

The third and higher powers of Eq. (2.79) form an infinite series of equations for the moments $\langle (dZ)^n \rangle$ each with zero RHS. Generally the equations are independent and the solution is that all moments $\langle (dZ)^n \rangle$ for $n \geq 3$ are zero. From this statistical reasoning we conclude that Eq. (2.79) becomes

$$dZ - \tfrac{1}{2} \frac{1}{T_L} \frac{dT_L}{dz} (dZ)^2 = T_L \, d\mu \,. \tag{2.81}$$

Note that dispersion in non-Gaussian inhomogeneous turbulence is described in Langevin models by a $d\mu$ whose higher moments are all of order dt. This characteristic of the model leads to the fact that we cannot derive a Markov Limit for these cases.

Solving the quadratic equation Eq. (2.81) we get for one root

$$dZ = \left(\frac{1}{T_L} \frac{dT_L}{dz}\right)^{-1} \left\{1 - \left(1 - 2 \frac{dT_L}{dz} d\mu\right)^{\frac{1}{2}}\right\} . \tag{2.82}$$

Any root $(1 + x)^{\frac{1}{2}}$ can be expressed as an infinite polynome in x. It is allowed to break this expansion off for an approximation in case the terms in the polynome converge to zero. To prove this for the root $(1-2\, T_L' \, d\mu)^{\frac{1}{2}}$ in Eq. (2.82) we use the fact that the third moment of $T_L' d\mu$ goes to zero in the limit $\alpha \to 0$, while $\alpha\beta^2$ is constant analogously to the third moment $T_L d\mu$. All higher moments of $T_L' d\mu$ are always zero in order dt. Reasoning with statistical arguments we break off the expansion of the root $(1-2\, T_L' \, d\mu)^{\frac{1}{2}}$ after the second term. This expansion then reads

$$1 - \frac{dT_L}{dz} d\mu - \tfrac{1}{2}\left(\frac{dT_L}{dz}\right)^2 (d\mu)^2 \quad \text{and}$$

Eq. (2.82) becomes

$$dZ = T_L \, d\mu + \tfrac{1}{2} T_L \frac{dT_L}{dz} (d\mu)^2 \,, \tag{2.83}$$

the Markov limit for Gaussian inhomogeneous turbulence.

In the large time limit we have that the third and higher moments of $T_L d\mu$ are zero and the first two moments are given by Eq. (2.80). We then can write

$$T_L \, d\mu = T_L \frac{d\sigma^2}{dz} dt + (2\, T_L \sigma^2)^{\frac{1}{2}} d\omega_t \,. \tag{2.84}$$

Substituting this in Eq. (2.83) this Markov Limit reads

$$dZ = (2\ T_L\ \sigma^2)^{\frac{1}{2}}\ d\omega_t + \frac{d(T_L\sigma^2)}{dz}\ dt\ , \qquad (2.85)$$

which is the Markov Limit used by Durbin (1980) and Durbin and Hunt (1980) (see Ch. 3), who however did not give a derivation for this equation. Durbin (1980) noted that the last term in Eq. (2.85) contains a drift velocity $V_d = d(T_L\sigma^2)dz$. Tracing back this term we find that both the damping term $-W/T_L$ as well as the first moment of $d\mu$ in the Langevin equation contribute to this drift velocity. We keep in mind that drift velocities in the Markov limit, an equation for dZ, are consistent with drift accelerations in the Langevin model, an equation for dW. This can be understood by investigating how e.g. $\langle d\mu \rangle$ appears in both equations. With these two ways to write the Markov limit for Gaussian inhomogeneous turbulence Eq. (2.83) and (2.85) we conclude this analysis. In the next section we derive their KME's.

2.5.5 KME of the Markov Limit in case T_L and σ are functions of z

We could derive the KME of the Markov limit in Gaussian inhomogeneous turbulence from Eq. (2.83). But it is much easier to start from Eq. (2.85). From Eq. (2.85) we can derive the moments needed in the KME:

$$\langle dZ\rangle = \frac{d(\sigma^2 T_L)}{dz}\, dt \;,$$

$$\langle (dZ)^2\rangle = 2\,\sigma^2 T_L dt \text{ and} \qquad (2.86)$$

$$\langle (dZ)^n\rangle = 0 \quad \text{for} \quad n \geq 3 \;.$$

Substituting these equations in the KME for a monovariate process Eq. (2.36), we see that this derivation results in the fact that the KME of the Markov limit of the Langevin model for W is also equal to the second order differential equation (Fokker Planck equation), the diffusion Eq. (2.72):

$$\frac{\partial P(z;t)}{\partial t} = \frac{\partial}{\partial z}\left(\sigma^2 T_L \frac{\partial P}{\partial z}\right) \;,$$

just like in homogeneous turbulence. We stress again that the constraints on K are necessary to obtain this result.

Intermezzo

Just for fun we also derive the KME of the Markov limit from Eq. (2.83). The moments $\langle (dZ)^n\rangle$ we need are as follows. The first moment reads

$$\langle dZ\rangle = T_L(z)a_1(z)dt + \tfrac{1}{2}\, T_L \frac{dT_L}{dz}\, a_2(z)dt$$

$$= \left(T_L(z)\,\frac{d\sigma^2}{dz} + \sigma^2\,\frac{dT_L}{dz}\right) dt = \frac{d(\sigma^2 T_L)}{dz}\, dt \;,$$

which is constant in the limit $T_L \to 0$ while $\sigma^2 T_L$ = constant.
The second moment in order dt is derived by squaring Eq. (2.84) and conditional averaging:

$$\langle (dZ)^2\rangle = T_L^2\, a_2(z)dt + T_L^2\, \frac{dT_L}{dz}\, a_3(z)dt \;.$$

The second term on the RHS of this equation can be written as

$$T_L^2 \frac{dT_L}{dz} a_3(z)dt = 3T_L^2 \frac{dT_L}{dz} \sigma^2 \frac{d\sigma^2}{dz} dt = 3\alpha(\alpha\beta^2)^2 T^2(z)S^2(z) \frac{dT}{dz}\frac{dS}{dz} dt .$$

This term goes to zero for $\alpha \to 0$ while $\alpha\beta^2$ is constant.
Thus $\langle(dZ)^2\rangle = T_L^2 a_2(z)dt = 2 \sigma T_L dt$.
The third moment $\langle(dZ)^3\rangle$, which is derived by taking Eq. (2.83) to the third power, contains a term $T_L^3 a_3(z)dt$. This term goes to zero in the limit according to Eq. (2.80). The other terms in the expression for $\langle(dZ)^3\rangle$ contain higher moments of $d\mu$ and are always zero in order dt. This also goes for all terms in the expressions for higher moments of dZ and summarizing we have again found the Eq. (2.86) and the rest of the derivation of the KME goes analogously.

2.5.6 Conclusions

The Langevin model for W is shown to give the correct large time behaviour in inhomogeneous Gaussian turbulence where T_L is either constant or a function of height. This behaviour is described by the ordinary diffusion equation and leads to a homogeneous steady state concentration distribution.

The Markov limit describing this behaviour is derived by putting constraints on the eddy diffusivity $K = \sigma^2 T_L$, while letting $T_L \to 0$. If we had not taken into account the constraints on K then in the case where σ^2 and T_L are function of height a Markov limit would have resulted, that is not equivalent with the diffusion equation. With these conclusions we end our chapter on theory of the Langevin equation for W.

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Ch. 3. REVIEW AND INTERPRETATION OF STOCHASTIC LAGRANGIAN DISPERSION MODELS, USED IN THE LITERATURE

Ch. 3 Review and interpretation of stochastic Lagrangian dispersion models

3.1 Introduction

Lagrangian dispersion models have been used to describe dispersion in a wide variety of atmospheric circumstances. The models differ in how the velocity of released particles is described. The first four models we discuss are partly determinsitic, partly stochastic models. Almost all other Lagrangian models are fully stochastic and based on one particular stochastic equation, the Langevin equation. The review of these models is based on the theory of the Langevin equation described in Ch. 2. Much of this theory will be used in this chapter.

First we discuss the relatively simple Langevin models for homogeneous turbulence. After this we turn to models for inhomogeneous conditions. The applicability of these models depends on the way the random forcing is prescribed. We show to which atmospheric situations certain models apply and indicate the errors if the models are applied outside their range of validity. Models were created that are successful in the neutral and stable surface layer, while the step to convective surface layers was more involved. This is because the still Gaussian turbulence intensity becomes height dependent. Langevin models for non-Gaussian turbulence velocity distributions (like in the convective boundary layer) are only recently made.

In Fig. 3.1 a schematic summary is given of the authors whose study we discuss. The order of the studies is given by their random forcing modelling. Also is indicated the situation the authors applied their model to. These situations are not necessarily identical to the atmospheric conditions the model can be applied to, as we will show in this chapter.

Partly Deterministic and Stochastic Models			
Lamb	1978		ch 3.2
Weil and Furth	1981	convective boundary layer	
Venkatram	1982		
Misra	1982		
Langevin Models for W			
Gifford	1982	homogeneous	ch 3.3
Reid	1979	neutral surface layer	ch 3.4
Ley	1982	neutral surface layer	
Legg	1982	neutral boundary layer	
Durbin	1980	neutral boundary layer	
Hall	1975	neutral and convective surface layer	
Durbin and Hunt	1980	neutral boundary layer	ch 3.5
Legg and Raupach	1982	neutral, within and above crop	
Davis	1983	neutral boundary layer	
Ley and Thomson	1983	stable and unstable surface layer	
Langevin Model for W/σ			
Wilson, Thurtell and Kidd	1981	homogeneous turbulence and neutral boundary layer	ch 3.6
	1983	inhomogeneous Gaussian turbulence	
Markov Limit for W/σ			
Durbin	1984	inhomogeneous Gaussian turbulence	ch 3.6
Theoretical Investigations			
Janicke	1981		ch 3.7
Thomson	1984		
van Dop, Nieuwstadt and Hunt	1985		
Langevin Model for W/σ			
Bærentsen and Berkowicz	1984	convective boundary layer	ch 3.8
Langevin Model for W			
de Baas, van Dop and Nieuwstadt	1986	convective boundary layer	ch 3.8

Fig. 3.1 Summary of models to be discussed.
The models are ordered according to their random forcing modelling.

3.2 Partly deterministic Lagrangian models

3.2.1 Lamb's model

Lamb (1978, 1984) made a 3D-Lagrangian model to simulate dispersion in the convective boundary layer (CBL). He calculated trajectories $\underset{\sim}{X}_i(t)$ of released particles. The velocity is split into a deterministic and a stochastic part. Lamb's model equation reads

$$\frac{d}{dt}\underset{\sim}{X}_i(t) = u_i(\underset{\sim}{X}_i(t),t) + U_i(t) \ . \qquad (3.1)$$

Here $u_i(\underset{\sim}{x},t)$ is the deterministic Eulerian velocity obtained from grid cell averages of a numerical model for turbulence in the CBL of Deardorff (1974) and U_i is a subgrid velocity due to scales of motion smaller than gridsize in Deardorff's model. Lamb considered U_i to be a Lagrangian random velocity, whose statistical properties are determined by the local subgrid scale turbulence. He described this Lagrangian part of the velocity by the following Langevin equation

$$U_i(t) = \alpha\ U_i(t-\Delta t) + \gamma\ E(X_i)r_i \ , \qquad (3.2)$$

where r_i is a random variable with zero mean and variance one. Note that Lamb did not use a Langevin equation for the total velocity. The variable E is proportional to the mean subgrid scale kinetic energy e nl. $E = (\frac{2}{3}\ e)^{\frac{1}{2}}$. The data for e are given by Deardorff's model. The constants α and γ are chosen such, that the form of the spectrum of the subgrid velocities and their integral timescale are represented. This subgrid velocity spectrum is a bandwidth limited spectrum (only subgrid scales are included) and its timescale is therefore very small.

With this model he simulated dispersion in the CBL from a continuous point source at several heights. The behaviour of plumes in the CBL was investigated before in a laboratory by the watertank epxeriments of Willis and Deardorff (1976, 1978, 1981). (see Ch. 1). Lamb compared his results with these watertank experiments of Willis and Deardorff and the surface data of the Prairie Grass experiment. He found that the results of his numerical model were in excellent agreement with these experiments. Both the laboratory and numerical plume showed the same involved behaviour (see Fig. 3.2). However, the maximum ground concentrations due to elevated sources were somewhat less in Lamb's model than in the tank experiments.

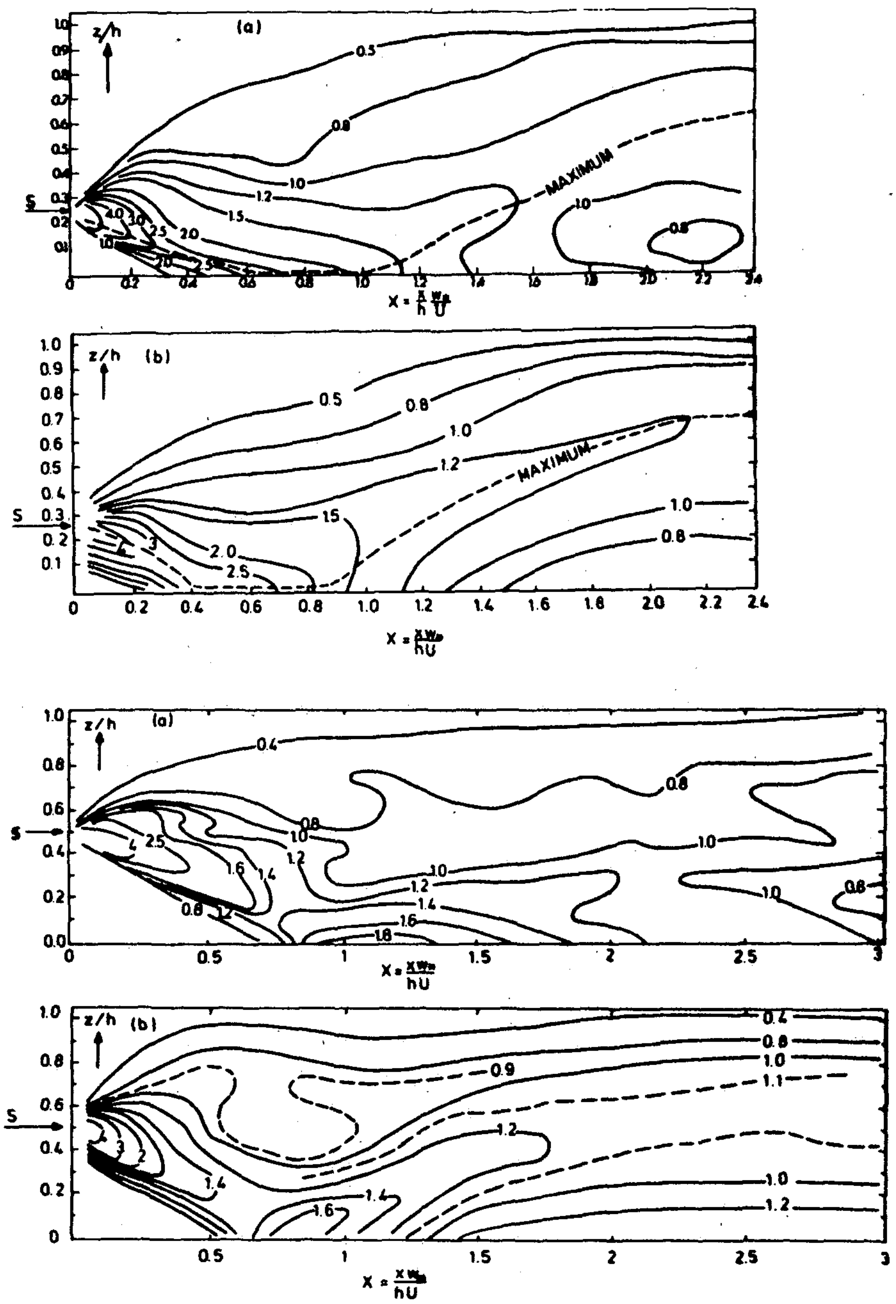

Fig. 3.2 Comparison of crosswind integrated concentration distributions

(a) predicted by the numerical model of Lamb (1978, 1984) with

(b) the corresponding field measured in the laboratory by Willis and Deardorff, (1978, 1981)

(From Lamb, 1984)

3.2.2 Weil and Furth's, Venkatram's and Misra's model

Three models were proposed in which the initial velocity of the particles is a stochastic process determined by the wind statistics at release time at the source. The velocity evolution of the particles is deterministically prescribed.

Weil and Furth (1981), Venkatram (1982) and Misra (1982) each proposed such a 1D-Lagrangian dispersion model to predict the ground level mean concentration in the CBL. These models were designed to be simple and to require short computer time.

We first discuss Venkatram's model, which is the simplest. Venkatram released particles with vertical velocities that adapt immediately to the turbulence. The particle velocities have the same skewed probability distribution as the vertical turbulence velocity in a CBL (see Fig.1.7). The particles keep this initial velocity and at the boundaries they only invert direction (Fig. 3.3). This implies that the Lagrangian timescale of the velocity process cannot be calculated from the velocity autocorrelation (Eq. (1.10)). Venkatram derived analytical expressions for the ground level concentration.

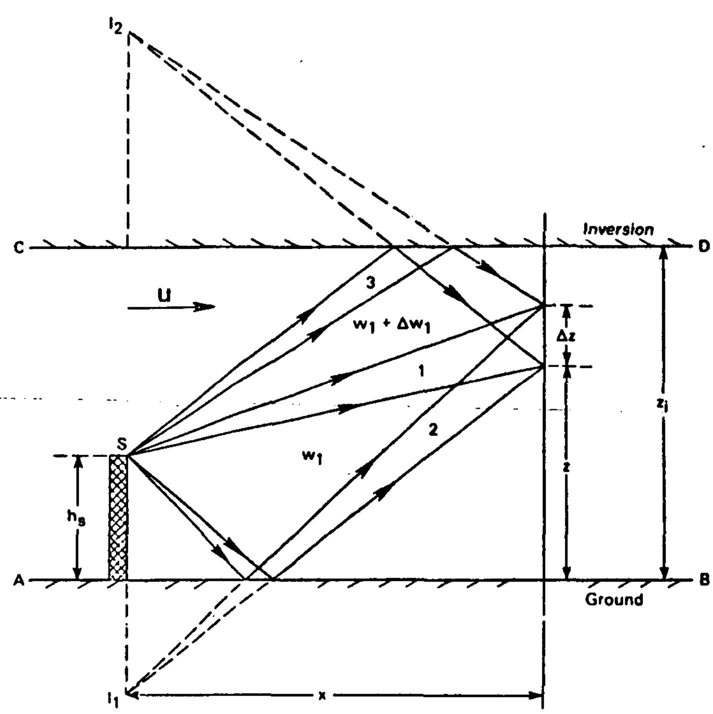

Fig. 3.3 Geometry of dispersion along straight lines in Venkatram's model. (From Venkatram, 1982).

Weil and Furth also released particles with velocities that adapt immediately to the turbulence. The skewed vertical velocity distribution was built up by making a distinction between upgoing and downgoing particles, which is based on the concepts of downdrafts and updrafts. At release 40% of the particles were situated in an updraft. These particles had a velocity probability distribution function (pdf) that is exponential with a mean upwards velocity $\overline{w}_u = 0.6\ w_*$, where w_* is the characteristic vertical velocity defined by Eq. (1.3). The 60% that move downwards after release also have an exponential velocity pdf with a mean downwards velocity $\overline{w}_d = -0.4\ w_*$. These numerical values are based on the studies of Lamb (1978, 1982). The particle velocity is constant untill the particle reaches a boundary, where "reflection" was imposed, given by $w_d = -2/3\ w_u$ or $w_u = -3/2\ w_d$. The particles remember their initial velocities at all time and again the Lagrangian timescale in this model cannot be calculated from Eq. (1.10).

In Misra's model particles are also released in up- or downdrafts, but the particles do not fully adapt to the turbulence. Their initial velocity distribution is Gaussian instead of skewed. The evolution of the velocity is specified by supposing that the downdrafts do not spread out. The particle velocity in such a downdraft w_d varies with height in a deterministic way. The initial downdraft velocity w_d is simply multiplied by a function of height. Of the updrafts less is specified. They are supposed to be well mixed before they reach the ground and only their impact on the ground level concentration is specified.

Despite their limitations these simple models reproduce most features of the ground level concentration in the CBL for sources at several heights (Fig. 3.4).

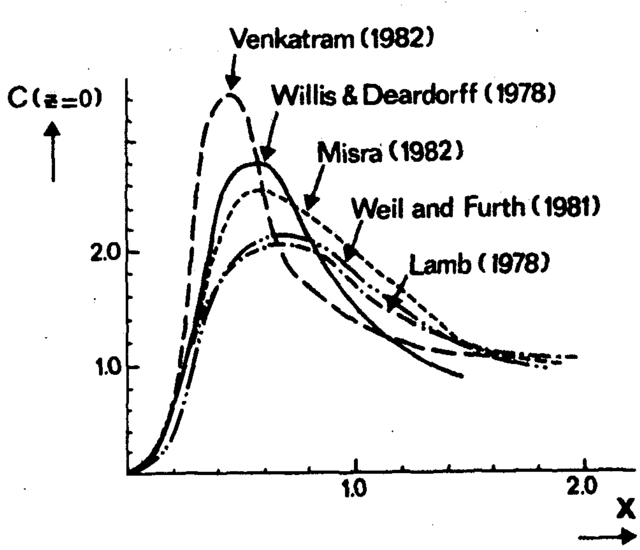

Fig. 3.4 Comparison of model results for a source at $z_s = 0.26\ z_i$. C(z=0) is the nondimensional (crosswind integrated) groundlevel concentration.

3.3 Homogeneous Langevin models

We discussed dispersion models that describe the velocity of the released particles in a partly determinsitic, partly stochastic way. We now turn to models in which the velocity of the particle is fully described as a stochastic process (Monte Carlo simulation). The motion of the particles is simulated by a stochastic differential equation. In analogy with the description of Brownian diffusion these models are based on one special stochastic equation, the Langevin equation which models the effect of the turbulence on the particles as a random force. This equation reads

$$dW = - \frac{W}{T_L} dt + d\mu \ , \tag{3.3}$$

where W is the particle velocity, T_L the Lagrangian time scale and $d\mu$ are the random velocity increments (random forcing).

In homogeneous turbulence the random forcing function is modelled by $d\mu = (2\sigma^2/T_L)^{\frac{1}{2}} d\omega_t$, where $d\omega_t$ is a white noise process with zero mean and variance dt. The Langevin equation then reads

$$dW = - \frac{W}{T_L} dt + (\frac{2\sigma^2}{T_L})^{\frac{1}{2}} d\omega_t \ . \tag{3.4}$$

We call this equation the homogeneous Langevin equation.

With this equation analytical expressions can be derived for the mean velocity $\overline{W}(t)$, displacement $\overline{Z}(t)$, their spreads $\overline{W^2}(t)$, $\overline{Z^2}(t)$, autocorrelation and spectra. Much of this theoretical work (of which we gave a description in Ch. 2) was done by Lin and Reid (1962).

3.3.1 Gifford's model

We discuss an application of the Langevin equation to homogeneous conditions by Gifford (1982). The input parameters are the initial velocity of the particles at the source, the (constant) Lagrangian timescale T_L and the (constant) turbulent energy σ^2. Gifford assigned values to these parameters by fitting the results of the Langevin model to atmospheric dispersion data for small and large time. He showed that the horizontal spread in tropospheric diffusion experiments, can very well be represented by this Langevin model. Not only tropospheric, but also stratospheric data are represented excellently over a very wide range of atmospheric diffusion scales which range from seconds to days, corresponding to distances from the source from several meters to several hundred kilometers (see fig. 3.5).

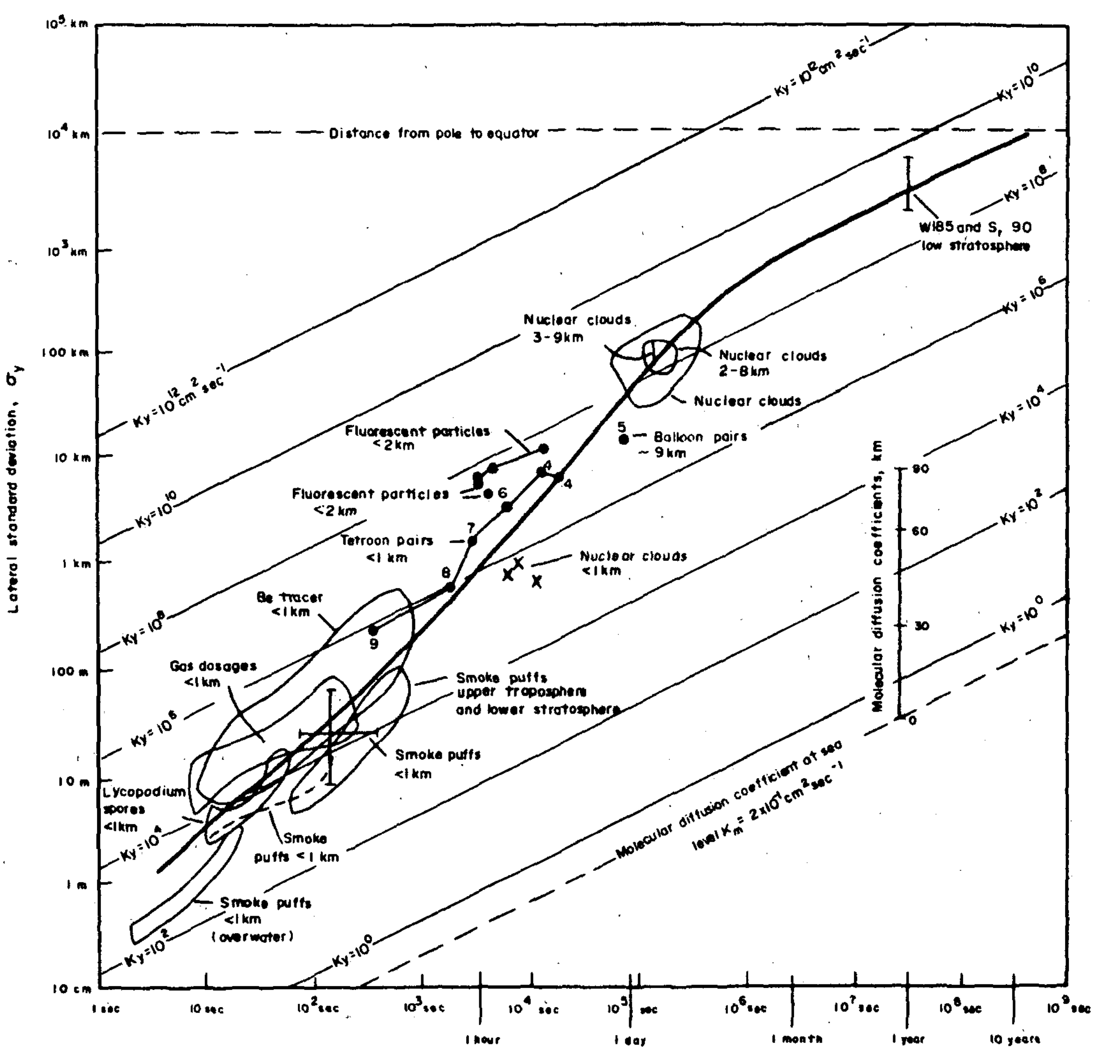

Fig. 3.5 Summary of data on horizontal atmospheric diffusion, from Hage and Church (1967). The solid curve illustrates Eq. (3.3.) (From Gifford, 1982a)

3.4 Langevin models for situations with a Gaussian height independent turbulence velocity distribution, where only T_L varies with height

In this section we study Langevin models, made for neutral surface layers. In neutral surface layer the turbulence is no longer homogeneous, because the timescale T_L varies proportionally with height. However, the intensity of the turbulence velocities σ^2 can be taken as constant and the velocity probability distribution as Gaussian. We investigate whether the homogeneous Langevin equation can also be used in neutral surface layers and we will show that this is indeed the case. Later we show this Langevin the formulation is erroneous when applied to a stable or convective surface layer.

3.4.1 Reid's model

Reid (1979) proposed a 1D-Langevin model for vertical dispersion in a neutral surface layer. He used the following discrete Langevin equation for the vertical velocity of the particle

$$W_{i+1} = \exp(-\frac{\Delta t}{T_L(z)})W_i + \sigma\, r_i\ (1-\exp)-\frac{2\Delta t}{T_L}))^{\frac{1}{2}} \quad , \tag{3.5}$$

which is in first order Δt a discrete form of the equation

$$W = -\frac{dt}{T_L(z)}\, W + (\frac{2\sigma^2}{T_L(z)})^{\frac{1}{2}} d\omega_t \ . \tag{3.6}$$

The random variable r_i and $d\omega_t$ are white noise processes with zero mean and variance resp. 1 and dt and σ^2 is the vertical turbulence velocity variance equal to $\sigma^2 = \overline{u_3^2}$. We see that his equation is formally equal to the homogeneous Langevin equation Eq. (3.4) only T_L has been substituted by $T_L(z)$.

Reid did not give a derivation for the formulation of this random forcing function, but assumed that the homogeneous formulation could be extended to dispersion in a neutral surface layer. It follows e.g. from Thomson's study (1984) that this is only true, if the Reynolds stresses $\overline{u_1u_2}$ and $\overline{u_2u_3}$ can be neglected. Thomson discussed the theory of 3-D dispersion, modelled by three Langevin equations. According to this study the correct random force in a neutral surface layer would be $\langle(d\mu)^2\rangle = 2\ \{\overline{u_1u_3} + \overline{u_3^2}\}dt/T_L$. In a neutral surface layer the wind varies with height resulting in a Reynolds stress $\overline{u_1u_3}$ which is nonzero. Thus even a 1D Langevin model should include more dimensional quantities, like $\overline{u_1u_3}$, in the random forcing $d\mu$. Deriving the KME of such a 1-D model we see that it has large time behaviour, which can not be described by a diffusion equation. The conclusion is that a 1-D formulation in a neutral surface layer is erroneous. We should go for a more dimensional Langevin model where we appropriately include the stresses in the random forcing formulation. Then we get a model with a large time behaviour described by a more dimensional diffusion equation, with diffusivity tensor $\overline{u_iu_j}$.

Model results

Reid discussed the results of his model applied for surface and elevated sources. The results of the surface sources were compared to the Porton data described by Pasquill (1961). To describe such a specific dataset, variables in the model were tuned to the measurements. Reid assumed that $\overline{Z}$ and varied the constant c from 0.3 to 0.5. This causes the mean particle height $\overline{Z}$ to vary by as much as 20% at a distance of x = 500 m. The formulation $T_L = 0.4\ z/u_*$ gave the best agreement with the Porton data (Fig. 3.6). Reid also compared his surface source results to similarity laws for the concentration profiles of Nieuwstadt and Van Ulden (1978) derived from the same Porton data and the Prairie Grass experiments and he found good agreement.

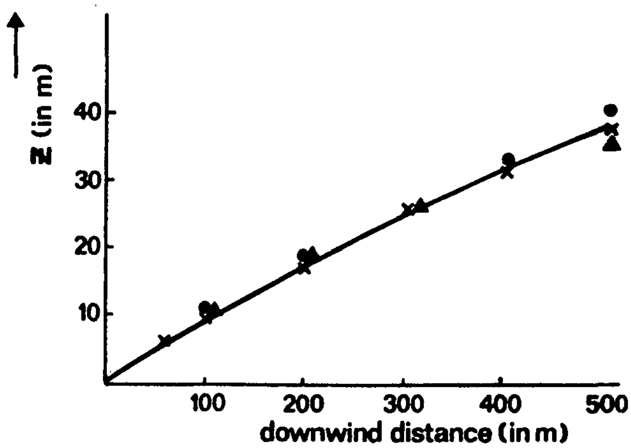

Fig. 3.6 Downwind variation of mean particle height $\overline{Z}$ for a surface source. The solid line represented the Porton data, further denotes a

. Reid's model,

x Ley's model (to be discussed in section 3.4.2) and

Δ Hall's model (to be discussed in section 3.4.3).

Reid compared his results for elevated sources to the Gaussian plume formula and Taylor's theorem although both formula's are in principle not valid in inhomogeneous turbulence. He allegedly finds discrepancies such as that in his model the mean height of the particles decreases just after their point of release, whereas in a Gaussian plume model $\overline{Z}/z_s$ increases monotonically. We can show from formula's derived by Hunt (1984) that his model shows the correct behaviour in contrast with the Gaussian plume model. Hunt derived an expression for the shorttime behaviour of the mean particle height $\overline{Z}$ not only as function of time but also an expressionas a function of downwind distance x. The last one reads

$$\frac{d\overline{Z}}{dx} = - \frac{\overline{uw}}{(\overline{u})^3} - \frac{x}{(\overline{u})^3} \left(\sigma^2 \frac{d\overline{u}}{dz} - \tfrac{1}{2} \overline{u} \frac{d\sigma^2}{dz}\right) . \qquad (3.11)$$

Generally the behaviour of $\overline{Z}$ depends on both $\frac{d\overline{u}}{dz}$, $\overline{uw}$ and $\frac{d\sigma^2}{dz}$. Depending on these variables $\overline{Z}$ might become larger or smaller.

In a situation with $\overline{uw} = 0$ and σ_w^2 constant (as in Reid's model) the shorttime behaviour reads

$$\frac{d\overline{Z}}{dx} = - \frac{\sigma^2}{(\overline{u})^3} \frac{d\overline{u}}{dz} \Big]_{z_s} x \; . \tag{3.12}$$

We see that $\overline{Z}$ decreases with distance in case $\overline{u}$ increases with height. This can be understood by considering particles at a distance x. We know that particles above source height z_s were transported by a larger horizontal wind and reached the point x therefore in a shorter time than particles under source height z_s. This means that particles above z_s had generally less time to disperse than particles under z_s. The averaged height $\overline{Z}$ becomes less. Reid finds indeed that $\overline{Z}$ decreases for short times.

Interesting is Reid's examination of the physics involved in dispersion. Reid discusses the effect of T_L varying with height. In comparing a case where T_L is constant with a case where T_L increases linear with z he comes to the conclusion that in the constant T_L case the mean height case $\overline{Z}$ is far less than in the varying case (Fig. 3.7a). This fact can be explained by the fact that drift terms up gradients in T_L occur as discussed in section 2.3.7 (second part).

The influence of the effect of varying T_L on the spread of the plume is not important for small downwind distances as can be xseen in Fig. 3.7b, while for large distances T_L being a function of z causes the plume to spread more rapidly. It is then empirically concluded that for the spread of the particles at short distances the windshear effect dominates T_L-variation effects, while for large distances they might be equally important or the T_L-effect might be larger.

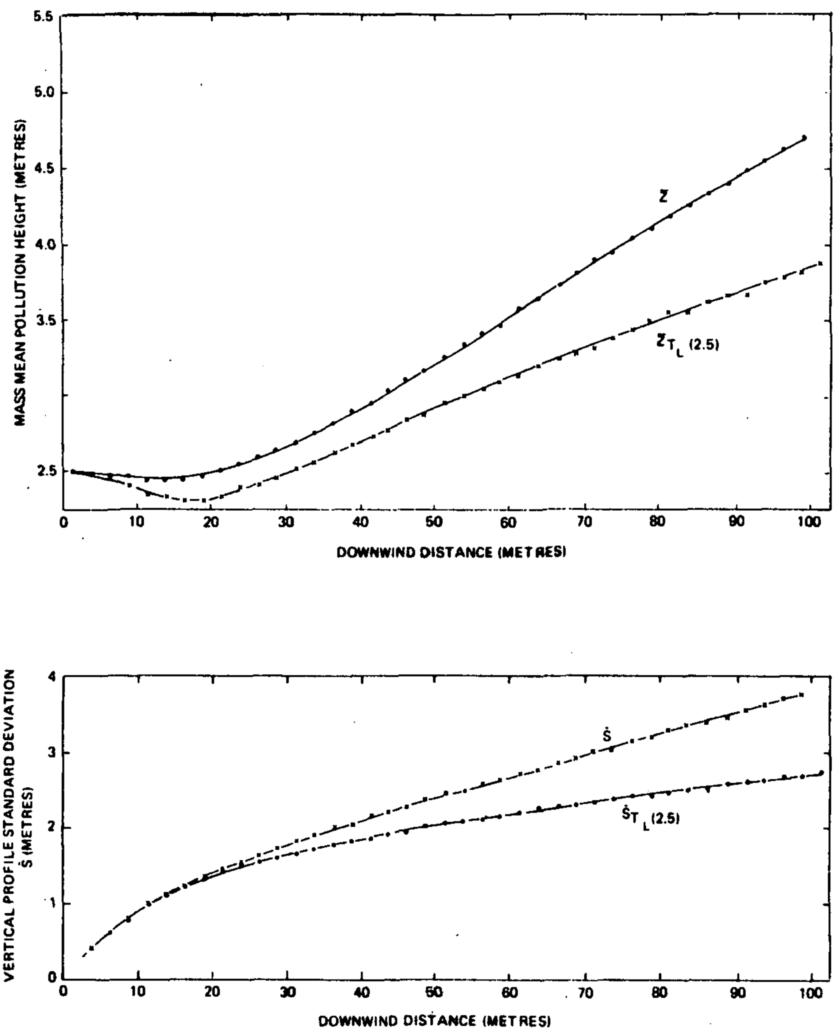

Fig. 3.7 Comparison of the height and standard deviation for a source at 2.5 m for T_L a function of height, $T_L(z) = 0.4\ z/u_*$ denoted by $\hat{s}$ and for $T_L = T_L(z = 2.5\ m)$ denoted by $s_{T_L(2.5)}$.
(From Reid, 1979)

3.4.2 Ley's model

Ley (1982) proposed a 2-D dispersion model for the neutral surface layer. The vertical dispersion is described by the homogeneous Langevin equation Eq. (3.4). The downwind dispersion is not described by a Langevin equation, but an alternative stochastic equation

$$dU = \overline{u} + \alpha U + \beta W + d\eta \ . \tag{3.13}$$

We first discuss the arguments (which we think are incorrect) leading to the formulation of the random forcing $d\mu$ in the vertical Langevin equation. We will see that the formulation of $d\mu$ is however correct in case the stress $\overline{u_1 u_3}$ can be neglected (as discussed in the former section).

Ley and later also Legg (1983, see section 3.4.3) started with the Langevin equation Eq. (3.3) in discrete form

$$W_{i+1} = (1 - \frac{\Delta t}{T_L(z)})W_i + \Delta\mu_i \ . \tag{3.14}$$

She squared this equation and took the ensemble average. Then she used the not always correct equation that

$$\overline{W^2_{i+1}} = \langle W^2_{i+1}\rangle = \overline{W^2_i} = \langle W^2_i\rangle = \overline{u^2_3} = \sigma^2_w \ . \tag{3.15}$$

In inhomogeneous circumstances this is only valid in the steady state. Then $\overline{W^2_{i+1}} = \overline{W^2_i}$ and the particle velocity statistics are equal to those of the turbulence velocities so that $\langle W^2_{i+1}\rangle = \langle W^2_i\rangle = \overline{u^2_3(z)}$. In this neutral case $\overline{u^2_3}$ is not a function of z and $\overline{W^2_i} = \langle W^2_i\rangle$ from which the above equation follows. From Eq. (3.15) she reached the equation

$$\sigma^2_w = (1 - \frac{\Delta t}{T_L})^2 \sigma^2_w + \langle(d\mu)^2\rangle + \langle 2(1 - \frac{\Delta t}{T_L})W_i\Delta\mu\rangle \ . \tag{3.16}$$

In this equation she neglected the last term on the RHS. This can indeed be justified, because the Lagrangian timescale T_L and the random forcing function $\Delta\mu$ are uncorrelated with the velocity W. (Note that T_L and $\Delta\mu$ are also uncorrelated, if we specify stochastic quantities occurring in the Langevin equation in the non-anticipating way (section 2.4). This non-anticipating specification implies that $T_L(z)$ is taken at the left end point

$z = Z_i$ of the interval $[Z_i, Z_{i+1}]$ over which $\Delta\mu$ is taken).

After neglecting the last term in Eq. (3.16) this equation gives

$$<(\Delta\mu)^2> = \frac{2\sigma_w^2}{T_L} \Delta t + O(\Delta t^2) .$$

As all other moments of $d\mu$ are zero this leads to the fact that the continuous random forcing function can be formulated as $d\mu = (2\sigma_w^2/T_L)^{½} d\omega_t$.

We discussed the Langevin modelling of the vertical velocity of the particles. We now discuss the modelling of the horizontal velocity of the particles Eq. (3.13). We denote the horizontal turbulence velocity in the downwind direction by u_1. The additional turbulence description needed to determine α, β and $d\eta$ is $\overline{u_1^2} = \sigma_u^2$ = constant, $R_u(dt) = \exp(-dt/T_u)$ and $\overline{u_1 u_3} = - u_*^2$. The determination of α, β and $d\eta$ is again based on equalities that are only valid in the steady state. The resulting formulation can not be compared with the theoretical results of Thomson (1984) as Thomson's results are for models, where both velocity components are modelled by a Langevin equation, while Ley's equation for the horizontal particle velocity is not a Langevin equation. The correlation between the two directions of motion should according to Thomson only be modelled in a joint moment of the random forcing functions $d\eta$ and $d\mu$. The difference with Ley's model is that there the correlation is also incorporated in a term proportional to W in the equation for U.

Model results

Ley discussed the results of surface sources, which were compared to the Porton data. Variables in the model were tuned to this dataset. Ley got the right results for $\overline{Z}$ by varying the von Karman constant k and the friction velocity u_* keeping u_*/k equal to 0.62. Varying k from 0.33 till 0.43 caused $\overline{Z}$ to vary as much as 20% at a distance of 500 m. The values k = 0.4 and u_* = 0.25 turned out to be the best for the Porton data (Fig. 3.6). We may conclude that both Reid's and Ley's model, although different, can be tuned to this dataset.

Ley also compared surface source results to the similarity laws derived from the Prairie Grass and Porton data by Nieuwstadt and Van Ulden (1978) and finds good agreement with the similarity shape of the concentration profiles just like Reid with his 1-D model.

Ley's examination of her 2-D formulation is interesting, although we can not directly apply her results to a 2D Langevin model. If no downwind dispersion is assumed (which reduces her 2-D model to a 1-D model) or when the downwind dispersion is uncorrelated with the vertical dispersion ($\beta = 0$, $\overline{uw} = 0$) the average height $\overline{Z}(x)$ of the particles becomes 8% lower.

3.4.3 Legg's model

Legg (1983) made a 2-D Langevin model for the neutral boundary layer in which the correlation between the two directions of motion is only modelled via the random forcing function. His equation for W is in first order Δt equal to Eq. (3.4) and for U he proposes

$$U_{n+1} = \frac{\Delta t}{T_L}\bar{u} + \left(1 - \frac{\Delta t}{T_L}\right)U_n + \left(\frac{2\sigma_u^2}{T_L}\right)^{1/2}\frac{\overline{u_1u_3}}{\sigma_u\sigma_w}\Delta\omega_t' + \left(\frac{2\sigma_u^2}{T_L}\right)^{1/2}\left(1-\frac{\overline{(u_1u_3)}^2}{\sigma_u^2\sigma_w^2}\right)^{1/2}\Delta\omega_t'' , \tag{3.15}$$

where $\sigma_w^2 = \overline{u_3^2}$, $\sigma_u^2 = \overline{u_1^2}$ and $\Delta\omega_t'$ and $\Delta\omega_t''$ are white noise processes with zero mean and variance Δt. Legg realised that in the derivation of the random forcing function it had to be argued that correlations between T_L, W and $d\mu$ pr $d\eta$ are neglected. As noted before this is exactly so because T_L and $d\mu$ or $d\eta$ are not correlated with W.

Thomson's (1984) theoretical investigation can be used to investigate this 2-D Langevin model of Legg. Thomson argued that in Gaussian turbulence, with σ^2 independent of height, the 2-D Langevin model should be

$$dW = -\frac{dt}{T_L}W + d\mu \text{ and}$$
$$dU = -\frac{dt}{T_L}U + d\eta , \tag{3.16a}$$

where the timescales in both equations are taken to be equal to T_L and

$$\langle d\mu\rangle = 0 \quad , \quad \langle d\eta\rangle = \frac{dt}{T_L}\bar{u} ,$$
$$\langle (d\mu)^2\rangle = 2\frac{dt}{T_L}(\overline{u_1u_3} + \overline{u_3^2}) \quad , \quad \langle (d\eta)^2\rangle = 2\frac{dt}{T_L}(\overline{u_1u_3} + \overline{u_1^2}) ,$$
$$\langle d\eta d\mu\rangle = \frac{dt}{T_L}(\overline{u_1^2} + 2\,\overline{u_1u_3} + \overline{u_3^2}) . \tag{3.16b}$$

We see that Legg's formulation of the random forcing differs considerably from Thomson's theoretical results.

Model results

Legg applied his model to an elevated source and compared the results to a heat dispersion experiment in a windtunnel. To reproduce the measurements Legg tried different descriptions of the windtunnel flow. One of these is a horizontally inhomogeneous boundary layer formulation. We note that in such cases the random forcing modelling becomes more involved than the ones in Eq. (3.4) and (3.16) and we refer for further details to Thomson (1984). Tuning the value of the timescale in the Langevin equation Legg could reproduce the results (Fig. 3.8). Legg also compared the 1-D formulation (line (a) and (b)) with the 2-D formulation (line (c)). He concluded that the inclusion in the dispersion model of streamwise velocity fluctuations and their correlation with vertical fluctuations increases the depth and rate of rise of the plume from an elevated source. It should be investigated, whether Thomson's formulation for a 2D model would show the same feature. Legg also modified his 2-D formulation to include the effect of skewness of the turbulence velocity. As the skewness in the windtunnel flow is small only little difference in the results appeared (line d).

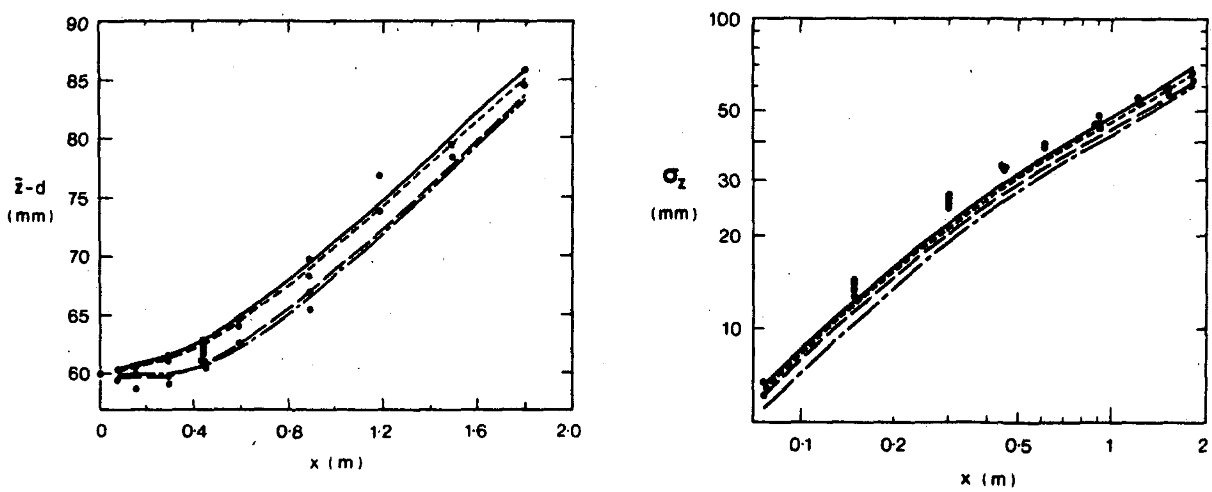

Fig. 3.8 Mean particle height $\overline{Z}$ and vertical plume spread σ_z against downstream distance in a neutral surface layer. Symbols (o) show experimental results and the lines show Markov chain similations with:

(a) long/short dashes: $\sigma_u = 0.63\ ms^{-1}$ $\sigma_u = 0.00\ ms^{-1}$

(b) long dashes : $\sigma_u = (0.68-0.05x) ms^{-1}$ $\sigma_u = 0.00\ ms^{-1}$

(c) short dashes : $\sigma_u = (0.68-0.05x) ms^{-1}$ $\sigma_u = (1.21-0.04x) ms^{-1}$

: $uw = -(0.28-0.033x) m^2 s^{-2}$ $T_L = 0.15$

(d) continuous As previous line but with a jointly skewed distribution of u' and w'.

(d is zero plane displacement) (From Legg, 1983)

3.4.2 Durbin's model

We further want to mention Durbin (1980), who studied open channel flow. He introduced an equation to describe the large time behaviour of dispersion. This equation is

$$dZ = \sigma^2 \frac{dT_L}{dz} dt + (2\,\sigma^2 T_L)^{1/2} d\omega_t \;. \tag{3.17}$$

We have shown in section 2.5 that this equation, the Markov limit of the Langevin equation Eq. (3.4), indeed describes the large time behaviour in turbulence with constant σ^2 and where T_L may be a function of z.
The KME of Eq. (3.17) is the diffusion equation

$$\frac{\partial P(z;t)}{\partial t} = \frac{\partial}{\partial z} (\sigma^2 T_L \frac{\partial P}{\partial z}).$$

The Markov limit is only applicable to dispersion for times large compared to T_L. However Durbin noted that in case of a surface source, the Markov limit is valid for all times. This is so if we accept like Durbin claims that the value of T_L to be used in the comparison of t with T_L is $T_L(z_s)$, which for a ground source is zero. However, for a surface source Durbin only shows large time results (Fig. 3.9) and his statement is not proved. On the other hand he does show that the Markov limit is not valid for small times for an elevated source where $T_L(z_s)$ is larger than t.

Note that the results of the Langevin equation (Eq. (3.4)) show many fluctuations as only a 100 particles are used to obtain ensemble averages, while the Markov limit results are obtained from an analytical solution of its KME.

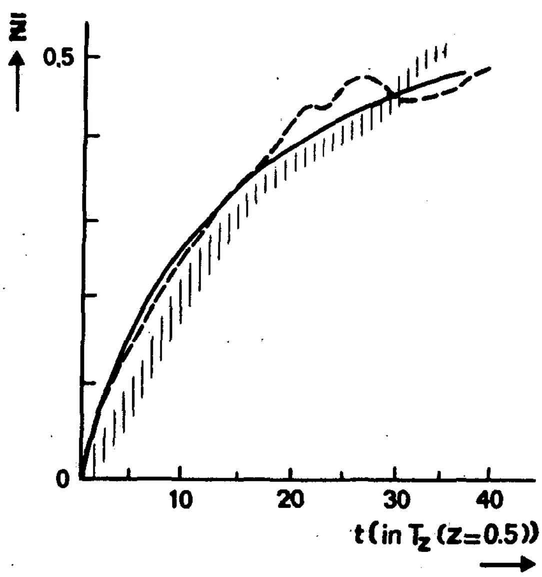

Fig. 3.9 Comparison of the Langevin equation Eq. (3.4), the Markov limit Eq. (3.17) and experimental data in an open channel flow with T_L = 0.8 z(1-z) and σ_w = 1.0, for a surface source.

Hatched lines: experimental data

Dashed line : Langevin equation

Solid line : Markov Limit

(From Durbin (1980), rescaled with the bottom of the channel at z = 0, the top at z = 1).

3.4.3 Hall's model

Hall (1975) made a 2-D model for the surface layer. It is a Langevin equation for the vertical velocity W and a zero order process for the horizontal velocity U

$$W_{i+1} = (1 - \frac{\Delta t}{T_L})W_i + (\frac{2\sigma_w^2}{T_L})^{1/2} \Delta\omega_t \quad , \tag{3.18}$$

$$U_{i+1} = \bar{u} + \Delta\eta_{i+1} \qquad \text{and}$$

$$Z_{i+1} = W_i \; \Delta t \quad .$$

This model does not take into account that the horizontal velocity process has a non-zero time scale. The random forcing formulation in the W-equation is only valid in Gaussian turbulence with a constant σ_w^2 and zero Reynolds stresses and as discussed in section 3.4.1, neglecting the Reynolds stress in $d\mu$ is also erroneus.
The moments of the random forcing function $d\eta$ are again derived assuming equalities between particle characteristics and turbulence velocity characteristics that are only valid in the steady state.

Model results

Hall did not only apply this model to a neutral-, but also to a convective surface layer. In the neutral surface layer only T_L and $\bar{u}$ are functions of height, while σ_w^2, σ_u^2 and $\overline{u_1 u_3}$ are constant. His results were compared to the Porton data and after tuning T_L they fit the measurements (Fig. 3.6). In the convective surface layer T_L and $\bar{u}$ but also σ_u^2 and σ_w^2 are functions of height, while $\overline{u_1 u_3}$ is still constant. Applying the homogeneous Langevin model to situations where the turbulence velocity characteristics are inhomogeneous is certainly not correct. This is apparent in his results compared to Porton data given by Pasquill (1961) for a surface source in a convective surface layer (L = - 5m). His model resulted in an underestimation of the measured cloud height at all distances (Fig. 3.10). This can be explained by the fact that his model does not incorporate the drift acceleration of particles in inhomogeneous turbulence due to gradients in σ_w^2. As we have seen in section 2.3.5 and 2.3.6 this should be modelled by a mean value of the random forcing in the z-direction equal to dt $d\sigma_w^2/dz$. Not including this drift velocity causes the particles to collect in regions of low turbulence variance, which in the convective surface layer is close to the ground. The mean height of the particles is then too low, as Hall indeed found in his simulations. We conclude that Hall's Langevin model is not applicable to a convective surface layer. Models that are applicable to such circumstances are discussed in the following section.

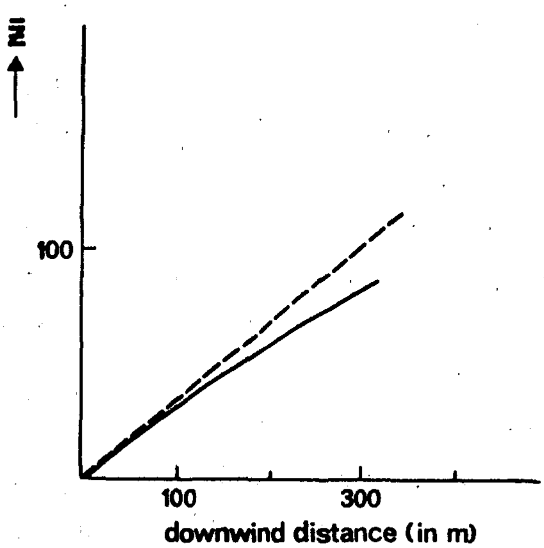

Fig. 3.10 Comparison of Hall's model (1975) with Porton data for a surface source in a convective surface layer (L = -5m).
Solid line : Hall's Langevin model Eq. (3.18)
Dashed line: Porton data.
(From Hall, 1975)

3.5 Langevin models for situation with height dependent Gaussian turbulence

In the previous section we discussed that the homogeneous Langevin equation is a correct formulation for dispersion in the surface layer where σ^2 is constant and where T_L can be constant or a function of z. The next group of models we want to discuss are models that take into account the effect of inhomogeneity in σ^2. The first attempt to model this was made by incorporating a mean drift acceleration in the homogeneous Langevin equation, or equivalently a drift velocity in its large time equation, the Markov Limit.

To avoid confusion about the concept drift velocity versus drift acceleration we note again that the effect of inhomogeneity described as a drift velocity $d(\sigma^2 T_L)/dz$ in the Markov limit is consistent with a drift acceleration $d\sigma^2/dz$ in the Langevin equation. This is shown in section 2.5.4.

3.5.1 Durbin and Hunt's model

Durbin and Hunt (1980) described dispersion in the neutral boundary layer in a windtunnel experiment of Shlien and Corrsin (1976). Near the surface the boundary layer is described by a constant $\sigma^2 = \overline{u_3^2}$ and T_L a function of height. In the larger part of the boundary layer σ^2 is on the contrary a function of height, while T_L is constant. To describe dispersion in this neutral boundary layer Durbin and Hunt used the homogeneous Langevin equation. Because they only show results in the surface layer where σ^2 is constant no inconsistencies between model results and measurements appear.

Besides this homogeneous Langevin model they also use a large time equation, the Markov limit, which incorporates the effect of inhomogeneity in σ^2 by a mean drift velocity $d(\sigma^2 T_L)/dz$:

$$dZ = \frac{d(\sigma^2 T_L)}{dz}\, dt + (2\sigma^2 T_L)^{\frac{1}{2}} d\omega_t \ . \qquad (3.19a)$$

This is a generalisation to height dependent σ^2-cases of Durbin's homogeneous Markov limit Eq. (3.17). According to the theory discussed in section 2.5 this Markov limit is the correct formulation for regions where σ^2 is a function of z. Durbin and Hunt based the incorporation of a drift velocity on arguments of Monin and Yaglom, who state that in horizontally homogeneous turbulence whose mean vertical velocity $\overline{u_3} = 0$, the pdf $P(z;t)$ should obey (1977, Ch. 10.3, Eq. 10.49).

$$\frac{\partial P(z;t)}{\partial t} = \frac{\partial}{\partial z} (K \frac{\partial P}{\partial z}) \ . \qquad (3.19b)$$

Any dispersion model should result in large time behaviour described by this diffusion equation. The KME of the Markov limit Eq. (3.19) is indeed equal to Monin and Yaglom's formulation in case $K = \sigma^2 T_L$ and we conclude that this Markov limit model gives the correct large time behaviour in turbulence with height dependent Gaussian velocity distributions.

The homogeneous Langevin equation Durbin and Hunt used has a Markov limit $dZ = (2\sigma^2 T_L)^{1/2} d\omega_t$. Comparing this Markov limit with the Markov limit Eq. (3.19) we see that the homogeneous Langevin equation and the Markov limit Eq. (3.19) are only consistent in homogeneous situations. The reason why no large discrepencies for large time between both models occur is that they only show results in the surface layer, where σ^2 is constant.

They apply their models to a surface source. As stated earlier by Durbin (section 3.4.4) the Markov limit should describe dispersion from surface sources at all times. To prove this statement they check whether the Langevin equation and the Markov limit describe the measurements equally well. They show direct simulations of the Langevin model while they however only derive an approximation for $\overline{Z}(x)$ from the KME of the Markov limit Eq. (3.19b) as follows. The mean height can be defined as M_1/M_0 where $M_n = \int_0^\infty z_n P(x,z) dz$. This equation can not analytically be solved in this neutral surface layer where K and u are functions of height and is therefore approximated. In comparing this result with the Langevin model we have to be careful. Both models start with $\overline{Z}(o) = z_s = 0$ and if differences with respect to each other exist, they only slowly accumulate. Within the restrictions of this Markov limit results it is hard to judge whether the Markov limit and the Langevin equation are indeed equivalent (see Fig. 3.11).

The statement that the Markov limit should describe dispersion from surface soruces of all times is based on the assumption that the relevant T_L is small compared to t (section 3.4.4). But if we argue for instance instead that the value of T_L that sould be taken in the comparison of t with T_L is T_L at mean plume height $T_L(\overline{Z})$ we find that the Markov limit is not equivalent to the Langevin equation for $x < 20\ z_i$.

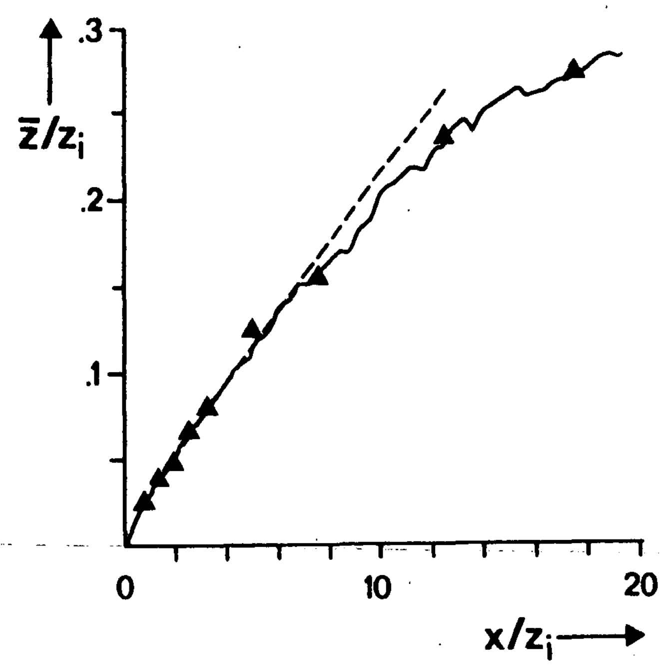

Fig. 3.11 Comparison of the Langevin Eq. (3.4) (solid line) and an approximation to the Markov limit Eq. (3.19) (dashed line) with windtunnel data (triangles) in a neutral surface layer. (From Durbin and Hunt, 1980).

3.5.2 Legg and Raupach's model

We now discuss a model proposed by Legg and Raupach (1982) for inhomogeneous turbulence. Legg and Raupach simulated dispersion within and above a crop canopy by means of the vertical 1-D Langevin equation

$$dW = (\exp(-\frac{dt}{T_L})-1)W + (1-\exp(-\frac{2dt}{T_L}))^{\frac{1}{2}}\sigma_w r + (1-\exp(-\frac{dt}{T_L}))T_L \frac{d\sigma_w^2}{dz} ,$$

which in first order dt is equal to

$$dW = -\frac{W}{T_L} dt + (\frac{2\sigma_w^2}{T_L})^{\frac{1}{2}} d\omega_t + \frac{d\sigma_w^2}{dz} dt . \qquad (3.20a)$$

This study incorporates the by now well familiar drift acceleration $d\sigma_w^2/dz$ in the Langevin equation to model the effect of inhomogeneity in the turbulence fluctuations $\sigma_w^2 = \overline{u_3^2}$. They base their arguments for the drift acceleration on the mean momentum equation that for stationary horizontally homogeneous flow reads

$$\frac{d\sigma_w^2}{dz} = -\frac{1}{\rho}\frac{\partial \bar{p}}{\partial z} .$$

This equation states that when there is a gradient in the vertical velocity variance $d\sigma_w^2/dz$ there is a mean force on the particle due to the mean pressure gradient. This force should be included in the Langevin model as a mean acceleration. The Langevin model with this term included Eq. (3.20a) can be written as

$$dW = -\frac{W}{T_L} dt + d\mu ,$$

$$\text{with} \quad \langle d\mu \rangle = \frac{d\sigma_w^2}{dz} dt , \qquad (3.21)$$

$$\langle (d\mu)^2 \rangle = \frac{2\sigma_w^2}{T_L} dt \quad \text{and}$$

$$\langle (d\mu)^n \rangle = 0 \quad \text{for} \quad n \geq 3 .$$

Model results

Legg and Raupach applied this model to dispersion in and above a crop. The flow field in the crop and in the first meter above it is described by

$$
\begin{aligned}
\bar{u}(z) &= \bar{u}(h)\ \exp \gamma(\tfrac{z}{h} - 1) && z \leq h \\
&= \frac{u_*}{k} \ln \left(\frac{z-d}{z_o}\right) && z > h \\
\sigma_w(z) &= 0.125\ u_* + 1.125\ \frac{z u_*}{h} && z \leq h \\
&= 1.25\ u_* && z > h \\
T_L(z) &= \frac{0.32(h-d)}{1.25\ u_*} && z \leq h \\
&= \frac{0.32(z-d)}{\sigma_w} && z > h
\end{aligned}
\qquad (3.22)
$$

where h is the crop height, d the zero plane displacement, z_o the roughness length and γ an extinction coefficient within the crop. Total reflection at the ground and at 1.5 h were assumed. An initially uniform distribution remained uniform in this model although the scatter near the ground becomes large. We can speculate on the reason why this model does preserve an initially uniform concentration distribution, while ours in its application to a convective boundary layer (Ch. 4) did not. Our speculation is that the boundaries might be a problem in case the characteristic length of the turbulence $\ell = T_L \sigma$ is large compared to the height of the layer (resp. h and z_i). Calculating ℓ by putting $\ell = T_L(\ell)\sigma(\ell)$ gives in Legg and Raupach's case $\ell/h = 0.05$ while in our model $\ell/z_i = 1.4$.

Let us investigate the random forcing in this model. In section 2.3.5 and 2.3.6 we showed that the first two moments of $d\mu$ are correctly modelled in case of inhomogeneous Gaussian turbulence. This model neglects the third moment of $d\mu$ for $z \leq h$, whereas the theory for the Langevin model in inhomogeneous conditions told us that the third moment of the random forcing function should be equal to $3\ \sigma_w^2\ d\sigma_w^2/dz$. We discuss the effect of omitting a nonzero third moment of the random forcing in inhomogeneous Gaussian turbulence. This can easiest be shown by considering the shorttime expansions around z_s, the point of release, of mean height, spread and third moment of the particle height. These expansions for height and spread will be derived in the coming section 5.3 and the expression for the third moment can be derived analogously. They read

$$\overline{Z-z_s} = \tfrac{1}{2}\, a_1(z)t^2 + \dots \qquad = \tfrac{1}{2}\,\frac{d\sigma^2}{dz}\, t^2 + \dots$$

$$\overline{(Z-z_s)^2} = \overline{u_3^2}\, t^2 + \frac{1}{3}\, a_2(z)\, t^3 \dots \qquad = \sigma^2\, t^2 + \dots \tag{3.23}$$

$$\overline{(Z-z_s)^3} = \tfrac{1}{4}\, a_3(z)t^4 + \dots \qquad = \frac{3}{4}\,\sigma^2\,\frac{d\sigma^2}{dz}\, t^4 + \dots$$

This first formula is consistent with Hunt's (1984) general expression for the mean height as function of x (Eq. (3.11)) which include effects of Reynolds stresses, windshear and skewness of the turbulence. Let us consider a source in the region where σ^2 increases with height. From Eq. (3.23) it follows that in the region near the ground, where $\frac{d\sigma^2}{dz} > 0$ the mean height of the cloud increases. At the same time the particle cloud becomes more and more skew with time because the third moment is non zero. The skewness is positive which means that the height at which the concentration is maximum decreases. This is schematically shown in Fig. 3.12. In a model where the third moment of $d\mu$ is zero no distinction is made between the mean height of the plume and the height where the concentration is maximum, boundary effects excluded. As Legg and Raupach start with a uniform concentration distribution errors due to this fact do not show in their results.

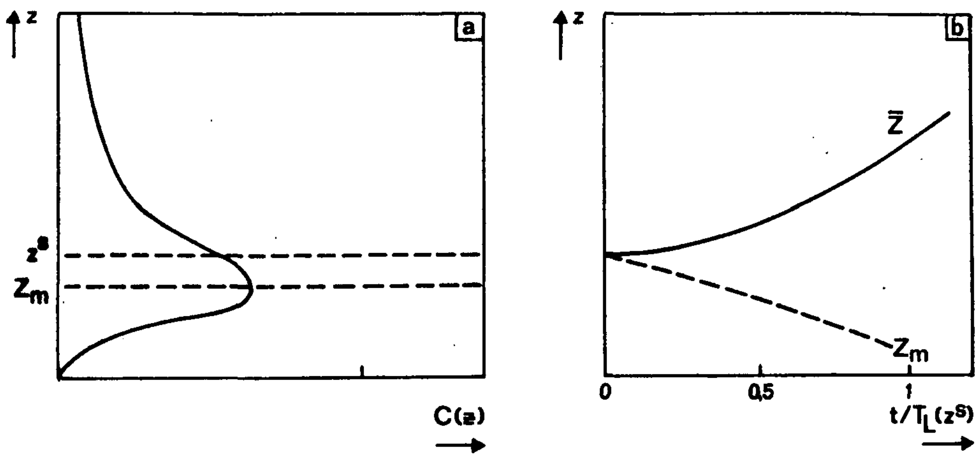

Fig. 3.12 (a) Concentration distribution of the vertical velocity close to the source.

(b) Mean plume or cloud height $\bar{Z}$ (solid line) and height of the maximum mean concentration Z_m in convective conditions $d\sigma_w^2/dz > 0$, $\overline{w^3} > 0$ $(z_s/z_i \sim 0.1)$.

(From Hunt (1984)

3.5.3 Davis' model

P.A. Davis (1983) made a 2D-model for the neutral boundary layer, in which all parameters $\overline{u}$, $\overline{uw}$, σ_w, σ_u, T_{L_w} and T_{L_u} depend on height. The vertical velocity is given by Legg and Raupach's Langevin Eq. (3.20a). The horizontal velocity fluctuation is modelled by

$$U(t + \Delta t) = S(t + \Delta t) + \beta W(t + \Delta t) \quad \text{and}$$
$$S(t + \Delta t) = \alpha\, S(t) + \gamma \eta\ , \qquad (3.24)$$

where S is a dummy variable. This equation is different from Ley's (1982) as the horizontal particle velocity does not depend on the history of the vertical velocity but only on its actual value. It is also different from Legg's (1983) model, as the horizontal particle velocity is not modelled by a Langevin equation. The derivation of the coefficients α, β and γ is again based imposing that the particles have the same velocity characteristics as the turbulence velocity, a requirement only valid in stationary turbulence.

Davis found that the effect of making a 2-D-model by taking the correlation between horizontal and vertical fluctuations into account did increase $\overline{Z}$ and σ_z at all downwind distances for elevated sources. The amount he found is less than found by Ley with her (different) 2-D-model in the surface layer. He also derives an analytical expression for the spread of the plume resulting from his model given as function of dimensionless parameters.

3.5.4 Ley and Thomson's model

Ley and Thomson (1983) made a 2-D model for diabatic (stable and unstable) conditions. They used Langevin formulations for the vertical velocity of the particles (Eq. (3.20a)) and for the horizontal velocity. The horizontal Langevin equation is a version of the one used by Legg (1983):

$$dU = (\exp(-\frac{dt}{T_L}) - 1)U + d\eta \ . \tag{3.25}$$

The derivation of the first two moments of $d\mu$ is analogous to the theory discussed in Ch. 2. The random forcing $d\eta$ is modeled by imposing that the particles mean horizontal velocity, horizontal velocity variance and covariance between vertical and horizontal fluctuations in the steady state should equal those of the air ($\overline{u}$, σ_u^2, $\overline{u_1u_3}$). In this study the equality is explicitly only required in the steady state but still their formulation of $d\mu$ and $d\eta$ is not consistent with the theory discussed in Ch. 2. In this Langevin model the random forcing function $d\eta$ and $d\mu$ are assumed to be Gaussian so that only the first two moments are specified. The fact that the third moment, which should be there from a theoretical point of view, is not taken into account, leads to errors as discussed in section 3.5.2.

Model results

Legg and Thomson applied their model to stable and unstable surface layers both with Gaussian velocity distributions. The turbulence is characterised by $\sigma_w^2(z) = \overline{u_3^2}$, $\sigma_u^2(z) \equiv \overline{u_1^2}$, $T_L(z)$ and $\overline{u_1u_3}(z)$. The profiles in the stable surface layer are given by profiles valid for the whole boundary layer

$$\sigma_w^2/u_*^2 = 2.25(1-z/z_i)^2 \ ,$$

$$\sigma_u^2/u_*^2 = 5.29(1-z/z_i)^2 \quad \text{and} \tag{3.26}$$

$$\overline{u_1u_3}/u_*^2 = (1-z/z_i)^2 \ ,$$

where z_i is the boundary layer height. These profiles give almost constant values for σ_w^2, σ_u^2 and $\overline{u_1u_3}$ in the surface layer ($z << z_i$).

The unstable surface layer is given by

$$\sigma_w^2/u_*^2 = 1.69(+ 3\|z/L)^{2/3} ,$$

$$\sigma_u^2/u_*^2 = (12 + 0.5\|z_i/L\|)^{2/3} \text{ and} \qquad (3.22)$$

$$\overline{u_1 u_3}/u_*^2 = 1$$

where L is the Monin Obukhov length. Thus in the unstable surface layer only σ_w^2 is a function of height.

For $\bar{u}(z)$ and $T_L(z)$ the similarity expressions of the surface layer are used:

$$\frac{d\bar{u}}{dz} = \frac{u_*}{kz}(1 + 5\ z/L) \qquad L > 0 \qquad \text{(stable)}$$

$$= \frac{u_*}{kz}(1 - 16\ z/L)^{-1/4} \qquad L < 0 \qquad \text{(unstable)}$$

$$(3.28)$$

$$T_L = ku_*z/(1 + 5z/L)\sigma_w^2 \qquad L > 0 \qquad \text{(stable)}$$

$$= ku_*z(1 - 16\ z/L)^{1/4}/\sigma_w^2 \qquad L < 0. \qquad \text{(unstable)}$$

In this study the values for T_L are determined from equating the eddy diffusivity K_{mass} to $T_L\sigma_w^2$ where $K_{mass} = ku_*z/\phi_m(z/L)$ with $\phi_m(z/L)$ the non-dimensional profile of mass transfer. Note that this description leads to the fact that T_L is u_* dependent even in unstable conditions, whereas free convection scaling states that T_L should depend on w_* instead of u_*.

It turned out that their model results could be tuned to measurements by varying the constants in the modelling of the turbulence. They compared their model with the Prairie Grass data, Porton data and Lagrangian similarity theory and find reasonable agreement within the limits of accuracy of the variable constants (Fig. 3.13).

With this study we end our discussion of models for dispersion in situations where both T_L and the Gaussian turbulence velocity distribution vary with height. Next we note studies with another Langevin model for W/σ. In Ch. 5 we will theoretically compare both Langevin models.

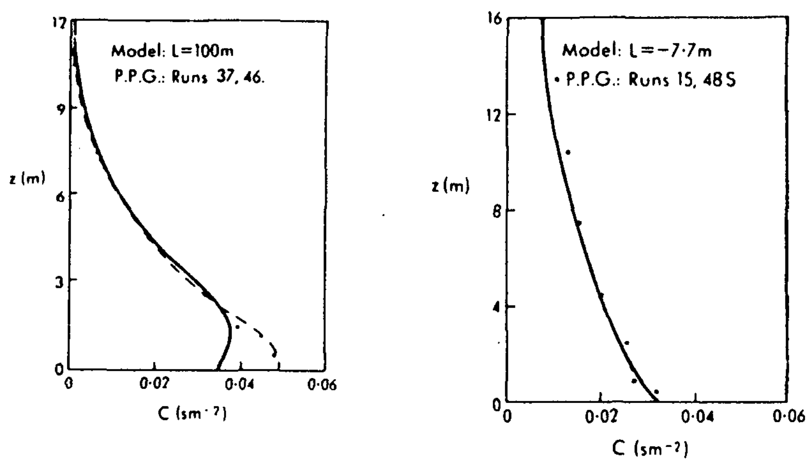

Fig. 3.13 Comparison of project Prairie Grass (P.P.G.) profiles with the Langevin model Eq. (3.20) and (3.25) The horizontal axis, C, represents cross-wind-integrated concentration per unit source strength for the P.P.G. data, and concentration per unit source strength for the model output. Continuous line: the model profile. Broken line: model profile. Dots: P.P.G. values. (From Ley and Thomson, 1983)

3.6 Langevin model for W/σ and its Markov limit

3.6.1a Wilson et al's Langevin model for W (1981a)

Wilson et al. (1981a) introduced a handy numerical method for the homogeneous Langevin model by scaling both time and particle height. Later he extended this idea to also transforming the particle velocity W by dividing it by σ. This led to a different Langevin model and well a Langevin model for the quantity W/σ. First we discuss their article (1981a) on simulation of dispersion in a neutral surface layer with $\sigma^2 = \overline{u_3^2}$ constant and T_L a function of height.

In this paper they only scale time and height. They showed that the homogeneous Langevin equation Eq. (3.4) can be scaled by introducing

$$dt' = dt \, \frac{T_L(H)}{T_L(z)} \text{ and } dz' = dz \, \frac{T_L(H)}{T_L(z)} , \tag{3.29}$$

where H is a reference height. This gives

$$dW(t') = -\frac{W(t')}{T_L(H)} \, dt' + \left(\frac{2\sigma^2}{T_L(H)}\right)^{1/2} d\omega_t' \quad \text{and}$$
$$dZ(t') = W(t')dt' \, . \tag{3.30}$$

This transformation leads to an equation with constant coefficients and is therefore more easy to handle. This equation can be solved analytically and the height of a particle at any time can be transformed back by the inverse of Eq. (3.29).

3.6.1.b Wilson et al. (1981b)

In a following article Wilson et al. (1981b) added an extra term to the homogeneous Langevin equation for W to model the effect of σ being a function of height. They assumed that the variation of σ in the turbulence considered is so slow that the gradient can be considered constant. They proposed the equation

$$dW = - W \frac{dt'}{T_L(H)} + \left(\frac{2\sigma^2(H)}{T_L(H)}\right)^{1/2} d\omega_t + \sigma(H) T_L(z) \frac{d\sigma(z')}{dz'} . \quad (3.31)$$

We discuss several aspects of this extra term.

In this last term $T_L(z)$ occurs, but we assume that is meant $T_L(H)$ as that is consistent with their later statements. The extra term implies then a height independent drift acceleration $\{\sigma(H)T_L(H)d\sigma/dz\}/dt$ that however goes to infinity in case $dt \to 0$, which is unrealistic. It can also be shown that this term is incorrect by transforming Eq. (3.31) back and comparing it to the theory of section 2.3.7.
The transformation in this article (1981b) is given by

$$dt' = dt \frac{T_L(H)}{T_L(z)} , \; dz' = dz \frac{T_L(H)}{T_L(z)} \frac{\sigma(H)}{\sigma(z)} \text{ and } C' = C \frac{\sigma(z)}{\sigma(H)} . \quad (3.32)$$

Executing the back transformation this gives the equation

$$dW = - \frac{W\,dt}{T_L(z)} + \left(\frac{2\sigma^2(H)}{T_L(z)}\right)^{1/2} d\omega_t + \sigma(z)\, T_L(z) \frac{d\sigma}{dz} , \quad (3.33)$$

which has a drift acceleration $\sigma(z)T_L(z) \frac{d\sigma}{dz} dt^{-1}$. Note that both the second term and the last term on the RHS of this Langevin equation are different from what they should be according to the theory discussed in Ch. 2. Based on this theory we showed in section 3.5.2 that the Langevin model in height dependent Gaussian turbulence should read (see Eq. (3.20))

$$dW = - \frac{W}{T_L(z)} dt + \left(\frac{2\sigma^2(z)}{T_L(z)}\right)^{1/2} d\omega_t \pm \tfrac{1}{2}\, \sigma(z) \frac{d\sigma}{dz} dt .$$

We see that in the second term on the RHS of Eq. (3.33) $\sigma^2(H)$ enters instead of $\sigma^2(z)$. The difference in the last term, the drift acceleration term is discussed in a later paper by Wilson et al. (1983). There it is wrongly assumed that Legg and Raupach (1982) used $d\overline{W} = T_L \frac{d\sigma^2}{dz}$ instead of $d\overline{W} = dt \frac{d\sigma^2}{dz}$. This might be explained by the fact that in the other studies the drift acceleration is expressed as

$$d\overline{W} = (1 - \exp(-dt/T_L) T_L \frac{d\sigma^2}{dz} .$$

The drift acceleration is then not given by $d\overline{W} = T_L \frac{d\sigma^2}{dz}$ but in first order dt by the correct expression $d\overline{W} = \frac{d\sigma^2}{dz}\, dt$.

We must conclude that Wilson et al.'s Langevin model (1981b) for W is not correct and therefore leave the discussion of this model. In the next chapter we will consider their W/σ Langevin model.

3.6.2 Wilsons' Langevin model for W/σ

In the paper (1983) Wilson et al. introduced a Langevin equation for W/σ. They were led to this model by their idea of scaling particle variables with relevant turbulence parameters. The Langevin equation for W/σ which they introduce reads in discrete form, in order Δt,

$$\left(\frac{W}{\sigma}\right)_{i+1} = \left(1 - \frac{\Delta t}{T_L}\right)\left(\frac{W}{\sigma}\right)_i + \left(\frac{2}{T_L}\right)^{\frac{1}{2}} \Delta\omega_t + \Delta t \frac{d\sigma}{dz} , \qquad (3.34a)$$

where $\Delta\omega_t$ is a white noise process with zero mean and variance Δt. Writing this in terms of W using $\sigma_{i+1} = \sigma_i + w_i \frac{d\sigma}{dz} \Delta t$ gives

$$W_{i+1} = \left(1 - \frac{\Delta t}{T_L}\right)W_i + \frac{W_i^2}{\sigma_i} \frac{d\sigma}{dz} \Delta t + \left(\frac{2\sigma^2}{T_L}\right)^{\frac{1}{2}}\Delta\omega_t + \tfrac{1}{2} \Delta t \frac{d\sigma^2}{dz} . \qquad (3.34b)$$

Wilson et al. state that this equation is negligibly different from their Langevin equation for W Eq. (3.33) in case $T_L \frac{d\sigma}{dz}$ does not vary much with height. This claim is not correct as Eq. (3.34b) is a nonlinear equation due to the extra second term on the RHS and the drift term is different from the one in Eq. (3.33). In Ch. 5 we will show that the Langevin model for W and for W/σ are essentially different. Dividing the Langevin equation (3.30) for W by σ is not a scaling when σ is not constant, but it changes properties of the model essentially with respect to the original Langevin equation for W. There is an essential difference between the models which, become clear in Ch. 5. In that chapter we will show that Wilson et al.'s Langevin equation for W/σ Eq. (3.34) is correct in case of Gaussian turbulence.

Wilson et al. applied their model for W/σ and Legg and Raupach's correct Langevin model for W to a case of Gaussian turbulence with $\bar{u}(z) = 0.50(z/z_i)^{0.15}$; $T_L(z) = (z/z_i)^{0.15}$ and $\sigma_w(z) = 0.30(z/z_i)^{0.15}$. They only show results at a downwind distance of 100 m. This corresponds to a travel time hundreds are more T_L. For such large times both the W/σ-model and the W-model results can be described by the diffusion equation (see Ch. 5) and this is indeed what Wilson finds (Fig. 3.14). We stress that this does not mean that the W/σ and W model are identical for all time with the diffusion equation.

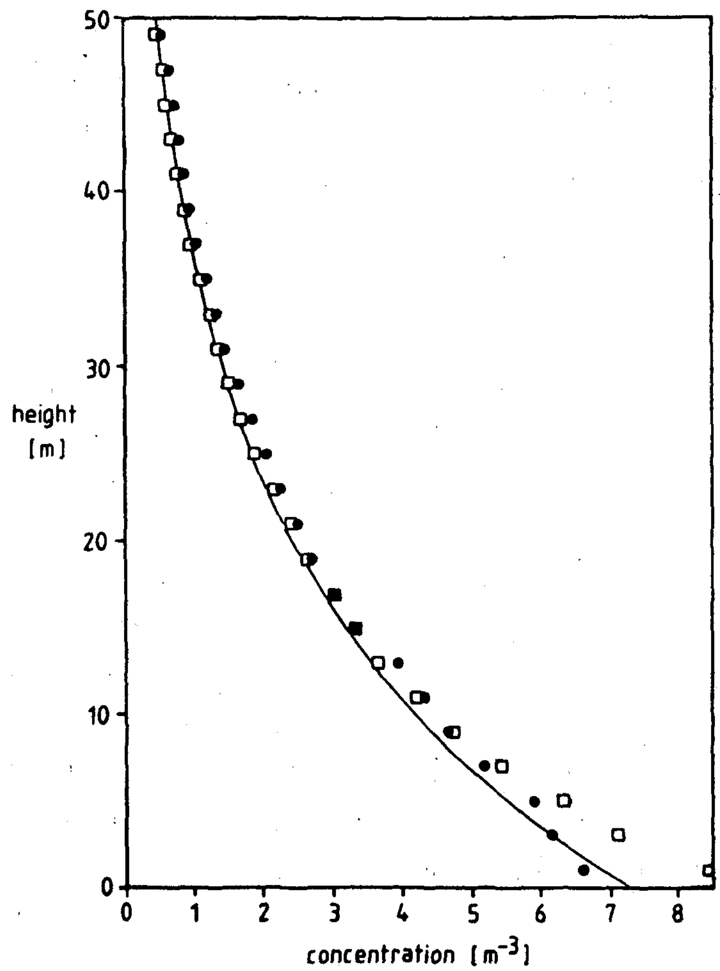

Fig. 3.14 The concentration profile for large times of a ground-level source in turbulence with power-law profiles of windspeed $\bar{u}$, σ^2 and T_L.

- diffusion equation with $K = \sigma^2 T_L$

. Langevin equation for W Eq. (3.20)

Langevin equation for W/σ Eq. (3.34)

(From Wilson et al., 1983)

3.6.3 Durbin's Markov limit model for W/σ model

Durbin (1984) wrote a paper in which he initiated the large time analysis of Langevin models. Note that already in an earlier study (1980) he used a large time equation, the Markov limit. In that study he did not base this Markov limit on large time analysis but on analogies with the diffusion equation. The large time an analysis is a strong tool when we want to investigate the random forcing function in the Langevin models. The modelling of the random forcing function should be such that the large time behaviour of the Langevin equation is described by a diffusion equation.

Durbin derives a Markov limit, which describes the large time behaviour of the Langevin model for W/σ in inhomogeneous Gaussian turbulence. He showed that the incorporation of a drift term $\frac{1}{2}\frac{d\sigma^2}{dz}\,dt$ ensures that the Markov limit of this Langevin equation is equal to the diffusion equation.

He wrote this paper as a comment on Wilson's et al. (1983) and Legg and Raupach's papers (1983) because his analysis shows the necessity of incorporating a drift term in the Langevin model for W/σ applied to inhomogeneous turbulence. We have to keep in mind though, that Durbin (1984) and Wilson et al. (1983) considered the Langevin model for W/σ, while Legg and Raupach (1983) considered the Langevin model for W. In Ch. 2 we showed however, that also in the Langevin model for W a drift term needs to be incorporated. Again only then the Markov limit for the W-model becomes equal to the diffusion equation.

3.7 Theoretical investigations into inhomogeneous Langevin models

The studies discussed above dealt exclusively with the first two moments of the random forcing in Langevin models. Janicke (1981) started a new path of development, by indicating a way to derive all moments of the random forcing. He himself however, still only considered the first two moments of the random forcing function, but his ideas were later generalised by other authors. Janicke assumed the random forcing function in the W-equation to be Gaussian. The KME of the W-model is then in inhomogeneous Gaussian turbulence a second order differential equation, the well-known Fokker Planck equation (Eq. 2.80). From this KME moment rate equations for W were derived (see also section 3.3.2). Janicke argued that in the steady state the moments of the particle velocity W should be equal to those of the turbulence velocity u_3. Using this in his comparison of the KME moment rate equations to the Eulerian equations, he finds that the first moment should be $\langle d\mu \rangle = dt \, \frac{d\sigma^2}{dz}$. This is the same drift term as was argued for by Legg and Raupach (1983) and Ley and Thomson (1983) on physical grounds. Janicke illustrates that this drift term indeed prevents particles from collecting in regions with low variance.

This idea is later generalised by Thomson (1984) and Van Dop et al. (1985) (see section 2.3). They do not restrict their analyses to Gaussian velocity and random forcing distributions but consider general pdf's with an infinite series of arbitrary moments. Thomson considered only the steady state requiring that then $\langle W^n \rangle = \overline{u_3^n}$. Van Dop et al. (1985) continued along this line carrying the idea further by considering an analysis of the moment rate equation for all time. Here we will not go into these last two theoretical studies but refer to the extensive discussion made in section 2.3.

3.8 Langevin models for situations with skewed turbulence velocity distributions

In the papers discussed above papers the Langevin equation was adapted to the dispersion in the neutral boundary layer and also to the convective and stable surface layer. The first and second moment of the random forcing in the model were modelled, while any higher (also nonzero) moments were neglected. These models are only applied to situations where the turbulence velocity distribution $P(u_3)$ was allowed to be height dependent but still Gaussian.

We now describe studies that deal with dispersion in boundary layers, where the turbulence $P(u_3)$ is no longer Gaussian but skew, which e.g. occurs in the convective boundary layer (CBL). The first model we discuss is the model of Baerentsen and Berkowicz. This model is not based on the theory of Langevin models described in Ch. 2, in contrast our own next model we shortly review. For a full description of our model and its application we refer to Ch. 4.

3.8.1 Baerentsen and Berkowicz's model

The first Langevin model, that deals with a skewed turbulence velocity distribution $P(u_3)$, was proposed by Baerentsen and Berkowicz (1984). They considered the convective boundary. Their model is based on the fact that the motion in the CBL consists of strong updrafts and weak downdrafts. The total turbulence velocity u_3 is modelled as the weighted sum of the velocities in the up- and downdrafts, whose distributions are assumed to be Gaussian. Both these distributions are characterised by the mean velocities $\overline{w}_+$ and $\overline{w}_-$ and variance σ_+ and σ_- for resp. the up- and downdrafts. A weighted sum of these two Gaussian distributions is made to represent the skewed distribution $P(u_3)$. This can be done by requiring that the weighted sum of these moments of the up- and downdrafts distributions is equal to the corresponding moment of the turbulence. The three equations for the first, second and third moment yield values for $\overline{w}_+$, $\overline{w}_-$, σ_+ and σ_- and the weight factor if an extra assumption (here $\overline{w}_+ = \sigma_+$ and $\overline{w}_- = \sigma$) is assumed.

Once these turbulence values are calculated, they are used in determining the particle velocity. The particles either move with an up- or downdraft. The motion of the particles within down- or updrafts is separately modelled, each by a Langevin model for W/σ:

$$W(t+dt) = \overline{w} + \frac{\sigma(Z(t+dt))}{\sigma(Z(t))} \exp(-\frac{dt}{\tau})W(t) + \sigma(z)(1-\exp(-\frac{2\Delta t}{\tau})^{1/2} d\omega_t + \tfrac{1}{2}\frac{d\sigma^2}{dz} dt \ , \tag{3.35a}$$

which in first order dt is equivalent to

$$dW = \overline{w} - \frac{dt}{\tau} W(t) + \frac{W^2}{\sigma}\frac{d\sigma}{dz} dt + (\frac{2\sigma^2}{\tau})^{1/2} d\omega_t + \tfrac{1}{2}\frac{d\sigma^2}{dz} dt \ . \tag{3.35b}$$

The drift term in this equation is correct in a Langevin model for W/σ (Thomson, 1984), although Baerentsen's and Berkowics's argument leading to it is not correct. Their argument is based on a Taylor expansion of the particle velocity W(t). This expansion should be made via $W(t) = u_3(Z(t))$. In making a Taylor expansion of u_3 it should be taken into account that the turbulence is three dimensional. The expansion around a point z_p should be (Hunt, 1984)

$$\begin{aligned} W(t) &= u_3(z_p) - \frac{du_3}{dx_j}\Big]_{\underset{\sim}{x}_p} (\underset{\sim}{X} - \underset{\sim}{x}_p) + \ldots \\ &= u_3(z_p) + t\, u_j \frac{du_3}{dx_j}\Big]_{\underset{\sim}{x}_p} + \ldots \\ &= u_3(z_p) + t \frac{du_3}{dx_j}\Big]_{\underset{\sim}{x}_p} + \ldots \end{aligned} \tag{3.36}$$

where in the last equality the three dimensional continuity equation is used. (see also Ch. 5). It follows with horizontal homogeneity that $d\langle W\rangle = dt\ d\overline{u_3^2}/dz$. Baerentsen and Berkowicz's did not take all these aspects into account and found thus a drift term with a factor ½ in front.

A drift term can straightforwardly be included in the linear Langevin model for W. But the W/σ-model nonlinear in W and including a drift term such that $d\langle W\rangle = dt\ d\overline{u_3^2}/dz$ is more involved. Pardoxically enough, the drift term that gives the desired result in this W/σ-model is the one used by Baerentsen and Berkowicz. For correct arguments leading to the driftterm in the W/σ-model we again refer to the discussion of the model for W/σ by Thomson (1984).

In Baerentsen and Berkowicz's model an exponential jump probability is further assumed that gives the probability to jump from an up- into a downdraft and vice versa. The four timescales involved, two in the Langevin equations and two in the jump probability functions, are in not-obvious-formulas related to the dissipation rate ε_t. By varying this ε_t they could tune their models to the watertank results of Willis and Deardorff (1976, 1978 and 1981).

An advantage of Baerentsen en Berkowicz's model is that only Guassian pdf's are used, which can be generated with high accuracy on a computer. However their model is specific for the CBL and is not applicable to other atmospheric turbulence situations.

3.8.2 Our model

For completeness we shortly review our own work. For a more detailed discussion we refer to the next chapter. The Langevin model we build is a Langevin model for W with the first three moments of the random forcing specified according to Thomson and van Dop et al.'s results discussed in section 2.3. The model is applicable to all atmospheric stabilities. To show the strength of the model we simulated dispersion in the strongly inhomogeneous convective boundary layer. The only parameters needed are profiles of T_L, $\overline{u_3^2}$ and $\overline{u_3^3}$. The agreement between model results and observations may be characterized as good. (see Figs. 4.2).

The theory for Langevin models requires that the third moment of the random forcing function should be nonzero in skew turbulence,

$$\langle(d\mu)^3\rangle = \left(\frac{3\overline{u_3^3}}{T_L} + 3\overline{u_3^2}\,\frac{d\overline{u_3^2}}{dz}\right)dt$$

in case the fourth moment of the turbulence velocity is modelled by a Gaussian assumption $\overline{u_3^4} = 3\overline{u_3^2}^2$. In our model we have found that this requirement is essential for the behaviour of dispersion near the source and also for large times. For short times this can theoretically be shown. The short time behaviour of height and spread in a Langevin model will be derived in Ch. 5.3 Eq. (5.10) and the third moment can be derived analogously. They read

$$\begin{aligned}
\overline{(Z-z_s)} &= \qquad + \tfrac{1}{2}\, a_1 t^2 && + \ldots \\
\overline{(Z-z_s)^2} &= \overline{u_3^2}\, t^2 + \left(\frac{1}{3}\, a_2 - \frac{\overline{u_3^2}}{T_L}\right)t^3 && + \ldots \\
\overline{(Z-z_s)^3} &= \overline{u_3^3}\, t^3 + \left(\tfrac{1}{4}\, a_3 - \frac{3}{2}\,\frac{\overline{u_3^3}}{T_L}\right)t^4 && + \ldots
\end{aligned}$$

Leaving the third moment of dμ out means that the skewness of the plume is not correctly represented leading to wrong concentration levels. For larger times the third moment of dμ is also important as we show in the next chapter. It is responsible for the fact that a much better uniform concentration is found in comparison with the case where the third moment is taken to be zero. The article in our model published in Quart. J. Met. Soc. (1986), is integrally included in Ch. 4 and redundancies might occur.

3.9 Discussion and conclusion

We discussed several dispersion models based on the Langevin equation. These models describe the vertical velocity of the dispersing particles by $dW = -\frac{W}{T_L} + d\mu$. In these models the parameters T_L and $d\mu$ are prescribed in such a way that the Langevin equation can be applied to different atmospheric situations.

Dispersion in the homogeneous conditions can be described by a Langevin equation in which only the second moment of the random forcing is nonzero. Dispersion in neutral surface layers where only T_L depends on height can be described by the same formulation of the random forcing. It is shown that this formulation is seriously in error when applied to more complex situations where turbulence intensity varies with height. Dispersion in such layers, like the stable and unstable layers, has to be described by a Langevin model for W in which more moments of the random forcing $d\mu$ are nonzero. The first attempts for such layers included a drift acceleration in the Langevin model by putting the first moment of $d\mu$ equal to $\frac{d\sigma^2}{dz}$ dt This is done to prevent that particles collect in regions of low turbulence intensity. This formulation is still not entirely correct because, even in Gaussian inhomogeneous turbulence, the third moment of $d\mu$ is nonzero. Neglecting this term means that the skewness of the plume is not represented, and as a result no distinction is made between the mean height and the height of maximum concentration. Results of the Langevin model for dispersion in skewed turbulence, like in the convective boundary layer, are also discussed. It will be shown in Ch. 4 that both short and large time behaviour improve considerably if the third moment of $d\mu$ is correctly modelled. Our Langevin model with the random forcing based on theoretical results of Thomson and Van Dop et al. will be shown to be a powerful model. It should be applicable to all atmospheric conditions.

In the above it is discussed that vertical dispersion is strongly influenced by the profiles of T_L and the turbulence velocities. But it also is by height variation of the mean horizontal wind. This effect can easily be modelled in a 1-D Langevin model by an advection term in the horizontal. The model results are then usually described as function of downwind distance x instead of time.

Another dispersion model the Langevin model for W/σ is introduced. In Ch. 5 we will investigate this model theoretically to show that the model for W is essentially different from and more correct than the model for W/σ The conclusion is that the Langevin equation for W is a powerful dispersion model, if the random forcing is specified by its first, second and third moment.

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Ch. 4. AN APPLICATION OF THE LANGEVIN EQUATION FOR INHOMOGENEOUS CONDITIONS TO DISPERSION IN A CONVECTIVE BOUNDARY LAYER

Ch. 4 An application of the Langevin equation for inhomogeneous conditions to dispersion in a convective boundary layer

4.1 Introduction

The dispersion in convective conditions has been first studied by Willis and Deardorff by means of a watertank (1976, 1978, 1981). The characteristics of the dispersion were quite unexpected at the time of its discovery. Material emitted at ground level first remains at the surface but then rises quickly to midlevel of the boundary layer, whereas particles released from elevated stacks first descend and then move to midlevel. These characteristics have since been confirmed by other observations of Poreh and Cermak (1984) in a wind tunnel and of Briggs (1983) in field experiments. Eulerian K-theory is unable to describe these phenomena, it does not give the proper vertical dispersion for small times. The rising of the plume would require negative K values, and in reality material emitted from elevated sources reaches the ground sooner and closer to the source than these models predict. An alternative is to use Lagrangian models in which the motion of individual fluid particles is considered. In these models the dispersion for times smaller than the Lagrangian timescale is better described. Besides that the conservation of mass is ensured and no problems occur with numerical stability of the equations used.

A Lagrangian model of Lamb (1978) simulated the above described dispersion phenomena by ascribing to particles a velocity that consists of two parts $W = W_d + W_s$. The first part W_d is the velocity determined by Deardorff's numerical model (1974): W_s is a stochastic velocity describing the subgrid part. Overall the agreement with the watertank experiment of Willis and Deardorff is very good.

Misra (1982), Weil and Furth (1981) and Venkatram (1982), arguing that the particle is either moved by an updraft or by a downdraft, set up two simple stochastic differential equations. By choosing the correct statistics for the updraft and downdraft they were able to simulate several aspects of convective diffusion.

Other models describe the movement of the particles by the Langevin equation in analogy with the description of Brownian diffusion.

The models based on the Langevin equation simulate dispersion in terms of a stochastic differential equation (random walk or Monte Carlo simulation). The stochastic term in the Langevin equation describes the forces exerted on the particles by the turbulence (Lin and Reid, 1962) and is expressed in terms of turbulence statistics

$$dW = -(W/T_L)dt + d\mu \qquad (4.1)$$

where W is the particle velocity, T_L the Lagrangian time scale and $d\mu$ are the random velocity increments.

The Langevin equation was first applied to describe dispersion in homogeneous turbulence (Lin and Reid, 1962; Gifford, 1982 a and b). This can be described by $\overline{d\mu} = 0$, $\overline{(d\mu)^2} = 2\overline{u_3^2}dt/T_L$ and $\overline{(d\mu)^3} = 0$ where $\overline{u_3^2}$ is the variance of the turbulence velocities. In this case analytical expressions for the velocity of a particle and its position may be obtained by successive integration of Eq. (4.1). The result is an exponential velocity autocorrelation, which is well known to be able to describe homogeneous dispersion adequately (Tennekes, 1979).

The Langevin equation has been furthermore applied to the surface layer, where the turbulence was taken to be homogeneous but the timescale varied with height. The resulting equation was solved numerically by Hall (1975), Reid (1979) and Ley (1982). Their results were tested against the known analytical solution of the diffusion equation valid for large times and against data like those of the Prairie Grass experiments.

However, the Langevin Eq. (4.1) derived for homogeneous turbulence can not be applied unmodified to a non-homogeneous boundary layer. For instance, particles have a tendency to become trapped in regions with small variances. To avoid this phenomenon Legg and Raupach (1982) and Ley and Thomson (1983) added an extra term to the Langevin equation. This adding an extra term is equivalent to a nonzero mean random forcing $\overline{d\mu} = dt\ \partial\overline{u_3^2}/\partial z$, but they still take $\overline{(d\mu)^2} = 2\overline{u_3^2}\ dt/T_L$. They base their arguments on the Navier Stokes equations and they state, that a gradient in the velocity variance induces a mean pressure force, which has to be added to the Langevin equation. Janicke (1981) derived the same expression for $d\mu$. He required that the Fokker-Planck equation (the Eulerian equivalent of the Langevin equation) should yield particle velocity moments, that for large times are equal to the turbulent velocity moments in equilibrium. Thomson (1984) extended these arguments, taking higher background velocity moments into account. By using moment-generating functions, he derived the moments of the random-forcing function by demanding that the probability density of the particles leads to a distribution of particles, that for large times has the same density distribution as the air.

A different approach is used by Van Dop et al. (1984) who deal with the general case of non-stationary and non-homogeneous turbulence. They consider the Langevin equation of the following form

$$dW = \{-(W/T_L) + a_1\}dt + a_2^{1/2}\, d\omega, \qquad (4.2)$$

with

$$\overline{d\omega_t} = 0, \qquad \overline{(d\omega_t)^2} = dt \ . \qquad (4.3)$$

This set of equations is equivalent to Eq. (1) if we take $\overline{d\mu} = a_1 dt$, $\overline{(d\mu)^2} = a_2 dt$. By means of Taylor expansion for small times of the rate equations fo $\overline{W}$ and $\overline{W^2}$, Van Dop et al. obtain expressions for a_1 and a_2. These expressions turn out to be equivalent to formulas for the moments of $d\mu$ found by Thomson. They also prove the validity of their results for all time by showing, that the moments obtained from Eq. (4.2) and (4.3) are consistent with the moments obtained from the Eulerian conservation equations.

Baerentsen and Berkowicz (1984) split the particle velocity into two parts on the same principle, the up- and downdrafts, as Misra, Weil and Furth and Venkatram did before, but Baerentsen and Berkowicz use two separate Langevin equations to describe them. They also allow a particle to jump from an updraft into a downdraft and vice versa with a given probability. These four processes involve separate timescales, which were tuned by testing the results against the watertank experiments of Willis and Deardorff. With this tuning their model compared very well with the water tank results.

Our approach differs from the study of Baerentsen and Berkowicz in that we do not split the particle velocity into two parts, but we use only one single Langevin equation to describe all particle velocities. The purpose of this paper is to consider, whether this single equation, with the moments of the random velocity increments as defined by Thomson, is able to describe dispersion in the horizontally homogeneous steady convective boundary layer. Moreover we will consider the influence of the moments of $d\mu$ on the solution. The results are compared with the water tank experiments of Willis and Deardorff (1976, 1978, 1981), the numerical experiments of Lamb (1978), the field experiments of Briggs (1983) and the windtunnel experiments of Poreh and

Cermak (1984).

The modelling of the Convective Boundary Layer (CBL) is described in the next section. The Langevin model we used to describe the dispersion in the CBL is explained, whereafter the results are given and discussed. In the last but one section we discuss some details of our simulation. The last section contains our conlusions.

4.2 Convective boundary layer

Usually during daytime the air is heated at the surface and the boundary layer becomes unstable. The vertical turbulence structure becomes organised in a pattern of updrafts and downdrafts, where on the average the updrafts move faster than the downdrafts. Because the vertical speed, averaged over a large horizontal area, should be zero, the downdrafts occupy a larger area than the updrafts at each level of the boundary layer. If the turbulence is inhomogeneous, the vertical velocity distribution is height dependent. Furthermore the vertical velocity distribution is skew. The Eulerian properties of the convection (outside the surface layer, where the stresses are constant) can be scaled with the convective velocity $w_* = (z_i \overline{w\theta_o} g/T)^{1/3}$ and the height z_i of the boundary layer if $-z_i/L > 10$ (L is Obukhov length, $\overline{w\theta_o}$ is the surface heat flux). Below this value the turbulence begins to be affected by shear stress (Willis and Deardorff, 1976, 1978 and 1981). This type of scaling is called mixed layer scaling. It is assumed that the Lagrangian and Eulerian correlation functions $\rho_L(t)$ and $\rho_E(t)$, are similar in shape but displaced by a scale factor β: $\rho_L(\beta t) = \rho_E(t)$ (Hanna, 1982). From the definition of T_L follows $\beta = T_L/T_E$. The Lagrangian properties then also scale with w_* and z_i. The various theoretical estimates of β all lead to the form βi = constant, where i is the turbulence intensity defined as $\sigma_u/\overline{u}$. The numerical values of the constant range from 0.35 to 0.8 (Pasquill and Smith, 1983). Hanna (1981) found for a convective boundary layer $T_E = 0.25\, z_i/\overline{u} = 0.69\, i z_i/w_*$, where $\sigma_u = 0.36 w_*$ is substituted (Hanna, 1982). Then we get

$$0.24\, z_i/w_* < T_L < 0.55\, z_i/w_* \,, \qquad (4.4)$$

but we have to keep in mind that there is a large uncertainty in the constants.

Many measurements have been carried out to determine the profiles of the second and third moments of the vertical turbulence velocity. Baerentsen and Berkowicz used the following profiles expressed in terms of mixed layer scaling:

$$\overline{u_3^2}/w_*^2 = 1.54 (z/z_i)^{2/3} \exp(-\, 2z/z_i) \qquad (4.5)$$

$$\overline{u_3^3}/w_*^3 = 0.8(z/z_i)(1 - z/z_i)(1 + 0.667z/z_i)^{-1} . \qquad (4.6)$$

In order to avoid difficulties, as will be discussed later, we use for the third moment a slightly modified expression:

$$\overline{u_3^3}/w_*^3 = 1.4(z/z_i)\exp(- 2.5\ z/z_i) \qquad (4.7)$$

(see Fig. 4.1).

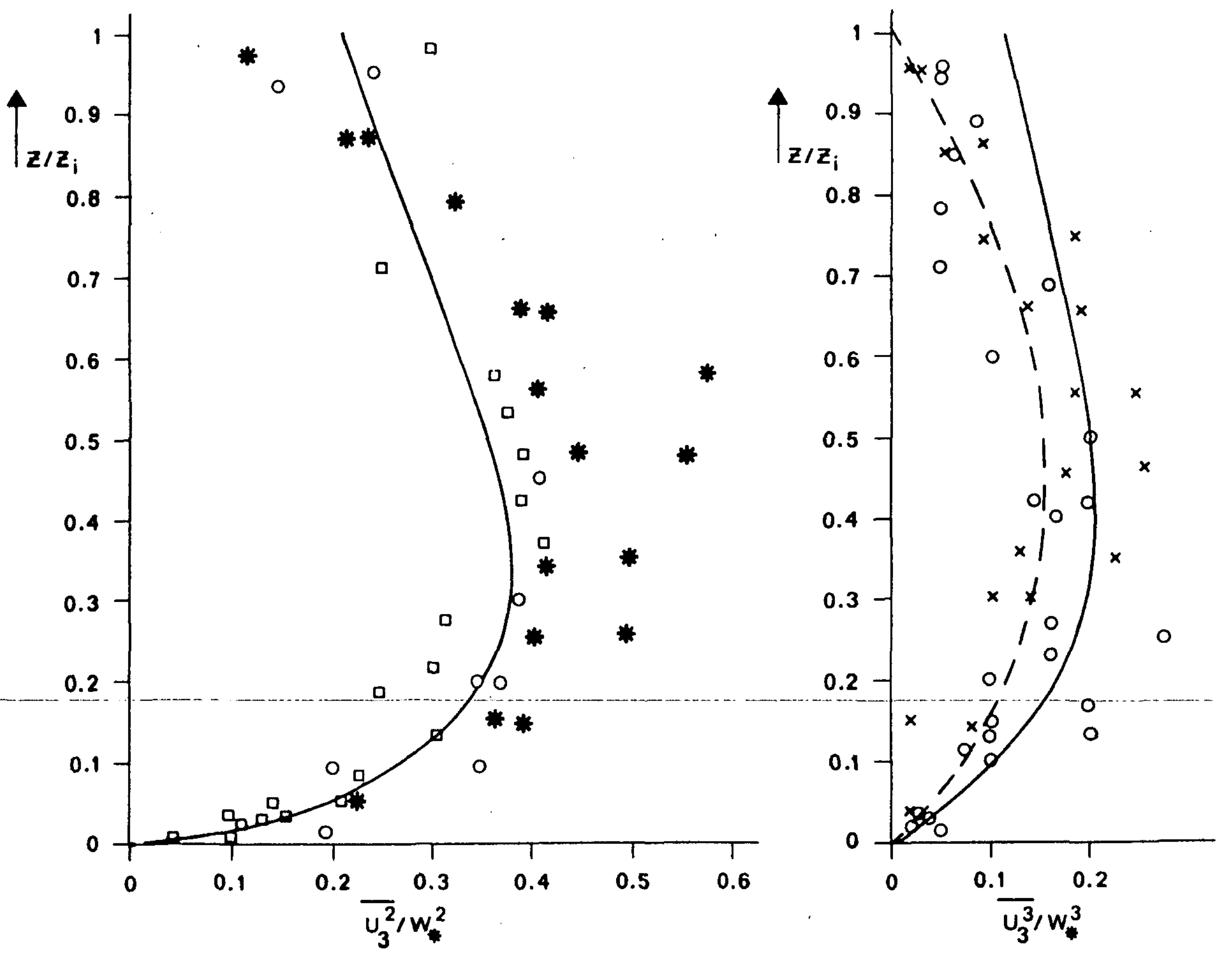


Fig 4.1

Second and third moments of turbulence vertical velocities as described by Eqs. (5) and (7) (solid line). Stars: water-tank data (Willis and Deardorff 1976); circles: aircraft measurements (Willis and Deardorff 1974); squares: Minnesota data (Izumi and Caughey 1976); crosses: water-tank data (Willis, published by Baerentsen and Berkowicz, 1984). Dashed line denotes $\overline{u_3^3}$ profiles of Baerentsen and Berkowicz (1984) (Eq. (6)).

4.3 The Langevin model

Next we consider the Langevin Eq. (4.1) for inhomogeneous conditions. The theory has been developed by Thomson (1984) and Van Dop et al. (1984). Their results lead to the following expressions for the moments of the random forcing function $d\mu$.

$$\overline{d\mu} = \Delta t\{\partial\overline{u_3^2}(z)/\partial z\}$$

$$\overline{(d\mu)^2} = \Delta t\{\overline{2u_3^2(z)}/T_L + \partial\overline{u_3^3(z)}/\partial z\} \qquad (4.8)$$

$$\overline{(d\mu)^3} = \Delta t\{3\overline{u_3^3(z)}/T_L + \partial\overline{u_3^4(z)}/\partial z - 3\overline{u_3^2(z)}\partial\overline{u_3^2(z)}/\partial z\} .$$

We solve the Langevin equation in a finite difference form. We use the following explicit scheme:

$$W(t + \Delta t) = W(t)(1 - \tfrac{1}{2}\Delta t/T_L)(1 + \tfrac{1}{2}\Delta t/T_L)^{-1} + d\mu(1 + \tfrac{1}{2}\Delta t/T_L)^{-1}\}$$

$$Z(t + \Delta t) = Z(t) + \tfrac{1}{2}\Delta t\{W(t + \Delta t) + W(t)\} \qquad (4.9)$$

with Δt the timestep used in the integration procedure. This scheme is unconditionally stable and doesn't cause computer time problems.

Finally to assign a value to the random forcing at each time step for each particle we construct the distribution density function $P(d\mu)$. This can be constructed from the Eq. (4.8) in the same mathematical way Baerentsen and Berkowicz (1984) constructed their distribution function for the velocity of the updrafts and downdrafts $P(u_3)$ (See appendix I).

4.4 Results

The Langevin model described above is applied to dispersion in a convective boundary layer, neglecting streamwise and cross-wind diffusion. The profiles used in Eq. (4.8) are Eq. (4.5) and Eq. (4.7) together with $T_L = z_i/w_*$, which relation will be discussed later. A slight adjustment is applied to the $\overline{u_3^2}$ profile near the ground. There we took $\overline{u_3^2}/w_*^2$ constant in a shallow layer of depth δ, where $\delta/z_i = 0.0025$. The velocity variance in this layer was put equal to $\overline{u_3^2}(\delta/z_i)/w_*^2$. The reason for this will be discussed later.

At the top and at the bottom reflection boundary conditions are imposed on the particle motion.

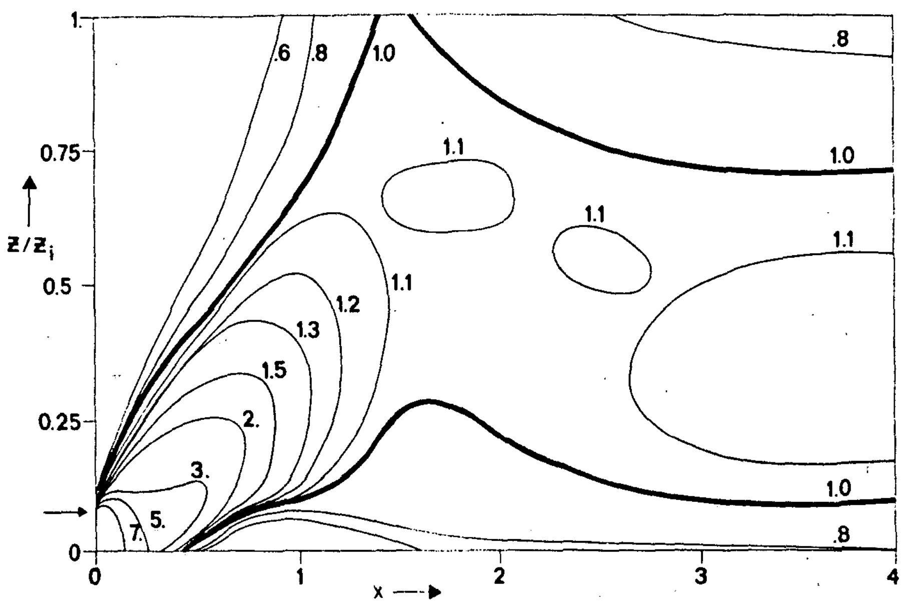
At t = 0 the particles released at $z = z_s$ are assigned initial velocities W such that

$$\overline{W}(t = 0) = 0,\ \overline{W^2}(t = 0) = \overline{u_3^2}(z_s) \text{ and } \overline{W^3}(t = 0 = \overline{u_3^3}(z_s) \ . \qquad (4.10)$$

The number of particles released was set at 2×10^4 and the timestep at $\Delta t/T_L = 0.05$. This choice was made to avoid inaccuracies in the generation of the random forcing funtion as will be discussed later. Computertime for a simulation of 2×10^4 trajectories up to $t = 4\ T_L$ on the CRAY XMP computer at ECMWF, Reading, U.K. was 13 seconds CPU time. The amount of particles was generally sufficient to obtain stable statistics.

The resulting concentration profiles are measured as the number of particles in an interval $\Delta z/z_i = 0.05$. They are nondimensionalised with the value Q/z_iU, which is the concentration when the particles are homogeneously distributed in height. The concentration profiles are given as function of nondimensional time t/T_L. This is equivalent to a nondimensional distance $X = (w_*/U)(x/z_i)$, where x is the distance over which particles are advected by the uniform mean wind U in a time t.

Contour plots were made of the concentration as function of height and time or downwind distance (Fig. 4.2) until the distribution reaches a steady state. They are compared with the results of the watertank experiments also given in Fig. 4.2. We see that the simulations describe the significant features found in the experiments remarkably well. Particles released at ground level first remain at the ground, then rise above mid-level before



LANGEVINMODEL

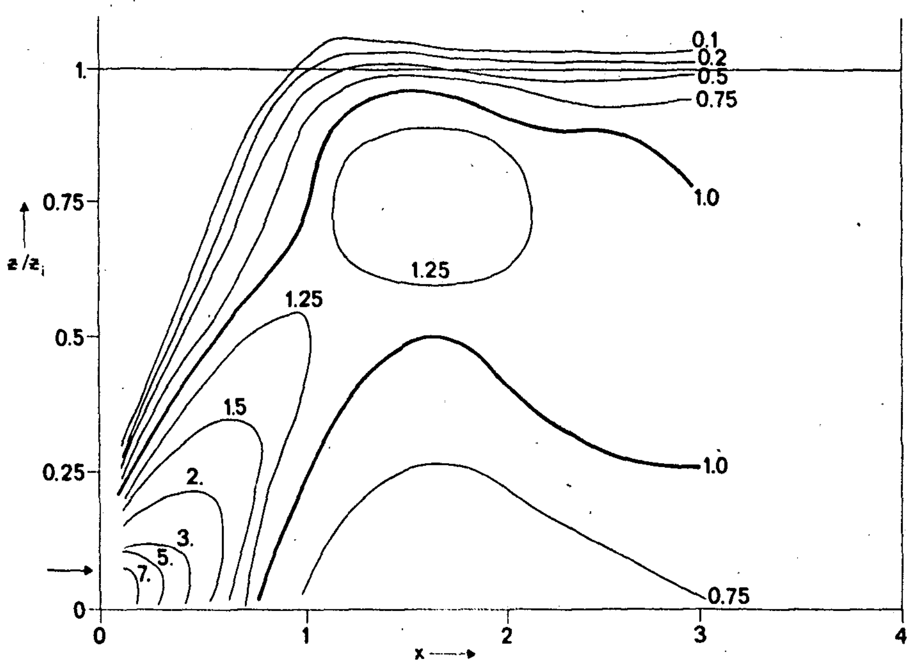


Fig 4.2 EXPERIMENT WILLIS & DEARDORFF

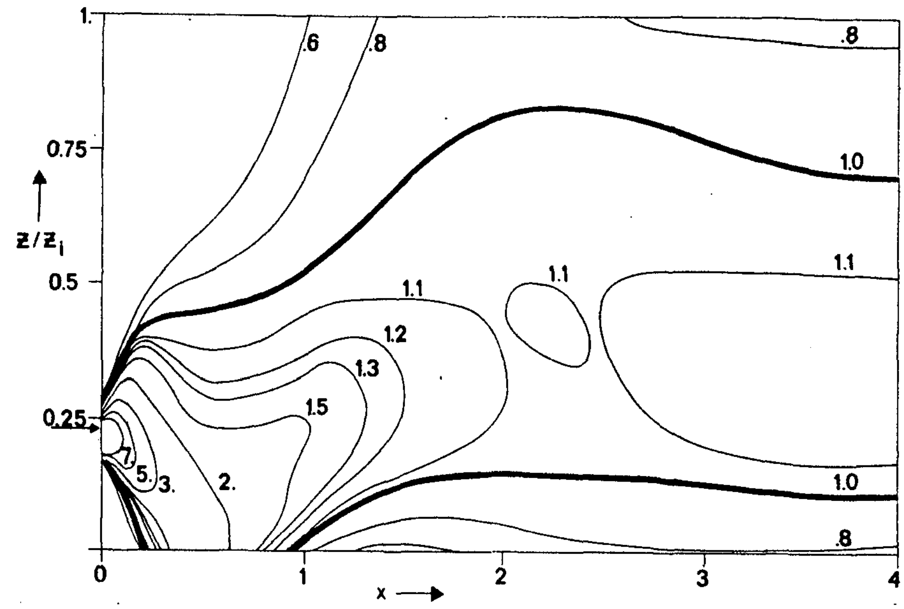
Contours in the vertical x,z plane of the dimensionless concentration presenting the results of our Langevin model (I) and of the cross wind integrated measurements of Willis and Deardorff (II) for the source heights

a) z_s/z_i = 0.067

b) z_s/z_i = 0.24

c) z_s/z_i = 0.49

Source height is indicated by arrow on ordinate.



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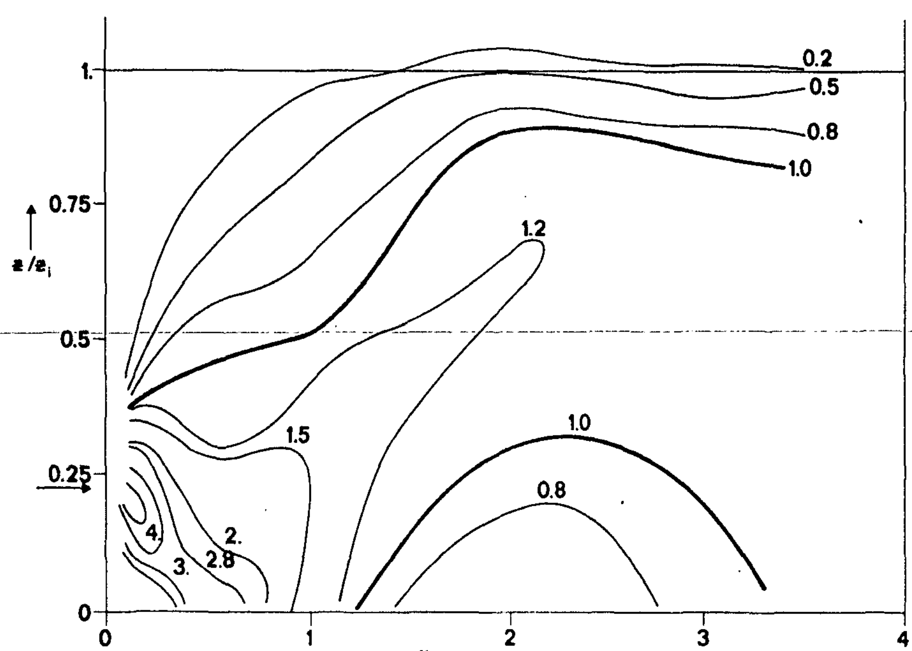
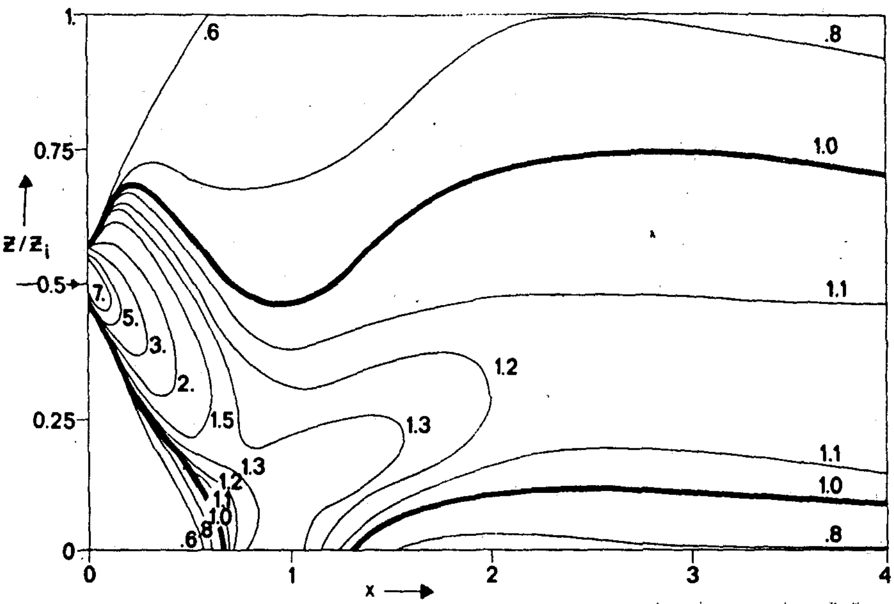
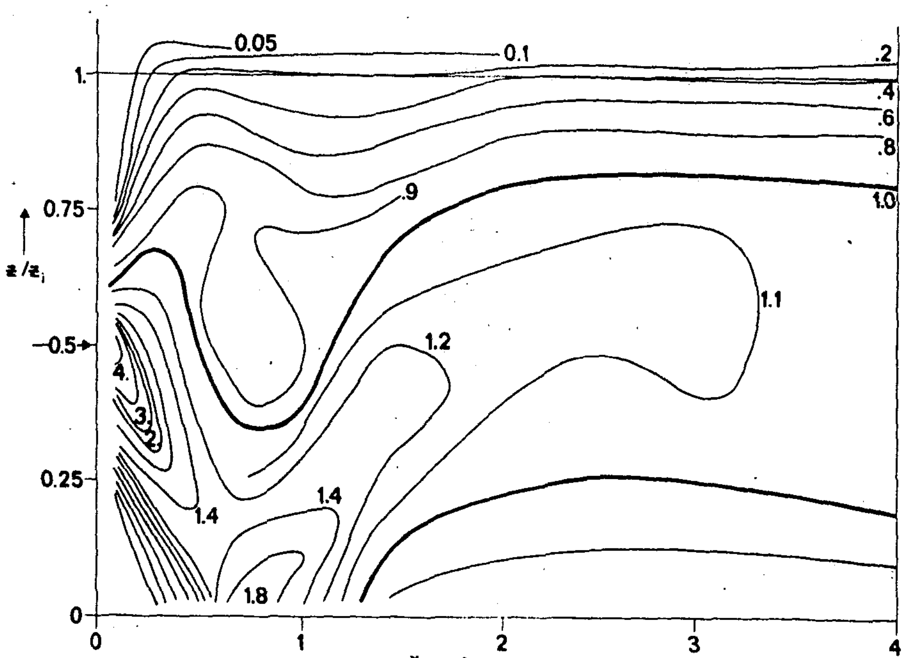


EXPERIMENT WILLIS & DEARDORFF

Fig 4.2 continued



LANGEVINMODEL



EXPERIMENT WILLIS & DEARDORFF

Fig 4.2 continued

reaching the equilibrium state. Particles released at a quarter of the boundary layer height and at mid-level are first swept downward, remain a small time at the surface and then rise to mid-level. Furthermore the observed concentration pattern is simulated not only qualitatively but also very satisfactorily quantitatively.

The maximum value in the center of the particle cloud, released at groundlevel, during lift off of the particles (Fig. 4.2) was slightly smaller than the experimental value of Willis and Deardorff during lift-off. It also appeared that our concentration profiles during lift-off are more peaked for $z/z_i < 0.2$. This is probably due to the fact that a point source is hard to simulate in experiments leading to less peaked concentration profiles.

In their windtunnel experiments Poreh and Cermak (1984) measured centerline concentrations for particle releases at $z_s/z_i = 0$ and $z_s/z_i = 0.133$ at six distances smaller than X = 1.2. We converted the centerline concentrations C(x,o,z) to cross wind averaged values $\overline{C}(x,z)$, assuming that the crosswind spread is Gaussian (Willis and Deardorff, 1976).

$$\overline{C}^y(x,z) = \int_{-\infty}^{\infty} C(x,y,z)\,\frac{dy}{z_i} = \int_{-\infty}^{\infty} C(x,0,z)\exp(-y^2/2\sigma_y^2)\frac{dy}{z_i} = \sqrt{(2\pi)}(\sigma_y/z_i)C(x,0,z) \qquad (4.11)$$

where we used Poreh and Cermak's measurements of $\sigma_y(X)/z_i$.
The results of our model for $z_s/z_i = 0.067$ and $z_s/z_i = 0.133$ compare very well with the calculated values of Poreh and Cermak (Fig 4.3). It seems though as if there is an inconsistency for the results at X = 1.06. Our results imply a larger value of $\sigma_y(X = 1.06)$ than the one given by Poreh and Cermak.

The mean height of the plume and its spread are calculated as a function of time until the distribution reaches a steady state (Fig. 4.4 - Fig. 4.5). These results were compared with cross-wind integrated results of the water tank experiments of Deardorff and Willis (1975) and Willis and Deardorff (1976, 1978, 1981) and the numerical results of Baerentsen and Berkowicz (1984).

The time at which the maximum height is reached agrees very well with the tank experiments, although the maximum height itself for groundlevel release is slightly less in our experiments (Fig. 4.4). In equilibrium the

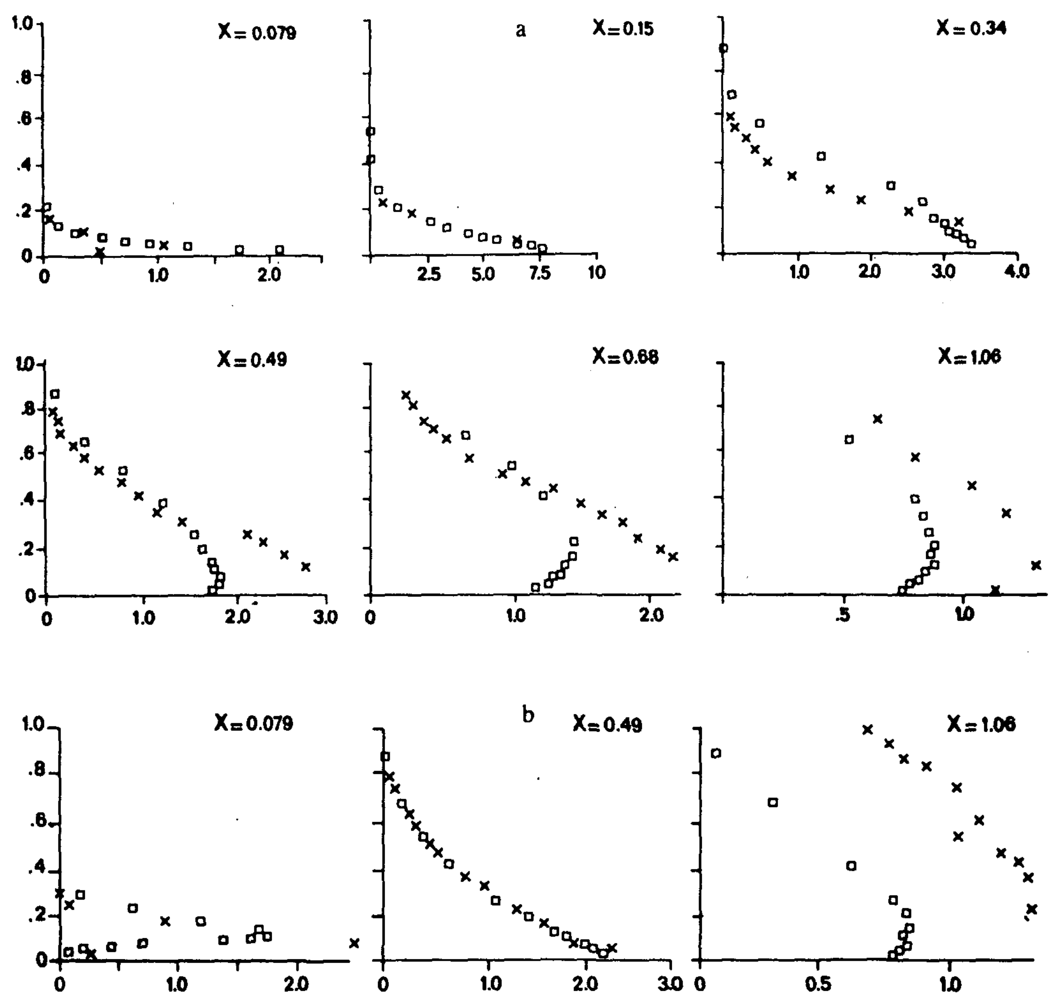


fig 4.3 Concentration profiles measured by Poreh and Cermak for $z_s/z_i = 0$ and $z_s/z_i = 0.133$ (squares), and our concentration profiles for $z_s/z_i = 0.067$ and $z_s/z_i = 0.133$ (crosses).

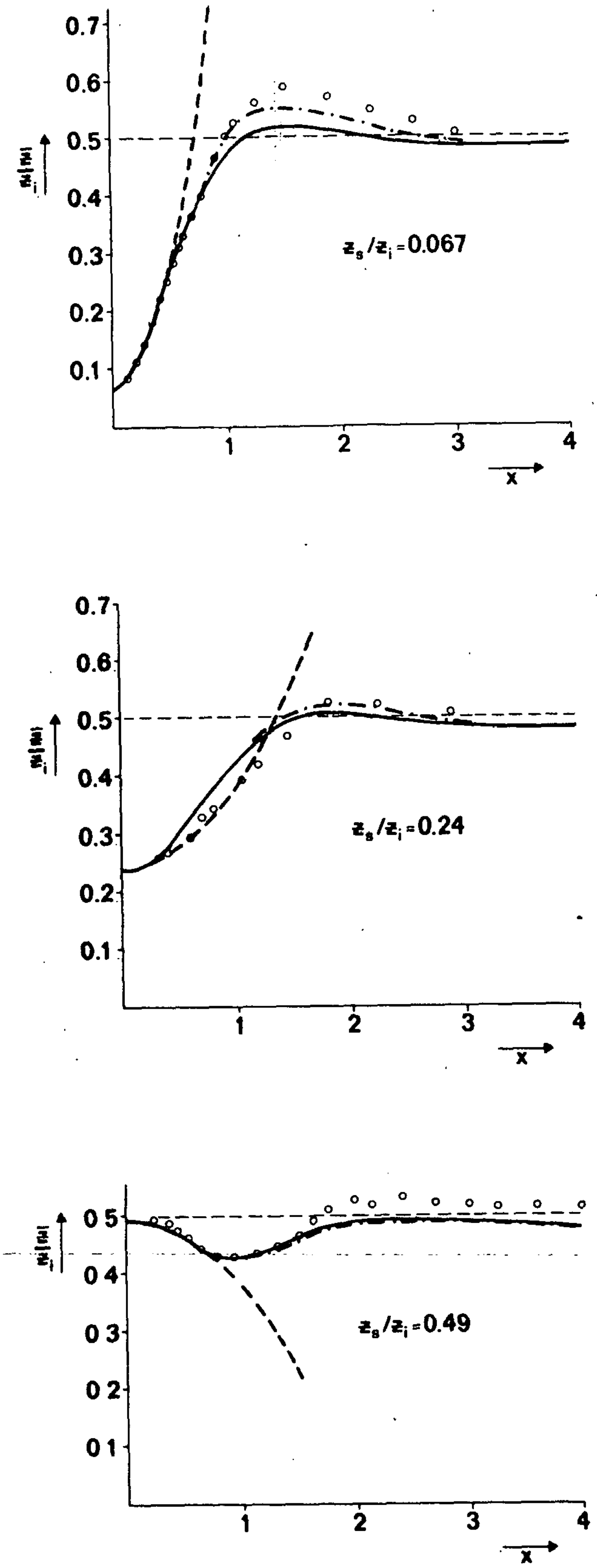


Fig 4.4

Mean particle height $\overline{z}/z_i$ as a function of downward distance X for source heights z_s/z_i = 0.067, z_s/z_i = 0.24 and z_s/z_i = 0.49. The results of our Langevin model are denoted by a solid line, the measurements of Willis and Deardorff by circles and the numerical experiments of Baerentsen and Berkowicz by (–.–). The short time Taylor series expansions (Eq. 13) are indicated by dashed lines.

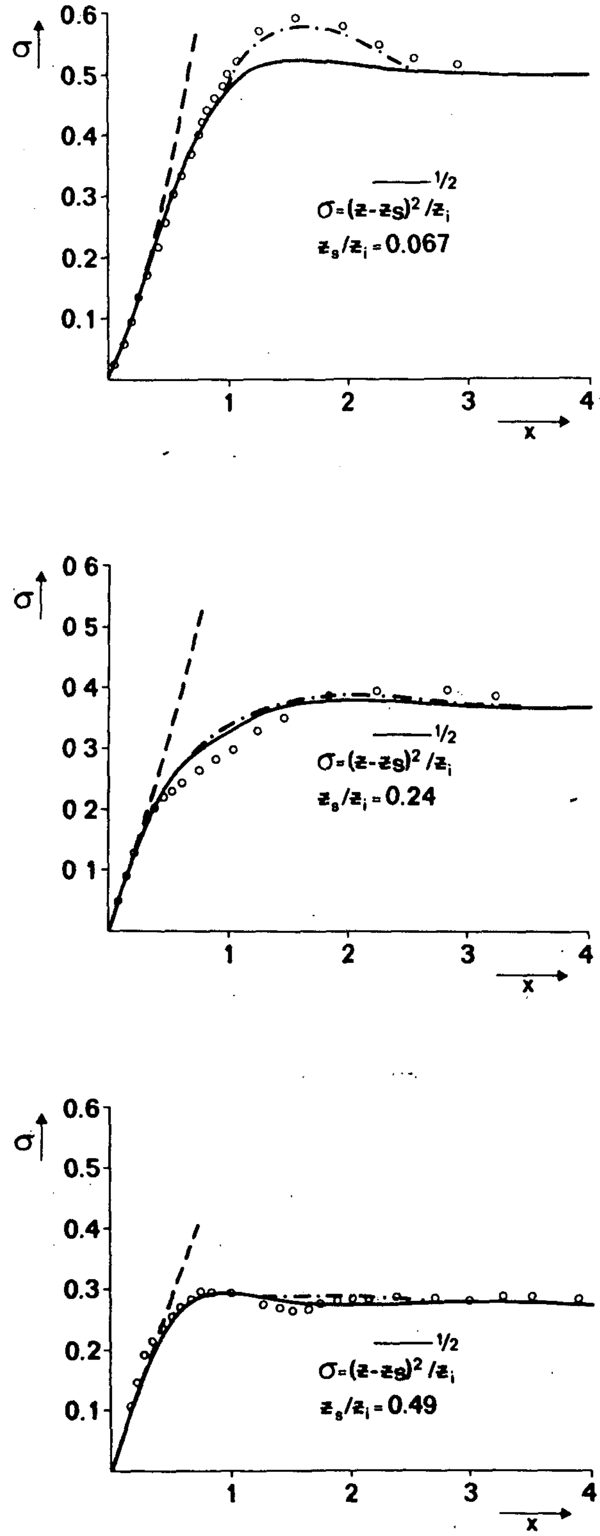


Fig 4.5

Mean variance $\overline{(z - z_s)^2}^{1/2}/z_i$ as a function of downwind distance X for source heights z_s/z_i = 0.067, z_s/z_i = 0.24 and z_s/z_i = 0.49. The results of our Langevin model are denoted by a solid line, the measurements of Willis and Deardorff by circles, and the numerical experiments of Baerentsen and Berkowicz by (–.–). The short time Taylor series expansions (Eq. 13) are indicated by dashed lines.

concentration should be homogeneous ($C(z) = 1$) and then the mean height is 0.5 z_i.

In our experiment, as well as in the experiments of Baerentsen and Berkowicz, the mean height is lower because the concentration distribution does not become homogeneous, as will be discussed later. Willis and Deardorff did find an equilibrium mean height of 0.5 z_i, although their equilibrium concentration is not homogeneous either. In their experiments the inversion height is not constant. At some places the particles reach beyond the average value leading to a larger mean height of the particles.

Our particle spread $\{\overline{(Z - z_s)^2}\}^{1/2}/z_i$, results agree very well with the tank experiments for all time although for the groundlevel release the maximum spread is again slightly less. Our equilibrium values are fair compared to the theoretical equilibrium value

$$\{\overline{(Z - z_s)^2}\}^{1/2}/z_i = \{(1/z_i)\int_0^{z_i}(z/z_i - z_s/z_i)^2 C(z)\,dz\}^{1/2} = \{\tfrac{1}{3} - z_s/z_i + (z_s/z_i)^2\}^{1/2} \tag{4.12}$$

which is equally true for the equilibrium values of Baerentsen and Berkowicz.

The dip in the spread between $X = 1$ and $X = 2$ for the case $z_s/z_i = 0.49$ is a feature that we were also able to simulate. This dip is due to the fact that the particles lift off the ground between $X = 1$ and $X = 2$. This results in a concentration distribution with such first and second moments, that the spread relative to z_s is smaller than the equilibrium value.

The small time exact Taylor series expansions for mean height and spread of the particles derived for an infinite boundary layer are (Hunt 1984)

$$\overline{Z - z_s} = \tfrac{1}{2}(\partial\overline{u_3^2}/\partial z)_{z_s}\, t^2 + O(t^3) \tag{4.13}$$

$$\overline{(Z - z_s)^2} = (\overline{u_3^2})_{z_s}\, t^2 + \tfrac{1}{2}(\partial\overline{u_3^3}/\partial z)_{z_s}\, t^3 + O(t^4)\ .$$

The results in Fig. 4.4 show indeed that the mean height increases the fastest the closer the source is to the surface. This is because $\partial\overline{u_3^2}/\partial z$ decreases with height.

Willis and Deardorff measured the mean height and spread for releases at $z_s/z_i = 0.05$ and $z_s/z_i = 0.067$. Our model run with a $\overline{u_3^2(z)}$ profile that is equal to Eq. (4.5) leads to good agreement with the short time results of $z_s/z_i = 0.067$. The results of Willis and Deardorff in case $z_s/z_i = 0.05$ are best simulated with $\overline{u_3^2(z)} = 1.8(z/z_i)^{2/3}$. This profile is also used by Van Dop et al. (1984), following Wyngaard et al. (1971). This might be explained by the fact, that maybe in each water tank experiment, the convective boundary layer established, should have been described by a different coefficient in the $\overline{u_3^2(z)}$ profile.

Groundlevel concentrations $C(x,z = 0)$ are presented in Fig. 4.6 where also the results of a source at $z_s/z_i = 0.75$ are given. These values are based on the average number of particles in the lowest interval $\Delta z/z_i = 0.05$, except for the ground level source at height $z_s/z_i = 0.067$, where the results of two layers were averaged to include the source height itself.

Particles released at the surface immediately lift off the ground, reducing the groundlevel concentration. Only after distances larger than $X = 0.5$ the groundlevel concentration increases again untill the particles get homogeneously distributed. The groundlevel concentration due to the phenomena shows a minimum between $X = 0.6$ and $X = 1.5$.

Particles from elevated sources are first transported downward with a nondimensional velocity of order $0.5\ w_*/U$. The higher the source, the longer it takes before the plume hits the ground and the more effective the diffusion already does its work. Therefore the maximum groundlevel concentration decreases with source height.

Briggs (1983) analysed a large number of dispersion field experiments. These are data for source heights in the lower half of the boundary layer. He came to the conclusion that groundlevel concentrations from elevated releases have a peak at $X = a\ z_s/z_i$ with $1.8 < a < 2.2$, due to a downward non-dimensionalised mean particle velocity of w_*/U. He also found that the maximum surface concentration can be described by

$$C_{max}(X,z=0) = 0.48(1 + 2z_s/z_i)(z_s/z_i)^{-1} \ . \qquad (4.14)$$

The values we found for the distances X at which the groundlevel concentration peaks agree very well with his formula (Fig. 4.6). But our maximum

Fig 4.6

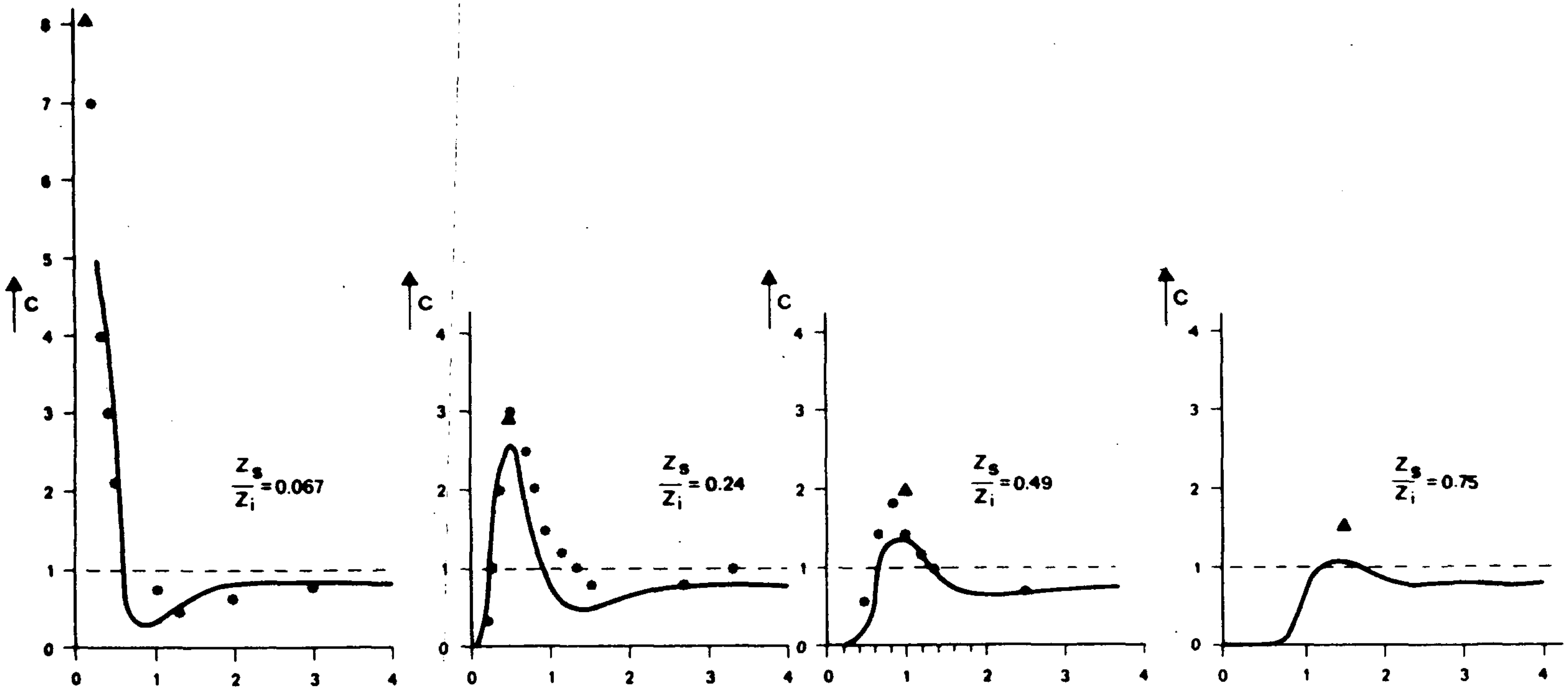


Figure 6. Ground level concentrations as a function of downwind distance X for the source heights $z_s/z_i = 0{\cdot}067$, $z_s/z_i = 0{\cdot}24$, $z_s/z_i = 0{\cdot}49$ and $z_s/z_i = 0{\cdot}75$. These concentrations are averaged values over the interval $z/z_i < 0{\cdot}05$ except for the source height $z_s/z_i = 0{\cdot}067$ where the average is over $z/z_i < 0{\cdot}1$. The results of our Langevin model are indicated by a solid line, the measurements of Willis and Deardorff by stars, and the maximum ground level concentration according to Briggs (Eq. 14) is indicated by ▲.

concentrations are smaller than those predicted by Briggs. This might be also due to the fact that the concentration gradient at the lower side of the particle cloud during lift off is very large in our experiment, resulting in lower groundlevel concentrations.

Simulations for longer times up to $t/T_L = 200$ show that the concentration distribution reached after $t/T_L = 3$ is approximately the equilibrium distribution. This concentration is homogeneous in the bulk of the boundary layer but reduces to 0.7 times the homogeneous concentration in two thin layers along the bottom and top with a thickness respectively of one tenth and one fifth of the boundary layer height, independent of source height.

These phenomena, although also quite accidentally measured by Willis and Deardorff, should be investigated further. It might be due to inconsistencies in the Lagrangian modeling and deserves our attention, because most applications will focus on a correct prediction of surface concentrations.

4.5 Discussion

In this section we will discuss some details of our simulation. First we consider the choice for T_L and for the turbulence velocity distribution. Next we consider the sensitivity of our model for the parameter Δt and for the modelling of the random forcing function. We conclude with a discussion of the results in comparison with observations.

The Lagrangian timescale was argued to be $T_L = cz_i/w_*$ (Eq.(4.4)). In this section 2 it is discussed that c lies between c = 0.24 and c = 0.55 based on one experiment by Hanna (1981). The choice of the constant c is critical. Each choice leads to different behaviour of the particles and therefore the choice for c can not be considered to be a scaling of the Langevin equation. This is because the equations for the moments of $d\mu$ depend both on $\Delta t/T_L$ and on Δt, leading to a nonscalable velocity and consequently to a nonscalable displacement.

The choice of c is restricted by the fact that the variance $\overline{(d\mu)^2}$ has to remain positive. For instance if we use the profiles of Baerentsen and Berkowicz in Eq. (4.8) we find that for c < 0.87 the requirement $\overline{(d\mu)^2} > 0$ is satisfied at all heights. However, these values of result in a too slow lift-off of the particles, suggesting that c should be larger. We chose c = 1 and in that case the profile of $\overline{u_3^3(z)}$ has to be changed slightly at the top to Eq. (4.7), which has a less negative gradient in this region.

Another small adjustment of the profiles was required. Near the ground ($z \to 0$) $\partial u_3^2/\partial z$ tends to infinity (cf Eq. 4.5) so that $d\mu$ may take arbitrary large values (Eq. 4.8). This, however, causes difficulties in the numerical procedure, which was chosen to determine $P(d\mu)$. These difficulties could be avoided by taking $\overline{u_3^2}/w_*^2$ to be constant in a small layer δ above the ground. Here δ is put equal to 0.0025. A larger δ causes the concentration in the layer $z < \delta$ to spread out more.

At the top and at the bottom reflection boundary conditions are imposed. This means that for some small quantity ε we get

$$u_3(-\varepsilon) = -u_3(\varepsilon) \text{ and } u_3(z_i + \varepsilon) = -u_3(z_i - \varepsilon) . \qquad (4.15)$$

This implies that $\overline{u_3(z)}$ and $\overline{u_3^3(z)}$ should be zero at the boundaries, while $\overline{u_3^2(z)}$ should be constant near the boundaries. At the ground the profiles given by Eq. (4.5) and Eq (4.7) are consistent with the boundary conditions. At the top the requirements $\overline{u_3^2}/w_*^2$ = constant and $\overline{u_3^3}/w_*^3 = 0$ are not met by the profiles. We did not adjust the profiles, because this would imply a too large gradient in u_3^3/w_*^2, which would lead to violation of the requirement $(d\mu)^2 > 0$.

The accuracy of the statistics of the constructed skew forcing function is a function of the number of particles and of the time step. This can be explained as follows. The skewness of the random forcing function is defined as $S = \overline{(d\mu)^3}/\{\overline{(d\mu)^2}\}^{3/2}$. This skewness is a function of the numerical time step $S \sim (\Delta t)^{-1/2}$. A small timestep implies a large value of S. A large skewness means that the probability density function has a tail. These large values of μ have a very small probability. If the generation is done with a limited number of particles, these large values of μ might be left out, causing the generated distribution to have a very inaccurate skewness. We choose $\Delta t/T_L = 0.05$ and the number of particles to be 20.000.

As we have seen we must prescribe the first three moments of the random forcing term in the Langevin equation. Let us now consider how sensitive our model results are for the exact prescription of those moments. The description of dispersion in non-homogeneous turbulence, when only $\overline{u_3^2(z)}$, but not its derivative, is taken into account, leads to accumulation of the particles in regions with a small variance (Janicke, 1981). Janicke (1981) and Thomson (1984) in their run 2 and 3 also took into account the derivative $\partial\overline{u_3^2}/\partial z$. They applied the full Eqs. (8a, b) with $\overline{u_3^3} = 0$. The higher moments are still assumed to be zero. This results in a concentration distribution for large times that is sometimes slightly the opposite, particles accumulate in regions with a large variance. This also happened in simulations with our model. Introducing a third moment of random forcing function $\overline{u_3^3(z)}$, in Eqs. (4.8b,c) improves the simulations very much.

Of the fourth moment, $\overline{u_3^4}$, no measurements are available. Therefore, we assumed a relationship between the fourth and the second moment, $\overline{u_3^4} = \alpha(\overline{u_3^2})^2$, with α between 2 and 5. Comparing the results with the watertank experiments it appears that the convective boundary layer is best modelled with the Gaussian assumption

$$\overline{u_3^4} = 3(\overline{u_3^2})^2 \ . \qquad (4.16)$$

4.6 Conclusions

Dispersion of particles into inhomogeneous turbulence in a convective boundary layer is modeled by a Langevin equation. The Langevin model is capable of simulating all the experimentally known features of dispersion in convective turbulence. The agreement with observations may be characterised as good. The theory for the Langevin model in inhomogeneous conditions requires that the third moment of the random forcing function should be nonzero. We have found that this requirement is essential for the behaviour of the model near the source, where it is responsible for the downward movement of an elevated plume. The requirement also holds for the behaviour for large time, where a much better uniform concentration is found in comparison with the case where the third moment is taken to be zero.

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Appendix

This skew distribution function $P(d\mu)$ can be constructed out of two Gaussian distributions: with a chance a_1 we choose $d\mu$ from the first Gaussian distribution function $P_1(x_1)$, and with a chance $(1 - a_1)$ we choose $d\mu$ from the second Gaussian distribution function $P_2(x_2)$. These $P_i(x_i)$ have mean m_i and variance σ_i^2. Four requirements

$$1 = a_1 \int P_1(x_1)dx_1 + a_2 \int P_2(x_2)dx_2 \qquad \text{(A1)}$$

$$\overline{(d\mu)^n} = a_1 \int x_1^n P_1(x_1)dx_1 + a_2 \int x_2^n P_2(x_2)dx_2 \qquad n = 1, 2, 3$$

lead to the equations

$$a_1 + a_2 = 1$$

$$a_1 m_1 + a_2 m_2 = \overline{d\mu} \qquad \text{(A2)}$$

$$a_1(m_1^2 + \sigma_1^2) + a_2(m_2^2 + \sigma_2^2) = \overline{(d\mu)^2}$$

$$a_1(m_1^3 + 3m_1\sigma_1^2) + a_2(m_2^3 + 3m_2\sigma_2^2) = \overline{(d\mu)^3} .$$

These equations still have two degrees of freedom. Because we're not interested in the specific form of $P(d\mu)$ but only in its first three moments the two other requirements were chosen to simplify the arithmatics. We chose

$$m_i^2 = \sigma_i^2 (i = 1,2).$$

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Ch. 5. COMPARISON OF LANGEVIN MODELS

Ch. 5 Comparison of Langevin models

5.1 Introduction

Dispersion in a turbulent atmosphere can be described by a Langevin model.Such a model describes the velocity of released particles. The changes of the velocity in time are modelled by a damping term and a random forcing term. The last term specifies the effect of turbulence eddies on the particle and can be formulated such, that the Langevin equation is able to describe dispersion in inhomogeneous turbulence. These facts were shown to be true in the former chapter, where we applied the Langevin equation to a convective boundary layer. The complicated behaviour of dispersion from a point source was satisfactorily described. Only in the equilibrium state the model results showed shortcomings: the particles were uniformly distributed, except near the ground and the top of the boundary layer. Another model, a Langevin model for the variable W/σ, shows a better homogeneous concentration distribution in the above mentioned application. This difference was the background of our theoretical investigation of both models.

To be able to make a comparison between the two models we investigate several of their characteristics. In particular we will consider short and large time behaviour. In addition we compare both Langevin models to the exact Eulerian conservation of mass equations. When we investigate the large time behaviour we do not only investigate the steady state of the Langevin models, but also their large time behaviour leading to this state, which is described by Markov limits previously discussed in Ch. 2. There the new large time analysis for inhomogeneous turbulence was applied to the Langevin model for W. In this chapter we extend the derivation to the W/σ-model and compare the two, to see whether the above described undesirable effect of a non-uniform concentration distribution in the W-model is inherent to this model.

5.2 Introduction of Langevin models for W and for W/σ

Two Langevin models have been used in the literature to describe dispersion in a turbulent atmosphere. The first model is a Langevin model for the vertical particle velocity W, which is already extensively discussed in Ch. 2. The second model describes W/σ, where $\sigma^2(z)$ is the variance of the vertical turbulence velocity fluctuations $\sigma^2(z) = \overline{u_3^2}(z)$.

This alternative model, first used by Wilson et al. (1983), is based on the Langevin equation for W/σ. It reads

$$d\frac{W}{\sigma} = -\frac{W}{\sigma(z)}\frac{dt}{T_L(z)} + d\chi(t) \text{ and}$$

$$dZ = Wdt \;, \tag{5.1a}$$

where dχ is a random process describing the random forcing of the particles consistent with this model. Eq. (5.1a) is equivalent to the equation

$$dW = -\frac{W}{T_L(z)}\,dt + W^2\frac{1}{2\sigma^2}\frac{d\sigma^2}{dz}\,dt + d\eta(t) \text{ and}$$

$$dZ = Wdt \;, \tag{5.1b}$$

where we substituted $d\eta = \sigma\, d\chi$ and used that $d\sigma^2 = \frac{d\sigma^2}{dz}\,dZ = \frac{d\sigma^2}{dz}\,W\,dt$.
For stationary turbulence the formula for the moments $\langle(d\eta)^n\rangle = b_n(z)dt$ were also derived by Thomson (1984) analogously to the derivation for the model for W. They can also be given in one general formula, which reads

$$b_n(z) = \frac{d\overline{u_3^{n+1}}(z)}{dz} + n\,\frac{\overline{u_3^n}(z)}{T_L} - \frac{n}{2\overline{u_3^2}}\,\frac{d\overline{u_3^2}(z)}{dz}\,\overline{u_3^{n+1}}(z) - \sum_{k=1}^{n-1}\binom{n}{k}\overline{u_3^{n-k}}\,b_k(z) \tag{5.2}$$

From Eq. (2.50) and (5.2) we evaluate the first three moments of both models.

For the W-model they read

$$a_1(z) = \frac{d\overline{u_3^2}}{dz} ,$$

$$a_2(z) = 2\,\frac{\overline{u_3^2}}{T_L} + \frac{d\overline{u_3^3}}{dz} \quad \text{and} \tag{5.3a}$$

$$a_3(z) = 3\,\frac{\overline{u_3^3}}{T_L} + \frac{d\overline{u_3^4}}{dz} - 3\,\overline{u_3^2}\,\frac{d\overline{u_3^2}}{dz} .$$

The first three moments in the W/σ-model read

$$b_1(z) = \tfrac{1}{2}\,\frac{d\overline{u_3^2}}{dz} ,$$

$$b_2(z) = 2\,\frac{\overline{u_3^2}}{T_L} + \frac{d\overline{u_3^3}}{dz} - \frac{\overline{u_3^3}}{\overline{u_3^2}}\,\frac{d\overline{u_3^2}}{dz} \quad \text{and} \tag{5.3b}$$

$$b_3(z) = 3\,\frac{\overline{u_3^3}}{T_L} + \frac{d\overline{u_3^4}}{dz} - \frac{3}{2}\,\frac{\overline{u_3^4}}{\overline{u_3^2}}\,\frac{d\overline{u_3^2}}{dz} - \frac{3}{2}\,\overline{u_3^2}\,\frac{d\overline{u_3^2}}{dz} .$$

From the characteristic function $\hat{f}$ of the random forcing function in the W-model we argued that in <u>Gaussian turbulence</u> the fourth and higher moments of dμ are zero in order dt, while

$$a_1(z) = \frac{d\sigma^2}{dz} ,$$

$$a_2(z) = 2\,\frac{\sigma^2}{T_L} , \tag{5.4}$$

$$a_3(z) = 3\,\sigma^2\,\frac{d\sigma^2}{dz} .$$

(see Eq. (2.56)).

Thomson (1984) derived the moment generating function of the random forcing function dη of the W/σ-model in Gaussian turbulence. From this we may find the characteristic function, which reads

$$\hat{f}(\theta) = 1 + dt\ \sigma_w \frac{\partial \sigma_w}{\partial z} \theta + \frac{dt}{T_L} \sigma_w^2 \theta^2 + O(dt^2) . \tag{5.5}$$

The moments $\langle (d\eta)^n \rangle$ are given by $\langle (d\eta)^n \rangle = (-i)^n \left. \frac{\partial^n \hat{f}}{\partial \theta^n} \right]_{\theta=0}$. Because the characteristic function Eq. (5.5) is a second order polynominal it follows that the third and higher moments of $d\eta$ are zero in order dt, while

$$\begin{aligned} b_1(z) &= \tfrac{1}{2} \frac{d\sigma^2}{dz} , \\ b_2(z) &= 2 \frac{\sigma^2}{T_L} . \end{aligned} \tag{5.6}$$

In homogeneous turbulence the models for W and W/σ are equivalent. However, in general turbulence conditions the models are not equivalent due to the nonlinear term in Eq. (5.1b). We will investigate this difference.

5.3 Short time behaviour of the models

5.3.1 Introduction

To compare the Langevin model for W and W/σ we investigate several aspects of them. The aspect of the Langevin models we consider here is the short time behaviour of particles released in stationary turbulence. We derive shorttime expansions of the mean particle height $\overline{Z(t)-z_s}$ and variance $\overline{(Z-z_s)^2}$ as given by the models (z_s is the source height) and compare these expressions to the exact Taylor expansions.

The exact Taylor expansions of the statistics of particle trajectories for the case of stationary turbulence are (Hunt, 1984)

$$\overline{(Z-z_s)} = \frac{1}{2}\frac{d\overline{u_3^2}}{dz}\Big]_{z_s} t^2 + \frac{1}{6}\frac{d^2\,\overline{u_3^3}}{dz^2} t^3 + \ldots = \frac{1}{2}\frac{d\overline{u_3^2}}{dz} t^2\left(1 + \frac{1}{3}\frac{t}{\tau_1}\right) + O(t^4) \tag{5.7a}$$

$$\overline{(Z-z_s)^2} = \overline{u_3^2}\Big]_{z_s} t^2 + \frac{1}{2}\frac{d\overline{u_3^3}}{dz}\Big]_{z_s} t^3 + \ldots = \overline{u_3^2}\, t^2\left(1 + \frac{1}{2}\frac{t}{\tau_2}\right) + O(t^4) \tag{5.7b}$$

where the dummy timescales τ_1 and τ_2 are given by Eq. (5.13a).

In the shorttime expansions of Langevin model result terms appear, that apart from T_L, also involve (still to be defined) timescales T_d, an artifact of the models. These terms specify the deviation from the exact Taylor expansions. The usual restriction on model shorttime expansions that they are valid for times smaller than T_L is therefore not necessarily correct. The model shorttime expansions deviate from the exact ones for times larger than either T_L or T_d and the T_d's might be smaller than T_L.

We will derive the shorttime expansions of the Langevin model and write them in such a form that similarities are easily noted. This will be done with the aid of dummy timescales. From them we define T_d and investigate the deviation of the models from the exact Taylor expansions in an application to convective turbulence.

5.3.2 General shorttime expansions of quantities in the Langevin models

The short time behaviour of mean height and variance as given by the Langevin models in stationary turbulence can be derived from the general formula for the particle displacement relative to the source z_s:

$$Z(t)-z_s = \int_{z_s}^{Z(t)} dZ = \int_o^t W(t')dt' = tW(t) - \int_{W(o)}^{W(t)} t'dW(t')$$

$$= W(o)t + t\int_{W(o)}^{W(t)} dW(t') - \int_{W(o)}^{W(t)} t'\, dW(t')$$

$$= W(o)t + \int_{W(o)}^{W(t)} (t-t')\, dW(t')\ .$$

Per definition we have that $W(o) \equiv u_3(z_s)$, so that

$$Z(t)-z_s = u_3]_{z_s}\, t + \int_{W(o)}^{W(t)} (t-t')\, dW(t')\ . \qquad (5.8)$$

This general equation can be used in both models.

Langevin model for W

To get expressions for the shorttime expansions in the first model we substitute the Langevin equation for W into Eq. (5.8). We get

$$Z(t)-z_s = u_3]_{z_s}\, t - \int_o^t (t-t')\, \frac{W(t')}{T_L(Z(t'))}\, dt' + \int_o^t (t-t')d\mu(t') \qquad (5.9)$$

Note that in inhomogeneous conditions $d\mu$ and T_L are implicit functions of t. To get a short time expansion we expand the terms on the RHS.

We can expand $\frac{W(t)}{T_L}$ using $W(t) \equiv u_3(\underset{\sim}{X}(t))$. Our Langevin model is a 1-D model for the vertical velocity W. However, the turbulence velocity is a 3-D quantity and should be expanded accordingly (Van Dop et al., 1985). In this expansion we use the continuity equation $d\underset{\sim}{u}_i/dx_i = 0$, which leads to the use of $u_j \frac{du_3}{dx_j} = \frac{d(u_3u_j)}{dx_j}$. This gives

$$\frac{W(t)}{T_L} = \{u_3]_{z_s} + (\underset{\sim}{X}-\underset{\sim}{x}_s)\frac{du_3}{dx_j}]_{\underset{\sim}{x}_s} + \ldots\} \frac{1}{T_L(z_s)}\{1-(Z-z_s)\frac{1}{T_L}\frac{dT_L}{dz}]_{z_s} + \ldots\}$$

$$= \{u_3]_{z_s} + (u_j\frac{du_3}{dx_j})]_{\underset{\sim}{x}_s} t + \ldots\} \frac{1}{T_L(z_s)} \{1-(u_3\frac{1}{T_L}\frac{dT_L}{dz})]_{z_s} t + \ldots\}$$

$$= \frac{u_3}{T_L}]_{z_s} + (\frac{1}{T_L}\frac{du_3u_j}{dx_j} - u_3^2\frac{1}{T_L^2}\frac{dT_L}{dz})]_{\underset{\sim}{x}_s} t + \ldots$$

We expand $d\mu(Z(t))$ as

$$d\mu(Z(t)) = d\mu(t=o) + \ldots$$

Substituting the expansions of $\frac{W(t)}{T_L}$ and $d\mu$ in Eq. (5.9a) we get

$$Z(t)-z_s = u_3]_{z_s} t + \int_o^t (t-t')d\mu(t=o) - \tfrac{1}{2}\frac{u_3}{T_L}]_{z_s} t^2 - \frac{1}{6}(\frac{1}{T_L}\frac{du_3u_j}{dx_j} - u_3^2\frac{1}{T_L^2}\frac{dT_L}{dz})]_{z_s} t^3 + \ldots \tag{5.9b}$$

To derive the shorttime expansion of the mean height we ensemble average Eq. (5.9b) and use the horizontal homogeneity to give $\frac{\overline{du_3u_j}}{dx_j} = \frac{\overline{du_3^2}}{dz}$:

$$\overline{Z(t)-z_s} = \int_o^t \overline{d\mu(t=o)}(t-t') - \frac{1}{6}(\frac{1}{T_L}\frac{d\overline{u_3^2}}{dz} - \overline{u_3^2}\frac{1}{T_L^2}\frac{dT_L}{dz})]_{z_s} t^3 + \ldots$$

$$= a_1(z_s)\int_o^t (t-t')dt' - \frac{1}{6}(\frac{1}{T_L}\frac{d\overline{u_3^2}}{dz} - \overline{u_3^2}\frac{1}{T_L^2}\frac{dT_L}{dz})]_{z_s} t^3 + \ldots \tag{5.10a}$$

$$= \frac{1}{2} \frac{d\overline{u_3^2}}{dz}\Big]_{z_s} t^2 - \frac{1}{6}\left(\frac{1}{T_L} \frac{d\overline{u_3^2}}{dz} - \overline{u_3^2} \frac{1}{T_L^2} \frac{dT_L}{dz}\right)\Big]_{z_s} t^3 + \ldots$$

$$= \frac{1}{2} \frac{d\overline{u_3^2}}{dz}\Big]_{z_s} t^2 \left(1 - \frac{1}{3} \frac{t}{T_L} + \frac{1}{3} \frac{t}{\tau_3}\right)\Big]_{z_s} + \ldots ,$$

where τ_3 is given by Eq. (5.13a) and the moments $\langle (d\mu(t))^n \rangle = a_n(z(t))dt$ in stationary turbulence by Eq. (2.50). To derive the shorttime expansion of the spread we square and ensemble average Eq. (5.9b). Using the fact that $u_3(z_s)$ and

$d\mu(z_s)$ are uncorrelated we get

$$\overline{(Z(t)-z_s)^2} = \overline{u_3^2}\Big]_{z_s} t^2 - \frac{\overline{u_3^2}}{T_L}\Big]_{z_s} t^3 + \int_0^t \int_0^t (t-t')(t-t'')\overline{d\mu(t'=0)d\mu(t'=0)} + \ldots.$$

$$= \overline{u_3^2}\Big]_{z_s} t^2 + \frac{1}{3} a_2(z_s)t^3 - \frac{\overline{u_3^2}}{T_L}\Big]_{z_s} t^3 + \ldots.$$

$$= \overline{u_3^2}\Big]_{z_s} t^2 + \frac{1}{3} \frac{d\overline{u_3^3}}{dz}\Big]_{z_s} t^3 - \frac{1}{3} \frac{\overline{u_3^2}}{T_L}\Big]_{z_s} t^3 + \ldots$$

$$= \overline{u_3^2}\Big]_{z_s} t^2 \left(1 - \frac{1}{3} \frac{t}{T_L} + \frac{1}{3} \frac{t}{\tau_2}\right)\Big]_{z_s} + \ldots , \qquad (5.10b)$$

where τ_2 is given by Eq. (5.13a). Note that τ_2 also appears in the exact Taylor expansions for the spread.

Langevin model for W/σ

The short time expansions of $\overline{Z-z_s}$ and $\overline{(Z-z_s)^2}$ for the Langevin model for W/σ can analogously be derived by substituting the Langevin Eq. (5.1b) into Eq. (5.8):

$$Z(t)-z_s = u_3]_{z_s} t+ \int_0^t A(Z(t'))W^2(t')(t-t')dt' - \int_0^t (t-t')\frac{W(t')}{T_L}dt' + \int_0^t (t-t')d\eta(t') \tag{5.11a}$$

with $A(z) = \frac{1}{2\sigma^2}\frac{d\sigma^2}{dz}$. To get a shorttime expansion we expand the terms on the RHS. We expand W, T_L and $d\eta$ like above and the square of the velocity W^2 and the quantity A(z) as

$$W^2(t) = \{u_3]_{z_s} + \frac{du_3u_j}{dx_j}]_{\underset{\sim}{x}_s} t + \ldots\}^2 = u_3^2]_{z_s} + 2\frac{u_3du_3u_j}{dx_j}]_{\underset{\sim}{x}_s} t + \ldots$$

$$= u_3^2]_{z_s} + \frac{\partial u_3^2u_j}{\partial x_j} t + \ldots \qquad \text{and}$$

$$A(z) = A(z_s) + u_3\frac{dA}{dz}]_{z_s} t + \ldots$$

Then Eq. (5.11a) becomes

$$Z(t)-z_s = u_3]_{z_s} t + \tfrac{1}{2}u_3^2 A]_{z_s} t^2 + (\frac{1}{6}\frac{du_3^2u_j}{dx_j}A + \frac{1}{6}u_3^3\frac{dA}{dz})]_{z_s} t^3 + \int_0^t (t-t')d\eta(t') - \tfrac{1}{2}\frac{u_3}{T_L}]_{z_s} t^2$$
$$- \frac{1}{6}(\frac{1}{T_L}\frac{du_3^2}{dz} - u_3^2\frac{1}{T_L^2}\frac{dT_L}{dz})]_{z_s} t^3 + \ldots \tag{5.11b}$$

Ensemble averaging Eq. (5.11b) using horizontal homogeneity the short time expression for the mean height becomes:

$$\overline{(Z(t)-z_s)} = \tfrac{1}{4}\frac{d\overline{u_3^2}}{dz}]_{z_s} t^2 + \tfrac{1}{2}b_1(z_s)t^2 - \frac{1}{6}(\frac{1}{T_L}\frac{d\overline{u_3^2}}{dz} - \overline{u_3^2}\frac{1}{T_L^2}\frac{dT_L}{dz})]_{z_s} t^3 + \frac{1}{6}\frac{d(\overline{u_3^3}A)}{dz}]_{z_s} t^3$$

$$= \tfrac{1}{2}\frac{d\overline{u_3^2}}{dz}]_{z_s} t^2(1 - \frac{1}{3}\frac{t}{T_L} + \frac{1}{3}\frac{t}{\tau_3} + \frac{1}{3}\frac{t}{\tau_4})]_{z_s} + \ldots, \tag{5.12a}$$

where τ_3 and τ_4 are given by Eq. (5.13b) and the moments $\langle(d\eta)^n\rangle = b_n dt$ in stationary turbulence by Eq. (5.2). The term with τ_3 is kept separate to compare the W- and W/σ-model. Squaring and ensemble averaging Eq.(5.11b) we get the expression for the spread:

$$\overline{(Z(t)-z_s)^2} = \overline{u_3^2}]_{z_s} t^2 + \overline{u_3^3} A t^3 - \frac{\overline{u_3^2}}{T_L}]_{z_s} t^3 + \int_0^t\int_0^t (t-t')(t-t'')\overline{d\eta(t')d\eta(t'')} + \ldots$$

$$= \overline{u_3^2}\Big]_{z_s} t^2 + t^3 \Big[\tfrac{1}{2}\frac{\overline{u_3^3}}{\sigma^2}\frac{d\sigma^2}{dz} + \frac{1}{3} b_2 - \frac{\overline{u_3^2}}{T_L}\Big]_{z_s} + \ldots$$

$$= \overline{u_3^2}\Big]_{z_s} t^2 + \Big(\frac{1}{3}\frac{d\overline{u_3^3}}{dz} + \frac{1}{6}\frac{\overline{u_3^3}}{\overline{u_3^2}}\frac{d\overline{u_3^2}}{dz}\Big)\Big]_{z_s} t^3 - \frac{1}{3}\frac{\overline{u_3^2}}{T_L}\Big]_{z_s} t^3 + \ldots$$

$$= \overline{u_3^2}\Big]_{z_s} t^2 \Big(1 - \frac{1}{3}\frac{t}{T_L} + \frac{1}{3}\frac{t}{\tau_2} + \frac{1}{6}\frac{t}{\tau_5}\Big)\Big]_{z_s} + \ldots , \qquad (5.12b)$$

where τ_5 is given by Eq. (5.13b). The term with τ_2 is kept seperate to compare the W- to the W/σ-model. In the next section we derive the deviation timescales T_d from the dummy timescales τ_1-τ_5.

Summary

The exact Taylor expansions Eq. (5.7) for mean height and spread are

$$\overline{Z(t)-z_s} = \tfrac{1}{2} \frac{d\overline{u_3^2}}{dz} t^2 \left(1 + \frac{1}{3}\frac{t}{\tau_1}\right) + O(t^4) \qquad \text{and}$$

$$\overline{(Z(t)-z_s)^2} = \overline{u_3^2}\, t^2 \left(1 + \tfrac{1}{2}\frac{t}{\tau_2}\right) + O(t^4)$$

The shorttime expansion of mean height and spread in the Langevin models are for the model for W Eq. (5.10):

$$\overline{Z(t)-z_s} = \tfrac{1}{2} \frac{d\overline{u_3^2}}{dz} t^2 \left(1 - \frac{1}{3}\frac{t}{T_L} + \frac{1}{3}\frac{t}{\tau_3}\right)\Big]_{z_s} + \ldots \text{ for } t \ll (T_L, \tau_1) \text{ and}$$

$$\overline{(Z(t)-z_s)^2} = \overline{u_3^2}\, t^2 \left(1 - \frac{1}{3}\frac{t}{T_L} + \frac{1}{3}\frac{t}{\tau_2}\right)\Big]_{z_s} + \ldots \text{ for } t \ll)T_L, \tau_2)$$

for the model for W/σ Eq. (5.12):

$$\overline{Z(t)-z_s} = \tfrac{1}{2} \frac{d\overline{u_3^2}}{dz} t^2 \left(1 - \frac{1}{3}\frac{t}{T_L} + \frac{1}{3}\frac{t}{\tau_3} + \frac{1}{3}\frac{t}{\tau_4}\right)\Big]_{z_s} + \ldots \text{for } t \ll (T_L, \tau_1, \tau_3) \text{ and}$$

$$\overline{(Z(t)-z_s)^2} = \overline{u_3^2}\, t^2 \left(1 - \frac{1}{3}\frac{t}{T_L} + \frac{1}{3}\frac{t}{\tau_2} + \frac{1}{6}\frac{t}{\tau_5}\right)\Big]_{z_s} + \ldots \text{ for } t \ll (T_L, \tau_2, \tau_4)$$

where the dummy timescales are defined by

$$\tau_1^{-1} = \frac{d^2\overline{u_3^3}}{dz^2} \Big/ \frac{d\overline{u_3^2}}{dz}\Big]_{z_s} \quad , \quad \tau_2^{-1} = \frac{1}{\overline{u_3^2}} \frac{d\overline{u_3^3}}{dz}\Big]_{z_s} \qquad (5.13a)$$

$$\tau_3^{-1} = \left(\overline{u_3^2}\frac{1}{T_L^2}\frac{dT_L}{dz}\right) \Big/ \frac{d\overline{u_3^2}}{dz}\Big]_{z_s} \quad , \quad \tau_4^{-1} = \left(\frac{d(\overline{u_3^3}A)}{dz} \Big/ \frac{d\overline{u_3^2}}{dz}\right]_{z_s} \qquad (5.13b)$$

$$\tau_5^{-1} = \frac{\overline{u_3^3}}{\overline{u_3^2}^2} \frac{d\overline{u_3^2}}{dz}\Big]_{z_s}, \qquad (5.13c)$$

with $A = \frac{1}{2\overline{u_3^2}} \frac{d\overline{u_3^2}}{dz}\Big]_{z_s}$ the factor appearing in the non-linear term of the W/σ Langevin equation.

5.3.3 Definition of deviation timescales T_d

In homogeneous turbulence the W- and W/σ-models are equal. In that case all mean height expansions are

$$\overline{Z - z_s} = 0.$$

The exact spread expansion resp. model expansion read

$$\overline{(Z - z_s)^2} = \overline{u_3^2} t^2 + O(t^4) \text{ and}$$

$$\overline{(Z - z_s)^2} = \overline{u_3^2}\, t^2 (1 - \frac{1}{3} \frac{t}{T_L}) + O(t^4).$$

In this homogeneous case the models deviate from the exact Taylor expansions in the spread for times that are no longer small compared to T_L, the only timescale appearing. For times t smaller than the only timescale T_L both models give the exact Taylor expansions. In homogeneous turbulence no deviation timescale T_d appears. However, it is interesting to investigate the model spread expansions with earlier derived expressions to show that the shorttime expansions are correct. The model spread equation is equal to the one derived from Taylor's theorem for an exponential autocorrelation Eq. (1.11) by Tennekes (1979). Tennekes gave the following interpretation of the last term. For small times the particle spread goes quadratic in time $\overline{(Z-z_s)^2} = \overline{u_3^2}\, t^2$. For larger time the dispersion slows down as small scale eddies are no longer effective in mixing the particles with the air. The correction term on the spread must therefore be negative and relate to the small-scale parameters ε, the energy dissipation rate per unit mass and time t. Dimensional analysis shows that

$$\overline{(Z-z_s)^2} = \overline{u_3^2}\, t^2 - \text{const}\ \varepsilon t^3.$$

Comparing this equation with the one derived from Taylor's theorem shows that $\varepsilon \sim \overline{u_3^2}/T_L$, so that ε, a small parameter, is determined by the large scale dynamics.

The deviation of the model shorttime expansions from the exact Taylor expansions in <u>inhomogeneous</u> turbulence is given by terms involving T_L and a (to be defined) deviation timescale T_d. We write the Taylor expansions generically as

$$\overline{(Z-z_s)^n} = g_n(t) + 0(t^4)$$

and the model expansions as (5.14)

$$\overline{(Z-z_s)^n} = g_n(t)(1 - \frac{1}{3}\frac{t}{T_L} + \frac{1}{3}\frac{t}{T_{d_n}}) + 0(t^4)$$

Mean height

In the mean height expressions Eqs. (5.10a) and (5.12a) for the model for W and for W/σ the deviation timescales T_{d_1} can be derived as follows. For the W-model we have using Eqs. (5.7), (5.10)and (5.14)

$$\overline{(Z-z_s)} = g_1(t)\,\frac{(1 - 1/3\ t/T_L + 1/3\ t/\tau_3)}{(1 + 1/3\ t/\tau_1)}$$

$$= g_1(t)(1 - 1/3\ t/T_L + 1/3(t/\tau_3 - t/\tau_1) + 0(t^4)$$

if $t \ll \tau_1$. So that

$$\frac{1}{Td_1^W} = \frac{1}{(\frac{1}{\tau_3} - \frac{1}{\tau_1})}\ .$$

Analogously we get for the W/σ-model

$$\overline{Z-z_s} = g_1(t)\,\frac{(1 - 1/3\ t/T_L + 1/3\ t/\tau_3 + \tfrac{1}{2}\ t/\tau_4)}{(1 + 1/3\ t/\tau_1)}$$

$$= g_1(t)\ (1 - 1/3\ t/T_L + 1/3\ t/\tau_3 + 1/3\ t/\tau_4 - 1/3\ t/\tau_1)$$

for $t \ll \tau_1$. So that

$$\frac{1}{T_{d_1}^{W/\sigma}} = 1/(\frac{1}{\tau_3} + \frac{1}{\tau_4} - \frac{1}{\tau_1})\ .$$

The timescales T_{d_1} are thus given by

$$T_{d_1}^{W} = \tau_1\tau_3/(\tau_1-\tau_3) \quad \text{and} \tag{5.15a}$$

$$T_{d_1}^{W/\sigma} = \tau_1\tau_3\tau_4/(\tau_4\tau_1 + \tau_3\tau_1 - \tau_3\tau_4) \tag{5.15b}$$

We note that in case T_L is constant no dummy timescale τ_3 appears in the model shorttime expressions. $T_{d_1}^{W}$ can be said to be $-\tau_1$ and $T_{d_1}^{W/\sigma} = \frac{\tau_1\tau_4}{\tau_1-\tau_4}$

The deviation of the models from the exact Taylor expansions are equal in case $T_{d_1}^{W} = T_{d_1}^{W/\sigma}$. We see that this is the case when $\tau_4 \rightarrow \infty$. This it does (see Eq. 5.13) in case $\frac{d(\overline{u_3^3 A})}{dz} \rightarrow 0$. This quantity is in turn a measure for the inhomogeneity of the turbulence. In homogeneous turbulence we have

$$\frac{d(\overline{u_3^3 A})}{dz} = 0.$$

Spread

The difference between the exact Taylor expansions for the spread and those of the models can be expressed as follows. In the exact expansions a term t/τ_2 appears with a factor ½, while in the model results a factor 1/3 appears. Using Eqs. (5.7), (5.10) and (5.14) we get for the W-model

$$\overline{(Z-z_s)^2} = g_2(t)\left(\frac{1 - 1/3\ t/T_L + 1/3\ t/\tau_2}{1 + ½\ t/\tau_2}\right) = g_2(t)\left(1 - \frac{1}{3}\frac{t}{T_L} - \frac{1}{6}\frac{t}{\tau_2}\right) + 0(t^4)$$

if $\|t/2\tau_2\| << 1$. We also defined

$$\overline{(Z-z_s)^2} = \left(1 - \frac{1}{3}\frac{t}{T_L} + \frac{1}{3}\frac{t}{T_{d_2}^{W}}\right) \text{ so that}$$

$$T_{d_2}^{W} = -\,2\,\tau_2 \tag{5.15c}$$

Analogously we get for the W/σ-model

$$\overline{(Z-z_s)^2} = g_2(t)\left(\frac{1 - \frac{1}{3}\ t/T_L + \frac{1}{3}\ t/\tau_2 + \frac{1}{6}\ t/\tau_5}{1 + ½\ t/\tau_2}\right)$$

$$= g_2(t)\left(1 - \frac{1}{3}\ t/T_L - \frac{1}{6}\ t/\tau_2 + \frac{1}{6}\ t/\tau_5\right) + 0(t^4)$$

if $\|t/2\tau_2\| << 1$.

So that

$$T_{d_2}^{W/\sigma} = \frac{2\ \tau_2 \tau_5}{\tau_2 - \tau_5} . \tag{5.15d}$$

The deviation of the models from the exact Taylor expansions are equal in case $T_{d_2}^{W} = T_{d_2}^{W/\sigma}$. This is the case if $\tau_5 \rightarrow \infty$, which happens when the turbulence becomes homogeneous $\overline{u_3^3} \rightarrow 0$ or $\frac{d\ \overline{u_3^2}}{dz} \rightarrow 0$. We summarize these timescales in Fig. 5.1 and investigate in the next section what these deviation timescales mean.

deviation time scale	W-model	W/σ-model
mean height	$T_{d1}^{W} = \frac{\tau_1\tau_3}{\tau_1 - \tau_3}$	$T_{d1}^{W/\sigma} = \frac{\tau_1\tau_3\tau_4}{\tau_4\tau_1 + \tau_3\tau_1 - \tau_3\tau_4}$
spread	$T_{d2}^{W} = -2\tau_2$	$T_{d2}^{W/\sigma} = \frac{2\tau_2\tau_5}{\tau_2 - \tau_5}$

$$\tau_1^{-1} = \frac{d^2\overline{u_3^3}}{dz^2} / \frac{d\overline{u_3^2}}{dz}\Big]_{z_s}$$

$$\tau_2^{-1} = \frac{1}{\overline{u_3^2}} \frac{d\overline{u_3^3}}{dz}\Big]_{z_s}$$

$$\tau_3^{-1} = \left(\overline{u_3^2} \frac{1}{T_L^2} \frac{dT_L}{dz}\right) / \frac{d\overline{u_3^2}}{dz}\Big]_{z_s}$$

$$\tau_4^{-1} = \frac{d(\overline{u_3^3}A)}{dz} / \frac{d\overline{u_3^2}}{dz}\Big]_{z_s}$$

$$\tau_5^{-1} = \frac{\overline{u_3^3}}{\overline{u_3^2}^2} \frac{d\overline{u_3^2}}{dz}\Big]_{z_s}$$

with $A = \frac{1}{2\overline{u_3^2}} \frac{d\overline{u_3^2}}{dz}$

Fig. 5.1. Deviation time scales Eq. (5.15) occurring in the short-time expansion.

5.3.4 Comparison Langevin model expressions to Taylor expansions

The expansions in both Langevin models are equal to the exact Taylor expansions for times smaller than all timescales involved (T_L and T_d). Which timescale plays a dominant role in the deviation from the exact expansions for larger times depends on the ratio of T_L and T_d, where T_d in turn depends strongly on the turbulence the models are applied to.

If the deviation timescale T_d is larger than the Lagrangian timescale T_L the term with T_L will be dominant over the term with T_d. In this case sufficient requirements for the model expansions to be valid is that t is smaller than T_L.

If the deviation timescale T_d is smaller than T_L, the term with T_d will be dominant over the term with T_L. In this case the shorttime expansions are certainly not valid for times smaller than T_L that are however larger than T_d. In the next section we illustrate these two cases in convective turbulence described by Eqs. (1.4) and (1.18).

We first concentrate on the mean height expressions. The mean height deviation timescales $T_{d_1}^{W}$ and $T_{d_1}^{W/\sigma}$ are strong functions of source height z_s/z_i (see Fig. 5.2a). We have $T_d \ll T_L$ for the W and W/σ-model in case of a source around $z_s/z_i = 0.3$. We investigate the mean height expressions for a source at $z_s/z_i = 0.36$. The deviation of the mean height from the exact expansions is dictated by the T_d-term. The difference in T_d for both models is small and the resulting difference in mean height is relatively small due to the factor $\frac{1}{2} \frac{d\overline{u_3^2}}{dz} t^2$ in front of the term $\frac{1}{3}\, t/T_d$. In Fig. (5.3a) we see indeed that for $t < T_L$ the W- and W/σ-model results remain close to the exact expansions.

We then focus on the spread expressions. In Fig. (5.2b) we see that in both models T_{d_2} is much larger than T_L except close to the ground. T_L is therefore the dominant timescale and both models remain close to the exact expansions for $t \ll T_L$ and deviate equally much for larger times dictated by the term $1/3\ t/T_L$ (Fig. (5.3.b)).

This explains why we have been very careful in deriving shorttime expansions. We cannot throw terms away before we know to what turbulence the models are applied, because the relative importance of terms containing T_L or T_d depends on the turbulence considered. We stress here that the requirement of times being small compared to T_L is not always sufficient for the validity of shorttime expansions. Even in cases where T_d is small the deviation caused by this term is not large in either of the models.

We conclude that the shorttime expansions for times smaller than T_L do not force us to conclude that either the model for W or for W/σ is a more correct description of dispersion in inhomogeneous circumstances.

We have discussed the shorttime behaviour of mean particle height and spread. These shorttime expansions only depend on the first two moments of the random forcing in the Langevin model. In the next section we discuss their large time behaviour and show that in this analysis all random forcing moments are involved.

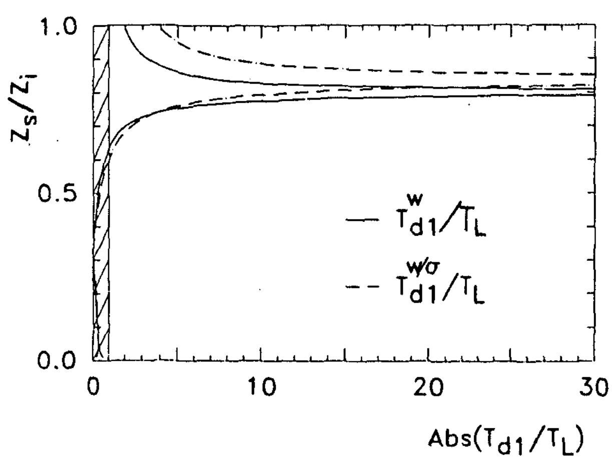

Fig. 5.2a

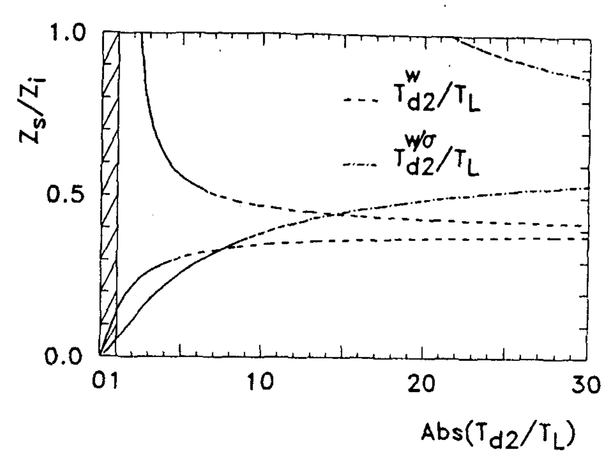

Fig. 5.2b

Fig. 5.2 Ratio of timescales T_d/T_L Eqs. (5.15) involved in shorttime expansions (SE) in convective boundary layer described by (1.4) and (1.18).

a) $T^W_{d_1}/T_L$, ratio of timescales involved in SE of mean height given by model for W

$T^{W/\sigma}_{d_1}/T_L$, ratio of timescales involved in SE of mean height given by model for W/σ

b) $T^W_{d_2}/T_L$, ratio of timescales involved in SE of spread given by model for W,

$T^{W/\sigma}_{d_2}/T_L$, ratio of timescales involved in SE of spread given by model for W/σ

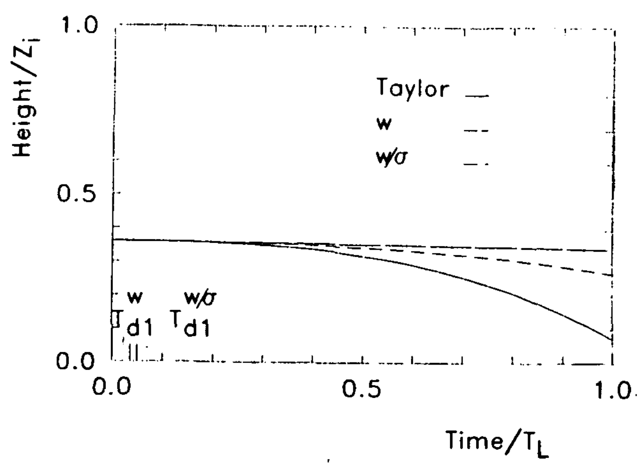

Fig. 5.3a

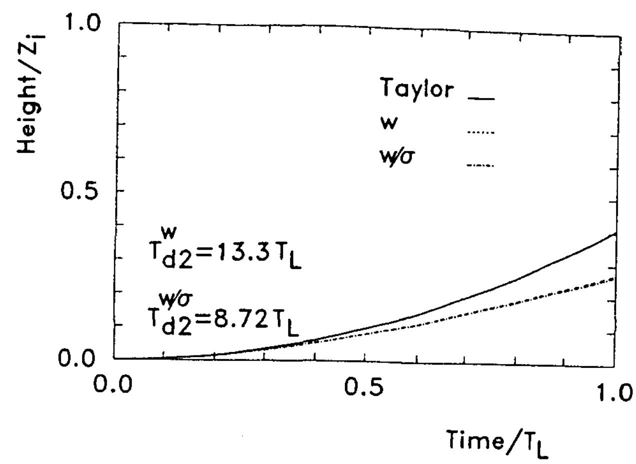

Fig. 5.3b

CONVECTIVE BOUNDARY LAYER

Fig. 5.3 Shorttime expansions mean height $\overline{Z-z_s}$ (Fig. 5.3a) and of $\sigma^2 = \overline{(Z - z_s)^2}$ (Fig. 5.3.b) in a convective boundary layer described by Eq. (1.4) and (1.18) for $z_s/z_i = 0.36$. The exact Taylor expansion Eq. (5.7) is denoted by a solid thick line, the expansions for the models for W and for W/σ Eqs. (5.10) and (5.12) are denoted by resp. a dotted line and a dot-dash line. The inhomogeneity timescales are marked on the time axis or given.

5.4 Large time behaviour of the models

5.4.1 Introduction

A noted difference between the W- and W/σ-models was that, implemented in a computer code, the model for W does not give a uniform concentration distribution in the limit to $t \to \infty$, whereas the model for W/σ does. We want to investigate this large time behavior in this section.

The large time behaviour depends on all moments of the random forcing. In general inhomogeneous turbulence these higher moments are non-zero and this complicates the analysis. Therefore we restrict ourselves to the asymptotic behaviour in Gaussian inhomogeneous turbulence. We must note, however, that turbulence in an inhomogeneous case is usually not Gaussian. In the convective boundary layer e.g. the turbulence velocity is positively skewed. So our treatment must be considered as a first approximation.

In section 5.4.2 we show that both Langevin models for both W and W/σ yield the correct steady state; their KME's have a concentration distribution as solution which is uniform in the steady state. The question remains, however, whether the models also show the correct behaviour leading to this steady state. This large time behaviour is described by Markov limits, which will be discussed in section 5.4.3. The new technique of deriving the Markov limit in inhomogeneous turbulence was introduced in section 2.5, where we derived the Markov Limit for the W-model. We shortly review this derivation and then discuss the derivation for the W/σ-model. Once these Markov limits are derived we investigate whether they describe the above difference between the models in concentration distribution results.

5.4.2 Steady state in inhomogeneous Gaussian turbulence

We start our large time analysis with an investigation of the steady state of the Langevin models for W and W/σ. In inhomogeneous turbulence the Langevin equation can not analytically be solved and a large time expansion of mean particle height and spread can not directly be derived. We therefore start the investigation from the Eulerian equivalents of the Langevin models, the KME's. We show that the restriction to inhomogeneous turbulence which is still Gaussian simplifies the analysis considerably, because in Gaussian turbulence the KME's reduce to a second and third order differential equation.

In Gaussian inhomogeneous turbulence the vertical turbulence velocity u_3 has a Gaussian distribution specified by $\sigma^2 = \overline{u_3^2}$. In section 2.3.7 we showed that in such Gaussian turbulence the random forcing function dμ in the Langevin model for W has a fourth and higher moments that are zero in order dt, while the Langevin model for W/σ has a random forcing dη, whose third and higher moments are zero in order dt (section 5.2). The moments $\langle d\mu^n\rangle = a_n(z)dt$ in Gaussian turbulence are given by Eqs. (5.4) while the moments $\langle (d\eta)^n\rangle = b_n(z)dt$ in Gaussian turbulence are given by Eq. (5.6). The fact that for both models the higher order moments are zero in order dt has some implications, because a distribution function with only the first moments being non zero does not exist. It can easily be shown that a correct (therefore positive) pdf has nonzero even moments, from which follows that the requirements Eqs. (5.4) and (5.6) can not be satisfied by a pdf.

We note that in an application of the models, like we did in Ch. 4 for the W-model, it is usually only required that the first few (e.g. three) moments of the random forcing are modelled correctly. In such an application the generated random forcing has nonzero higher moments which do not satisfy the general equation for the moments. The deviation of the higher moments causes anomalies in the higher moments of particle characteristics (velocity, height). This fact, that the Langevin models cannot meet requirements on the higher moments of the random forcing in inhomogeneous Gaussian turbulence, is considered to be of minor importance when we are only interested in the lower moments of the particle statistics, the mean height, spread and skewness of the concentration distribution.

Accepting these deficiencies of Langevin models we proceed to find their large time behaviour. We derive the KME's of both models by substituting the moments of the random forcing Eqs. (5.4) and (5.6) into the general KME for a bivariate process (Eq. (2.35)).
For the model for W the KME in Gaussian inhomogeneous turbulence reads:

$$\frac{\partial P}{\partial t}(z,w;t) + w\frac{\partial P}{\partial z} = \frac{\partial}{\partial w}\{(\frac{w}{T_L} + \frac{d\sigma^2}{dz})P\} + \frac{\partial^2}{\partial w^2}\{\frac{\sigma^2 P}{T_L}\} - \frac{\partial^3}{\partial w^3}\{\frac{\sigma^2}{2}\frac{d\sigma^2}{dz}P\}. \quad (5.16)$$

For the models for W/σ it reads:

$$\frac{\partial P}{\partial t}(z,w;t) + w\frac{\partial P}{\partial z} = \frac{\partial}{\partial z}\{[\frac{w}{T_L} + \tfrac{1}{2}\frac{\partial\sigma^2}{\partial z}(\frac{w^2}{\sigma^2} + 1)]P\} + \frac{\partial^2}{\partial w^2}\{\frac{\sigma^2}{T_L}P\}. \quad (5.17)$$

We see that the general KME for the model for W and W/σ break off after the third and second term respectively. A real probability distribution, has a KME which is either a Fokker-Planck equation or a differential equation of infinite order (v. Kampen, 1983, p. 280). The model for W does not give either one as a consequence of the formulation of its random forcing function dμ.

In the steady state (in a bounded area) the models should yield a uniform concentration distribution and the probability density of the particle velocities should become equal to that of the turbulence velocities. In Gaussian turbulence the turbulence velocity distribution can be characterized by its moment generating function earlier given in Eq. (2.57) $\hat{g}(\theta) = \exp(-\tfrac{1}{2}\sigma^2\theta^2)\rho$ where $\sigma^2 = \overline{u_3^2}$ and $\rho = \int P(z,u_3)du_3$. The requirements imply that for steady state conditions the pdf of the bivariate process Z, W of the particles should read

$$P(z,w) = (2\pi\sigma^2(z))^{-\frac{1}{2}} \exp(-\frac{w^2}{2\sigma^2(z)}) ; \quad (5.18)$$

then the concentration distribution defined by $C(z,t) = \int P(z,w;t)dw$ is uniform in the steady state and $\langle w^n\rangle = \overline{u_3^n}(z)$. This pdf Eq. (5.18) has to be the steady state of the KME's. By substitution it can be shown that Eq. (5.18) is a solution of both the KME Eqs. (5.16) and (5.17). We conclude that both Langevin models have a KME with a uniform concentration distribution as steady state solution, so that both Langevin models are correct in this respect. In the next section we discuss the large time behaviour leading to this steady state.

5.4.3 Markov limit of the Langevin models and their KME

We are interested in the concentration distribution determined by the Langevin equations for W and for W/σ. This concentration distribution can be determined from the Eulerian equivalent of the Langevin equations, the KME's, which are differential equations describing the time evolution of P(z,w;t). Once we know P(z,w;t), we know P(z;t) via the relation $P(z;t) = \int P(z,w,;t)dW$. Via the fundamental theorem Eq. (1.6) which reads C(z,t) = QP(z;t) we can derive the concentration distribution. Inspection of the KME's Eqs. (5.16) and (5.17) shows, that we cannot simply integrate its terms over dw to get an expression for the whole time evolution of P(z;t). However, the large time behaviour of P(z;t) can be deduced, as we showed in section 2.5 for the W-model. In that section a Lagrangian equation, the Markov limit was derived, describing the large time behaviour of Z(t). Its KME is a large time equation for P(z;t) or the concentration C(z,t). The Markov limit of the W-model was derived for both homogeneous and inhomogeneous turbulence. We shortly review the results for the W-model and in this section we analogously derive the Markov limit for the W/σ-model. We also calculate the Eulerian equivalent of this Markov limit, its KME and compare the large time behaviour of the concentration in both Langevin models.

Model for W

Here we summarize the large time behaviour of the Langevin model for W as derived in section 2.5. For details we refer to this section.

In homogeneous turbulence the limit $T_L \to 0$ is equivalent to the limit $t \to \infty$. The so-derived Markov limit for the model of W in homogeneous turbulence is then given by Eq. (2.71):

$$dZ = (2\sigma^2 T_L)^{1/2} d\omega_t \ ,$$

where with large times are meant times large compared to T_L.

In inhomogeneous turbulence more timescales than only T_L play a role. However, the limit $T_L \to 0$ still describes the behaviour for large times in weakly inhomogeneous Gaussian turbulence under the restriction that while $T_L \to 0$ we let $\sigma^2 \to \infty$ such that the eddy diffusivity K remains the same function of height. The Markov limit is given by Eqs. (2.83) or (2.85):

$$dZ = T_L \, d\mu + \tfrac{1}{2} T_L \frac{dT_L}{dZ} (d\mu)^2 \quad \text{or} \quad dZ = \frac{d(\sigma^2 T_L)}{dz} dt + (2\sigma^2 T_L)^{1/2} d\omega_t .$$

With large times in this case is meant times large compared to T_L but still small compared to the inhomogeneity timescale.

The Markov limit has a KME which is given by Eq. (2.72):

$$\frac{\partial P}{\partial t}(z;t) = \frac{\partial}{\partial z}\left(\sigma^2 T_L \frac{\partial P}{\partial z}\right) .$$

As expected from arguments of Monin & Yaglom (1977, Ch. 10.3) for large times dispersion should be described by a ordinary diffusion equation for its pdf like Eq. (2.80). A schematic summary of the relation between the Langevin equation, the Markov limit and their KME is given in Fig. 2.1 (section 2.5.3).

Model for W/σ

Introduction

We want to derive the large time behaviour of the Langevin equation for W/σ and compare this behaviour with that of the Langevin model for W. The model for W was discussed in section 2.5, where first the large time behaviour for homogeneous turbulence and subsequently for inhomogeneous turbulence was derived. Here we follow the same line in the derivation for the W/σ model.

In inhomogeneous turbulence other timescales than T_L play a role, namely timescales T_i due to the inhomogeneity. We only consider weakly inhomogeneous Gaussian turbulence, where T_i is much larger than T_L. By large times we then mean times large compared to T_L but still small compared to T_i. We can not investigate this large time behaviour by only letting $T_L \to 0$, because this would mean a change in the dispersive character of the turbulence given by the eddy diffusivity $K = \sigma^2 T_L$. We replace the limit $t \to \infty$ by letting the relevant timescale T_L go to zero, modifying σ^2 such that the dispersive character of the turbulence given by the eddy diffusivity $K = \sigma^2 T_L$ remains unchanged (see also section 2.5.1). In this limit goes the turbulence lengthscale $\ell = \sigma^2 T_L$ also to zero. We basically follow Durbin's (1983) derivation for the W/σ-model, but we add the above constraint on the replacement of the limit $t \to \infty$ by the limit $T_L \to 0$. We call the resulting equation, describing the large time behaviour of Z(t), again a Markov limit.

Markov limit and KME of homogeneous Langevin equation for W/σ

We derive the large time behaviour of the Langevin equation for W/σ. The W/σ-model reads (Eq. 5.1a)

$$d(\frac{W}{\sigma}) = -\frac{W}{\sigma}\frac{dt}{T_L} + d\chi \qquad \text{and}$$
$$dZ = W(t)dt. \tag{5.19}$$

In homogenous turbulence the Langevin model for W/σ is equal to the Langevin model for W. The Markov Limit for Gaussian turbulence is thus Eq. (2.71) (See section 2.5.2).

$$dZ = (2\ \sigma^2 T_L)^{\frac{1}{2}}\ d\omega_t\ ,$$

and its KMML is equal to Eq. (2.72)

$$\frac{\partial P}{\partial t}(z;t) = \frac{\partial}{\partial z}(\sigma^2 T_L \frac{\partial P}{\partial z})\ .$$

Markov Limit of inhomogeneous Langevin equation for W/σ

In inhomogeneous turbulence the analysis becomes more complicated by the fact that T_L and σ are functions of height. We formally deal with the inhomogeneity by splitting T_L and σ in a shape factor T(z) resp. S(z) and an amplitude α resp. β so that $T_L(z) = \alpha\ T(z)$ and $\sigma(z) = \beta\ S(z)$. We replace the limit $t \to \infty$ by a rescaling of the turbulence. We rescale the turbulence such that the eddy diffusivity $K(z) = T_L(z)\sigma^2(z)$ remains the same function of z, that is we let $\alpha \to 0$ and $\beta^2 \to \infty$ while $\alpha\beta^2$ = constant.

Putting W/σ = U and multiplying the Langevin equation with α gives

$$\alpha\ dU = -\frac{U(z)}{T(z)}\ dt + \alpha\ d\chi(t)\ . \tag{5.20}$$

Integration of this equation gives

$$\int_o^t (\frac{U(z)}{T(z)}\ dt' - \alpha\ d\chi(t')) = -\ \alpha[U(t)-U(o)]\ . \tag{5.21}$$

The factor U(t)-U(o) is bounded (Durbin, 1983) and the RHS of Eq. (5.21) goes to zero in the limit $\alpha \to 0$. We keep the term on the LHS that contains α, as this term might contain terms that involve $\alpha\beta^2$. These terms remain constant in our limit process.
Subsituting $U(z)dt = \frac{dZ}{\beta\, S(z)}$ in Eq. (5.21) it becomes in the limit:

$$\int_{z_s}^{Z} \frac{dZ'}{T(Z')S(Z')} = \int_{z_s}^{Z} \alpha\beta\, d\chi(Z(t')). \tag{5.22}$$

To differentiate Eq. (5.22) we have to use Itô calculus (see section 2.4). Applying this rule to a general integral

$$\psi = \int_{z_s}^{Z} \frac{dZ'}{A(z')} ,$$

we get

$$d\psi = \frac{dZ}{A(z)} - \tfrac{1}{2}\frac{1}{A^2}\frac{dA}{dz}(dZ)^2 + \frac{1}{6}\left(\frac{2A'^2}{A^3} - \frac{A''}{A^2}\right)(dZ)^3 + \dots , \tag{5.23}$$

where a prime denotes derivation with respect to z.
Using this in differentiating Eq. (5.22) by putting $A(z) = S(z)T(z)$ we get

$$\frac{dZ}{A(z)} - \tfrac{1}{2}\frac{1}{A^2}\frac{dA}{dz}(dZ)^2 + \frac{1}{6}[A''A^{-2} - 2A^{-3}(A')^2](dZ)^3 +.. = \alpha\beta d\chi . \tag{5.24}$$

This is a differential equation for dZ whose solution, the Markov limit, we want to derive. As an illustration we will first solve it for homogeneous turbulence to show that Eq. (5.24) gives indeed the results as discussed above for homogeneous turbulence.

<u>Intermezzo: homogeneous turbulence</u>

In homogeneous turbulence σ and T_L are constant with height and Eq. (5.24) becomes

$$\frac{dZ}{TS} = \alpha\beta\, d\chi \quad \text{or} \quad dZ = T_L\sigma\, d\chi. \tag{5.25a}$$

In homogeneous Gaussian turbulence the random forcing function can be written as $d\chi = (\frac{2}{T_L})^{1/2} d\omega_t$. (From Eq. (5.6) with $\langle(d\chi)^n\rangle = \langle(d\eta)^n\rangle/\sigma^n = b_n dt/\sigma^2$).

The Markov Limit we so derive from the differential equation Eq. (5.25a) reads

$$dZ = T_L \ \sigma \ d\chi = (2\sigma^2 T_L)^{1/2} \ d\omega_t, \tag{5.25b}$$

which is indeed equivalent to the Markov limit for the W-model given by Eq. (2.71) as expected from the fact that in homogeneous turbulence the W and W/σ-model are equivalent.

We already showed in section 2.5.3 that this Markov limit has a KME that is equal to the diffusion equation Eq. (2.72). For future use we show how the diffusion equation can also be derived from Eq. (5.25a). The moments $\langle (dZ)^n \rangle$, that we need in the KME of this Markov limit, are by Eq. (5.25) equal to the averages of powers of $T_L \sigma \ d\chi = T_L d\eta$. The moments of $d\eta$ in order dt are given in Eq. (5.6). In homogeneous Gaussian turbulence only the second moment of $d\eta$ is nonzero.
We have

$$\begin{aligned}
\langle dZ \rangle &= T_L \sigma \langle d\chi \rangle = T_L \langle d\eta \rangle = T_L \ b_1 \ dt = 0 \\
\langle (dZ)^2 \rangle &= T_L^2 \sigma^2 \langle (d\chi)^2 \rangle = T_L^2 \ \langle (d\eta)^2 \rangle = T_L^2 \ b_2 \ dt = 2T_L \sigma^2 dt \qquad (5.26) \\
\langle (dZ)^3 \rangle &= T_L^n \sigma^n \langle (d\chi)^n \rangle = T_L^n \ \langle (d\eta)^n \rangle = T_L^n \ b_n \ dt = 0 \quad \text{for} \quad n \geqq 3 \ .
\end{aligned}$$

We subsitute these moments of dZ in the general KME for a monovariate process Eq. (2.35) and get a KME that is equal to the diffusion equation Eq. (2.72):

$$\frac{\partial P(z;t)}{\partial t} = T_L \sigma^2 \frac{\partial^2 P}{\partial z^2} = \frac{\partial}{\partial z} (\sigma^2 T_L \frac{\partial P}{\partial z}). \tag{5.27}$$

We see that the preliminary equation Eq. (5.24) gives us the correct Markov limit and KME for the W/σ-model in homogeneous circumstances. So far our intermezzo.

Inhomogeneous turbulence

In case T_L and/or σ are a function of z Eq. (5.24) does not always reduce to a simple form which can generally be solved for dZ to give the Markov Limit. However, in Gaussian turbulence it does reduce to a solvable equation In case of Gaussian turbulence we have in order dt from Eq. (5.6) that

$$\langle\sigma d\chi\rangle = \langle d\eta\rangle = \tfrac{1}{2}\frac{d\sigma^2}{dz}\,dt = \sigma\sigma'\,dt \quad \rightarrow \langle d\chi\rangle = \sigma'\,dt\,,$$

$$\langle(\sigma d\chi)^2\rangle = \langle(d\eta)^2\rangle = \frac{2}{T_L(z)}\,\sigma^2\,dt \quad \rightarrow \langle(d\chi)^2\rangle = \frac{2}{T_L(z)}\,dt\,, \qquad (5.28)$$

$$f(\sigma d\chi)^n\rangle = \langle(d\eta)^n\rangle = 0 \quad \rightarrow \langle(d\chi)^n\rangle = 0 \quad \text{for } n \geqq 3\,.$$

We use the fact that the higher moments of $d\chi$ are zero (in order dt) as follows. Taking Eq. (5.24) to the third and higher power and ensemble averaging, we see that this results in a infinite series of equations for the moments $\langle(dZ)^n\rangle$ with $n \geqq 3$, with in the RHS the third and higher moments of $d\chi$ which are equal to zero. Generally this series consist of independent equations and the only solution is that all moments $\langle(dZ)^n\rangle$ with $n \geqq 3$ are zero. From this statistical reasoning we conclude that Eq. (5.24) becomes

$$\frac{dZ}{\sigma T_L} - \frac{1}{2\sigma^2 T_L^2(z)}\,\frac{d(\sigma T_L(z))}{dz}\,(dZ)^2 = d\chi \qquad (5.29)$$

Solving this quadratic equation for dZ we get

$$dZ = \frac{\sigma T_L(z)}{(\sigma T_L)'} - \frac{\sigma T_L}{(\sigma T_L)'}\,(1 - 2(\sigma T_L)'d\chi)^{\frac{1}{2}} \qquad (5.30)$$

where a prime denotes derivation with respect to z.
We can expand the square root in Eq. (5.30) as
$(1 + x)^{\frac{1}{2}} = 1 + \frac{1}{2}x - \frac{1}{8}x^2 + \ldots$
If we can show that the higher order terms in this infinite sum converge to zero, we can approximate the root by breaking off this sum. To prove that the terms indeed converge to zero we use the fact that the third and higher moments of $d\chi$ are zero in order dt (see Eq. 5.28).
(Note that in the derivation for the W-model we had that the third moment of $d\mu$ is nonzero; only in the limit $\alpha \rightarrow 0$ does the third moment of $T_L d\mu$ disappear, which is a weaker statement).

The fact that the third and higher moments of $d\chi$ are zero implies that the third and higher moments of $x = 2(\sigma T_L)'d\chi$ are zero. From these statistical arguments we reason that we can break the expansion of the root $(1 + x)^{1/2}$ off after the quadratic term. The last term in Eq. (5.30) becomes

$$\frac{\sigma T_L}{(\sigma T_L)'}(1 - 2(\sigma T_L)'d\chi)^{1/2} = \frac{\sigma T_L}{(\sigma T_L)'} - (\sigma T_L)d\chi - \tfrac{1}{2}(\sigma T_L)'(\sigma T_L)(d\chi)^2 .$$

Equation (5.30) becomes

$$dZ = \sigma T_L d\chi + \tfrac{1}{2}\frac{d(\sigma T_L)}{dz}\sigma T_L(d\chi)^2 . \tag{5.31}$$

In inhomogeneous Gaussian turbulence $d\chi$ has only two non-zero moments and we can write $d\chi$ as

$$d\chi = \frac{d\sigma}{dz}dt + \left(\frac{2}{T_L}\right)^{1/2} d\omega_t . \tag{5.32}$$

Substituting this into Eq. (5.31) we get the Markov limit of the W/σ-model in inhomogeneous Gaussian turbulence

$$dZ = \frac{d(\sigma^2 T_L)}{\partial z}dt + (2\sigma^2 T_L)^{1/2} d\omega_t . \tag{5.33}$$

Comparing this with Eq. (2.85) we see that also in inhomogeneous Gaussian turbulence the Markov limit of the W/σ-model is equal to the Markov limit of the W-model. It then follows that its KME is also given by the diffusion equation Eq. (2.72).

Conclusions

After investigating the Markov limit of the Langevin models for W and for W/σ, we conclude that they show a large time behaviour which can be described by the diffusion equation. This diffusive behaviour is what we require on physical ground for any dispersion process in both homogeneous and inhomogeneous Gaussian turbulence. The large time behaviour leads to the correct steady state solution, a uniform concentration distribution.

We showed that the constraint on the eddy diffusivity while taking the limit $T_L \to 0$ is necessary to obtain these physically correct results. Only when this constraint is taken into account the analysis yields a large time behaviour, which can be described by the diffusion equation.

Here we come back to the reason why we started the investigation, nl. differences between the two models implemented in computer codes. We found that the difference in large time behaviour (inhomogeneous concentration distributions for the W-model, homogeneous for the W/σ-model) are not due to a theoretical deficiency of the W-model but must be due to differences inherent to the implementation.

5.5 Comparison Langevin models with Eulerian conservation laws

In this section we compare the Lagrangian models for W and W/σ with the Eulerian motion equations to investigate whether differences occur between the two models. Van Dop et al. (1985) made this analysis for the model for W, which study is discussed in section 2.3.6. We make a similar derivation for the model for W/σ.

5.5.1 Model for W/σ

We first derive the KME of the Langevin equation Eq. (5.1b)

$$\frac{dW}{\sigma} = -\frac{W}{\sigma}\frac{dt}{T_L} + d\eta \ ,$$

where T_L and $\langle (d\eta)^n \rangle = b_n dt$ are not yet specified. These variables should be modelled such that the correspondence of the KME with the Eulerian conservation equations is optimal. In the KME we need the moments of dW. These can be derived from this Langevin equation:

$$\langle dW \rangle_w = [-\frac{w}{T_L(z)} + \frac{w^2}{2\overline{u_3^2}(z)}\frac{d\overline{u_3^2}(z)}{dz} + b_1(z)]dt \quad \text{and}$$

$$\langle (dW)^n \rangle_w = b_n(z)dt \qquad \text{for } n \geqq 2. \tag{5.34}$$

Substituting Eq. (5.34) in the general equation for a KME Eq. (2.35) we get the KME of the model for W/σ

$$\frac{\partial P(z,w;t)}{\partial t} + w\frac{\partial P}{\partial z} = \frac{\partial}{\partial w}\left\{\left(\frac{w}{T_L(z)} - \frac{w^2}{2\overline{u_3^2}}\frac{d\overline{u_3^2}}{dz}\right)P\right\} + \sum_{\nu=1}^{\infty}\frac{(-1)^\nu}{\nu!}b_\nu(z)\frac{\partial^\nu P}{\partial w^\nu} \ . \tag{5.35}$$

From this equation we can derive a series of rate equations for the moments $\langle W^n \rangle$ by multiplying the KME with w^n and integrating over w. We use Eq. (2.8) again to obtain the first three moment equations:

$$\frac{\partial C}{\partial t} = -\frac{\partial \overline{u_3 c}}{\partial z} \, , \tag{5.36a}$$

$$\frac{\partial \overline{u_3 c}}{\partial t} = -\frac{\partial \overline{u_3^2 c}}{\partial z} - \overline{u_3^2}\,\frac{\partial C}{\partial z} + \left[b_1 - \tfrac{1}{2}\frac{\partial \overline{u_3^2}}{\partial z}\right] C - \frac{\overline{u_3 c}}{T_L} + \frac{1}{2\overline{u_3^2}}\frac{\partial \overline{u_3^2}}{\partial z}\,\overline{u_3^2 c} \quad \text{and} \tag{5.36b}$$

$$\frac{\partial \overline{u_3^2 c}}{\partial t} = -\frac{\partial \overline{u_3^3 c}}{\partial z} - \overline{u_3^3}\,\frac{\partial C}{\partial z} + \overline{u_3^2}\,\frac{\partial \overline{u_3 c}}{\partial z} + 2\overline{u_3 c}\,\frac{\partial \overline{u_3^2}}{\partial z} - 2\overline{u_3 c}\left(\frac{\partial \overline{u_3^2}}{\partial z} - b_1\right)$$

$$+ \left[b_2 - \frac{2\overline{u_3^2}}{T_L} - \frac{\partial \overline{u_3^3}}{\partial z} - \frac{\partial \overline{u_3^2}}{\partial t} + \frac{\overline{u_3^3}}{\overline{u_3^2}}\frac{\partial \overline{u_3^2}}{\partial z}\right] C - \frac{2\overline{u_3^2 C}}{T_L} + \frac{1}{\overline{u_3^2}}\frac{\partial \overline{u_3^2}}{\partial z}\,\overline{u_3^3 c} \, . \tag{5.36c}$$

To get the third term on the RHS of Eq. (5.36c) use is made of Eq. (5.36a).

The first moment equation Eq. (5.36a) is equivalent to the first Eulerian conservation equation Eq. (2.49a). The higher order Eqs. (5.36b) and (5.36c) are in stationary turbulence only equivalent to the Eulerian conservation Eqs. (2.49b) and (2.49c) when b_1 and b_2 are described by Eqs. (5.6) and when in addition it is assumed that

$$\overline{c\frac{du_3}{dt}} = -\frac{\overline{u_3 c}}{T_L} + \frac{1}{2\overline{u_3^2}}\frac{d\overline{u_3^2}}{dz}\,\overline{u_3^2 c} \quad \text{and} \tag{5.37a}$$

$$\overline{(u_3 c)\left(\frac{du_3}{dt}\right)'} = -\frac{\overline{u_3^2 c}}{T_L} + \tfrac{1}{2}\frac{d\overline{u_3^2}}{dz}\left[\frac{\overline{u_3^3 c}}{\overline{u_3^2}} - \overline{u_3 c}\right]. \tag{5.37b}$$

Note, that in assuming b_1 to be described by Eq. (5.6), the 5th term on the RHS of Eq. (5.37c) does not cancel. This term contributes to Eq. (5.37b).

The Langevin model for W and for W/σ give different closures expressed in the assumptions Eqs. (2.51) and (5.37). These relations will now be examined. From the equations of motion we can obtain an exact expression for these correlations. Neglecting buoyancy, molecular and Coriolis forces the equations of motion yield

$$\overline{c\frac{du_3}{dt}} = -\frac{1}{\rho}\,\overline{c\frac{\partial p}{\partial z}} \tag{5.38a}$$

$$\overline{(u_3c)(\frac{du_3}{dt})'} = -\frac{1}{\rho}\overline{u_3c\frac{\partial p}{\partial z}} \ . \qquad (5.38b)$$

Deardorff (1978) presented closures for the Eulerian equation of motion for dispersion from a single source in homogeneous turbulence (see section 2.3.7), which read

$$\frac{1}{\rho}\overline{\frac{c\partial p}{\partial z}} = \frac{\overline{u_3c}}{T_L} \quad \text{and} \quad \frac{1}{\rho}\overline{u_c c\frac{\partial p}{\partial z}} = \frac{\overline{u_3^2c}}{T_L} \ .$$

These equations imply that the assumptions Eqs. (2.51) for the Langevin model for W are consistent with Deardorff's closure relations, whereas, the assumptions Eqs. (5.37) for the Langevin model for W/σ are more involved. Even with a Gaussian assumption on the third and fourth order correlations, that is $\overline{u_3^2c} = 0$ and $\overline{u_3^3c} = 3\overline{u_3^2}\ \overline{u_3c}$, the W/σ-closures still read

$$\overline{\frac{cdu_3}{dt}} = -\frac{1}{\rho}\overline{c\frac{\partial p}{\partial z}} = -\frac{\overline{u_3c}}{T_L} \quad \text{and} \qquad (5.39a)$$

$$\overline{u_3c(\frac{du_3}{dt})'} = -\frac{1}{\rho}\overline{u_3c\frac{\partial p}{\partial z}} = -\frac{\overline{u_3^2c}}{T_L} + \tfrac{1}{4}\,\overline{u_3c}\,\frac{\partial\overline{u_3^2}}{\partial z} \ . \qquad (5.39b)$$

Extra terms appear with respect to Deardorff's closure relations, which have no obvious interpretation.

5.5.2 Discussion

From the comparison of the Langevin models with the exact Eulerian equations we conclude, that the model for W corresponds better with the Eulerian conservation equations. We base this on the fact that the closures in the W-model Eqs. (2.51) have some justification as discussed by Van Dop et al. (1985). This is supported by Deardorff, who stated that these relations are exactly valid in Eulerian models in the restricted case of particles released at a particular time in homogeneous turbulence. On the contrary, do the closures of the W/σ-model not have an obvious interpretation.

5.6 Conclusions from the comparison of the W- and W/σ-model

Dispersion models based on the Langevin equation are simple in use and can easily be adapted to different atmospheric conditions. Two Langevin models are often used in the literature, the model for W and the model for W/σ.

The short time behaviour of mean height and variance of the particles in the model for both W and W/σ are investigated and shown to be equal to the exact Taylor expansions in a first approximation valid for times smaller than all timescales involved. In homogeneous turbulence the only timescale involved is T_L but in inhomogeneous turbulence these timescales are T_L and T_d, a timescale imposed by the turbulence. Usually the shorttime analysis interest only exists for times smaller than T_L. In case T_L is smaller than the timescale T_d imposed by the turbulence further investigation into the validity of the shorttime expansion is not necessary. In that case is the shorttime expansion always valid for the times of interest t small compared to T_L. In situations where T_d is smaller than T_L on the other hand, we have to be careful because times smaller than T_L can be larger than T_d. For these times the models start to deviate from the exact Taylor expansions in a rate, depending strongly on the turbulence values of T_L, $\overline{u_3^2}$ and $\overline{u_3^3}$ and their derivatives at source height. The conclusion is that shorttime expansions in the Langevin models can only be said to be valid for $t < T_L$ in case T_L is the smallest timescale involved. If T_d is the smallest timescale the expansions for both models are different from each other and from the exact Taylor expansions for $t < T_L$. However, in an application to the convective boundary layer these deviations are shown not to be so large that a distinction in the performance of the models can be made based on the short time expansions.

The large time behaviour of both Langevin models, in homogeneous as well as in inhomogeneous Gaussian turbulence, is shown to be physically correct. They both yield a large time behaviour described by the ordinary diffusion equation. This is indeed confirmed by the study of Wilson et al. (1983) who show large time results of the correct W- and W/σ-Langevin equation for inhomogeneous Gaussian turbulence and results of the diffusion equation with $K = \sigma^2 T_L$ (see section 3.6.2) and both models lead to a uniform steady state concentration in a bounded area. The fact that our computer model for the Langevin model for W gave a steady state concentration distribution which decreased near the boundaries must be due to other (numerical) facts.

Comparing the Langevin models for W and for W/σ with the Eulerian conservation laws shows that the model for W corresponds best. This leads to the final conclusion that the Langevin model for W is theoretical superior to the Langevin model for W/σ and its practical application should be investigated further.

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Curriculum Vitae

Anne Francisca de Baas werd geboren op 12 april 1957 te Driebergen-Rijsenburg. Na het behalen van het Atheneum-B diploma aan het Eindhovens Protestants Lyceum studeerde zij Technische Natuurkunde aan de Technische Hogeschool Eindhoven, maar stapte over naar de Rijks Universiteit Utercht waar zij doctoraal examen in de geologie en geofysica, hoofdrichting meteorologie deed op 25 juni 1983.

De Nederlandse stichting zuiver wetenschappelijk onderzoek gaf haar gelegenheid tot een driejarig promotie-onderzoek op het KNMI onder begeleiding van prof. Schuurmans en drs. Nieuwstadt en van Dop afgerond met dit proefschrift.

Sinds 1 september 1987 is zij aangesteld als wetenschappelijk onderzoeker op de afdeling Meteorologie en Windenergie van het nationale onderzoeksinstituut Risø te Roskilde, Denemarken.

EIGENSCHAPPEN VAN HET LANGEVINMODEL VOOR VERSPREIDING

Anne F. de Baas

Samenvatting:
De Langevin-vergelijking wordt gebruikt voor het beschrijven van verontreinigingverspreiding in de atmosfeer. De teoretische achtergrond voor de vergelijking wordt uitgebreid bediscussieerd en een overzicht over eerdere verhandelingen en toepassingen gegeven.
We tonen aan dat de Langevin-vergelijking verspreiding in complexe omstandigheden kan beschrijven. In het bijzonder verspreiding in een convectieve atmosferische grenslaag, waar het de metingen nauwkeurig reproduceert.

Twee vormen van de Langevin-vergelijking, die beide worden gebruikt in praktische toepassingen, worden vergeleken en de conclusie is dat, in termen van hun teoretische eigenschappen, ze niet erg verschillend zijn, ondanks belangrijke verschillen in praktische toepassingen.

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Some properties of the Langevin model for dispersion

Anne F. de Baas

Date January 1988

Department or group

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Abstract (Max. 2000 char.)

The Langevin equation is used to describe dispersion of pollutants in the atmosphere. The theoretical background for the equation is discussed in length and a review on previous treatments and applications is given. It is shown that the Langevin equation can describe dispersion in complex circumstances. In particular the equation is applied to dispersion in a convective boundary layer, where it reproduced the measurements accurately.

Two forms of the Langevin equation, which have both been used in practical applications, are compared and it is concluded that in terms of their theoretical properties, they are not very different in spite of important differences in practical application.

Descriptors – EDB

BOUNDARY LAYERS; DIFFUSION; LAGRANGE EQUATIONS; LANGEVIN EQUATIONS; LEVELS; METEOROLOGY; MONTE CARLO METHOD; POLLUTANTS; RANDOMNESS; STOCHASTIC PROCESSES; TURBULENT FLOW; VELOCITY; WIND

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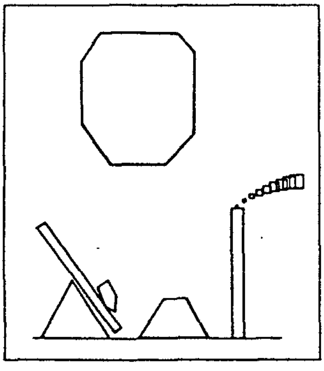

inspired by B. van der Lek

1

Variance measurements can lead to large overestimates of dispersion because such transporting and nontransporting mechanisms as turbulence and waves contribute to the variance.

Anne F. de Baas and A.G.M. Driedonks (1985)
Internal gravity waves in a stably stratified boundary layer,
BLM, **31**, p. 303.

2

For the mean flow in complex terrain the spectral methods are extremely powerful because they allow simple scale-dependent closures that are easy to understand.

Ib Troen and Anne F. de Baas (1986)
A spectral diagnostic model for wind flow simulation in complex terrain. Proceedings of EWEC'86 European Wind Energy Association, Conference and Exhibition, Rome.

3

The turbulence quantities in flow over hills cannot be modeled unless anisotropy is taken into account.

Otto Zeman and Niels Otto Jensen (1987)
Modification of turbulence characteristic in flow over hills.
Quart. J. Roy. Met. Soc., **113**, *55-80.*

4

Some simple equations are hard to analyze without powerful computers (e.g. the Langevin equation and the Lorentz equation).

5

Even if a model adequately describes the empirical data, we still may not regard the problem as solved until we have established a complete theory correctly argued from basic principles.

6

Geophysical years sometimes harvest their fruits around thirty years after.

7

Fuzzy transform: what is fuzzy in clear space is clear in fuzzy space and vice versa.

8

The average result of a random differential equation differs at random from the result of the average differential equation.

9

It it scandalous that 250 years after women first entered universities the need is still felt to make statements on feminism. Here is my own: the little chance for promotion for women often leads to the result that women excel men in the same organizational position.

19 January 1988
Anne F. de Baas