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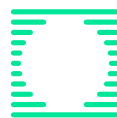
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A random walk model for turbulent diffusion  
*Ein Lagrange-Modell für turbulente Diffusion*

Lutz Janicke

August/*August* 2000



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# A random walk model for turbulent diffusion

Lutz Janicke

August 2000

## Abstract

An algorithm of a random walk model is presented that is not restricted to time steps small with respect to the smallest Lagrangian correlation time. The correct relation for the drift velocity under these circumstances is derived. The increased value of the time step makes it possible in many cases to perform the dispersion calculation within a shorter time or with higher accuracy.

In addition, an empirical expression for the drift velocity is given that is also valid for a spatially varying time step. The algorithm described is implemented in the Lagrangian dispersion model LASAT.



# 1 Introduction

Random walk models are used for the calculation of the turbulent diffusion of tracers in the atmosphere. The atmospheric transport is determined by the following quantities:

- $\mathbf{V}(\mathbf{x})$  : Vector of the mean wind velocity
- $\mathbf{\Sigma}(\mathbf{x})$  : Tensor of the wind fluctuations
- $\mathbf{K}(\mathbf{x})$  : Diffusion tensor

The wind field  $\mathbf{V}(\mathbf{x})$  can be assumed to be incompressible, i.e.  $\nabla \cdot \mathbf{V} = 0$ .

A random walk model treats a cloud of tracer material as a collection of many individual particles and calculates the dispersion of the cloud by following the trajectories of these particles. Here, the action of the turbulence on the movement of the particles is simulated by a random process. All particles are moving independently.

Two basic types of algorithms for calculating the particle trajectories can be distinguished (for simplicity only the one-dimensional case is considered):

- Simulation of classical diffusion

During a time step  $\tau$  a particle is moved by the wind field  $V$  and displaced in addition by a random amount  $x_r$ ,

$$x_{\text{new}} = x_{\text{old}} + \tau V + x_r.$$

The displacement  $x_r$  is chosen at random and statistically independent for each time step. This algorithm simulates the behaviour of colliding molecules changing their flight direction with each collision at random.

- Simulation of turbulent diffusion

In the case of turbulent diffusion the role of molecular collisions is played by turbulent eddies. Here, the process of a “collision” takes a rather long time. Accordingly, the particles have a velocity  $u$  representing the wind fluctuations within the turbulence and this velocity  $u$  is changed slowly by a random process. The time scale of the change is the Lagrangian correlation time  $T$ . Therefore, the path of a particle is generated by the following algorithm:

$$\begin{aligned} u_{\text{new}} &= (1 - \tau/T)u_{\text{old}} + u_r, \\ x_{\text{new}} &= x_{\text{old}} + \tau V + \tau u_{\text{new}}. \end{aligned}$$

As a rule, the time step  $\tau$  has to be small with respect to the Lagrangian correlation time  $T$ . The velocity change  $u_r$  is chosen at random and statistically independent for each time step.

Turbulent diffusion studied on a time scale that is large with respect to the Lagrangian correlation time shows a behaviour similar to that of classical diffusion, because on this time scale the action of an eddy on a particle takes a short time and is therefore comparable to a collision process.

The problem in defining a Lagrangian model consists in the difficulty to specify the parameters of the random process in such a way that exactly the prescribed situation is



simulated. In particular, the task is to correctly specify the first and second moment of the random number distribution, i.e. mean value and variance, as functions of  $\mathbf{V}$ ,  $\Sigma$  and  $\mathbf{K}$ .

## 2 The algorithm

We will discuss the algorithm implemented in the Lagrangian dispersion model LASAT (Lagrangian Simulation of Aerosol Transport).<sup>1,2,3</sup> For the present a constant time step  $\tau$  is used and all quantities are computed for the times  $t_n = n\tau$ . If at time  $t_n$  a particle is located at position  $\mathbf{x}_n$  with a velocity  $\mathbf{u}_n$ , then position and velocity at time  $t_{n+1}$  are calculated using the following algorithm:

$$\mathbf{u}_{n+1} = \Psi(\mathbf{x}_n) \cdot \mathbf{u}_n + \mathbf{W}(\mathbf{x}_n) + \Lambda(\mathbf{x}_n) \cdot \mathbf{R}, \quad (1)$$

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \tau[\mathbf{V}(\mathbf{x}_n) + \mathbf{u}_{n+1}]. \quad (2)$$

Note, that the mean wind velocity  $\mathbf{V}$  is not part of the particle velocity  $\mathbf{u}$  in this formulation but is rather added as a separate term in equation (2) to calculate the new particle position. The model parameters to be determined are  $\Psi$ ,  $\mathbf{W}$  and  $\Lambda$ . The components of the vector  $\mathbf{R}$  are random numbers chosen with a probability density  $p(\mathbf{R})$ . Here, we use a normal distribution. Because mean value and variance are effectively set by  $\mathbf{W}$  and  $\Lambda$ , we can restrict  $p$  by the following conditions:

$$\int p(\mathbf{R}) d^3\mathbf{R} = 1, \quad (3)$$

$$\int \mathbf{R} p(\mathbf{R}) d^3\mathbf{R} = \overline{\mathbf{R}} = 0, \quad (4)$$

$$\int \mathbf{R}\mathbf{R} p(\mathbf{R}) d^3\mathbf{R} = \overline{\mathbf{R}\mathbf{R}} = \mathbf{I}. \quad (5)$$

## 3 The density distribution in phase space

In the following, only a single time step from  $t = 0$  to  $t = \tau$  is considered. In order to simplify the notation, position and velocity before the time step (at  $t = 0$ ) are denoted by  $\hat{\mathbf{x}}$  and  $\hat{\mathbf{u}}$ , respectively, values during the time step (for  $0 < t \leq \tau$ ) by  $\mathbf{x}(t)$  and  $\mathbf{u}$ . If only a single particle is considered, the suffix p is used. Therefore, the algorithm can be written in the following way:

$$\mathbf{u}_p = \Psi(\hat{\mathbf{x}}) \cdot \hat{\mathbf{u}} + \mathbf{W}(\hat{\mathbf{x}}) + \Lambda(\hat{\mathbf{x}}) \cdot \mathbf{R}, \quad (6)$$

$$\mathbf{x}_p(t) = \hat{\mathbf{x}} + t[\mathbf{V}(\hat{\mathbf{x}}) + \mathbf{u}_p]. \quad (7)$$

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<sup>1</sup>L. Janicke: Particle simulation of inhomogeneous turbulent diffusion, *in*: "Air Pollution Modeling And Its Application II", C. de Wispelaere, ed., Plenum Press, New York, p. 527 (1983).

<sup>2</sup>L. Janicke: Particle simulation of dust transport and deposition and comparison with conventional models, *in*: "Air Pollution Modeling And Its Application IV", C. de Wispelaere, ed., Plenum Press, New York, p. 759 (1985).

<sup>3</sup>L. Janicke: The embedding of the Lagrangian dispersion model LASAT into a monitoring system for nuclear power plants, *in*: "Air Pollution Modeling And Its Application X", S-V. Gryning and M.M. Millán, eds., Plenum Press, New York, p. 405 (1994).



A particle has a point like shape and its density  $n_p$  is given by Dirac's delta-function<sup>4</sup>

$$n_p(\mathbf{x}, t; \hat{\mathbf{x}}, \hat{\mathbf{u}}, \mathbf{R}) = \delta(\mathbf{x} - \mathbf{x}_p(t)). \quad (8)$$

The density is a function of position  $\mathbf{x}$  and time  $t$  and depends parametrically on the starting values  $\hat{\mathbf{x}}$  and  $\hat{\mathbf{u}}$  and the chosen random number  $\mathbf{R}$ . In phase space with coordinates  $\hat{\mathbf{x}}$  and  $\hat{\mathbf{u}}$ , the density is

$$f_p(\mathbf{x}, \mathbf{u}, t; \hat{\mathbf{x}}, \hat{\mathbf{u}}, \mathbf{R}) = \delta(\mathbf{x} - \mathbf{x}_p(t)) \delta(\mathbf{u} - \mathbf{u}_p). \quad (9)$$

Consider a group of particles, all starting from the same position  $(\hat{\mathbf{x}}, \hat{\mathbf{u}})$  in phase space but with different random vectors  $\mathbf{R}$  chosen according to the probability density  $p(\mathbf{R})$ . The particle density in phase space is given by

$$f(\mathbf{x}, \mathbf{u}, t; \hat{\mathbf{x}}, \hat{\mathbf{u}}) = \int f_p(\mathbf{x}, \mathbf{u}, t; \hat{\mathbf{x}}, \hat{\mathbf{u}}, \mathbf{R}) p(\mathbf{R}) d^3\mathbf{R}. \quad (10)$$

Now let the particles start from different positions and with different velocities. If their distribution density at time  $t = 0$  is  $f(\hat{\mathbf{x}}, \hat{\mathbf{u}}, 0)$ , then the distribution density at time  $t$  is given by

$$f(\mathbf{x}, \mathbf{u}, t) = \int f_p(\mathbf{x}, \mathbf{u}, t; \hat{\mathbf{x}}, \hat{\mathbf{u}}, \mathbf{R}) f(\hat{\mathbf{x}}, \hat{\mathbf{u}}, 0) p(\mathbf{R}) d^3\mathbf{R} d^3\hat{\mathbf{x}} d^3\hat{\mathbf{u}}, \quad (11)$$

$$= \int f(\hat{\mathbf{x}}, \hat{\mathbf{u}}, 0) p(\mathbf{R}) \delta(\mathbf{x} - \hat{\mathbf{x}} - t[\mathbf{V}(\hat{\mathbf{x}}) + \mathbf{u}]) \delta(\mathbf{u} - \mathbf{S}(\hat{\mathbf{x}}, \hat{\mathbf{u}}, \mathbf{R})) d^3\mathbf{R} d^3\hat{\mathbf{x}} d^3\hat{\mathbf{u}}, \quad (12)$$

with the abbreviation

$$\mathbf{S}(\hat{\mathbf{x}}, \hat{\mathbf{u}}, \mathbf{R}) = \Psi(\hat{\mathbf{x}}) \cdot \hat{\mathbf{u}} + \mathbf{W}(\hat{\mathbf{x}}) + \Lambda(\hat{\mathbf{x}}) \cdot \mathbf{R}. \quad (13)$$

This equation describes how a cloud of particles develops during the period  $0 < t \leq \tau$  if each particle is moved by the algorithm in equations (6) and (7).

The algorithm uses the parameters  $\mathbf{V}$ ,  $\mathbf{W}$ ,  $\Psi$ , and  $\Lambda$ . However, the system to be simulated is described by  $\mathbf{V}$ ,  $\Sigma$  and  $\mathbf{K}$ . The task of the following sections is to derive a relation between these quantities.

## 4 The drift velocity

An important step is to determine the drift velocity  $\mathbf{W}(\mathbf{x})$  that is added to the given wind field  $\mathbf{V}(\mathbf{x})$ . It prohibits the accumulation of particles in regions of low turbulence. It guarantees that a uniform distribution of particles remains uniform. Let us assume that the system is in such a uniform state, hence  $f(\mathbf{x}, \mathbf{u}, \tau) = f(\mathbf{x}, \mathbf{u}, 0)$  and  $n(\mathbf{x}, \tau) = n(\mathbf{x}, 0) = \text{const}$ . In the following we study what restrictions on the model parameters are posed by this requirement.

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<sup>4</sup> $\delta(\mathbf{x}) = \delta(x_1)\delta(x_2)\delta(x_3)$  for a vector  $\mathbf{x}$  with components  $x_1$ ,  $x_2$  and  $x_3$ .  $\int f(x)\delta(x) dx = f(0)$  for an arbitrary function  $f(x)$  if the origin is within the interval of integration, otherwise the integral has the value 0.



The calculation becomes much simpler if the random vector  $\mathbf{R}$  is replaced by the variable  $\mathbf{S}$  with a corresponding probability density  $q(\mathbf{x}, \mathbf{u}, \mathbf{S})$ . The mean value of a quantity  $X(\mathbf{u}, \mathbf{S})$  with respect to the distribution density  $g(\mathbf{x}, \mathbf{u}, \mathbf{S})$ ,

$$g(\mathbf{x}, \mathbf{u}, \mathbf{S}) = f(\mathbf{x}, \mathbf{u}, 0) q(\mathbf{x}, \mathbf{u}, \mathbf{S}), \quad (14)$$

is defined as

$$\bar{X}(\mathbf{x}) = \frac{\int X(\mathbf{x}, \mathbf{u}, \mathbf{S}) g(\mathbf{x}, \mathbf{u}, \mathbf{S}) d^3\mathbf{u} d^3\mathbf{S}}{\int g(\mathbf{x}, \mathbf{u}, \mathbf{S}) d^3\mathbf{u} d^3\mathbf{S}}. \quad (15)$$

The mean value of  $\mathbf{S}$  for example becomes

$$\bar{\mathbf{S}} = \frac{1}{n} \int (\boldsymbol{\Psi} \cdot \mathbf{u} + \mathbf{W} + \boldsymbol{\Lambda} \cdot \mathbf{R}) g(\mathbf{x}, \mathbf{u}, \mathbf{S}) d^3\mathbf{u} d^3\mathbf{S}, \quad (16)$$

$$= \boldsymbol{\Psi} \cdot \bar{\mathbf{u}} + \mathbf{W}. \quad (17)$$

Using these variables, equation (12) can be written for  $t = \tau$  as

$$f(\mathbf{x}, \mathbf{u}, \tau) = \int g(\hat{\mathbf{x}}, \hat{\mathbf{u}}, \mathbf{S}) \delta(\mathbf{x} - \hat{\mathbf{x}} - \tau[\mathbf{V} + \mathbf{u}]) \delta(\mathbf{u} - \mathbf{S}) d^3\mathbf{S} d^3\hat{\mathbf{x}} d^3\hat{\mathbf{u}}. \quad (18)$$

From this equation, we derive momentum equations (with respect to  $\mathbf{u}$ ) and expand the right hand side for small values of  $\tau$ . To be more precise about the meaning of “small”, we define a characteristic velocity  $u_0$  and a characteristic length  $l_0$  and require

$$\varepsilon = \tau u_0 / l_0 \ll 1. \quad (19)$$

The expansion uses the following ordering scheme:

$$\mathbf{V} = O(u_0), \quad (20)$$

$$\boldsymbol{\Sigma} = O(u_0^2), \quad (21)$$

$$\mathbf{K} = O(l_0 u_0), \quad (22)$$

$$\boldsymbol{\Psi} = O(1), \quad (23)$$

$$\boldsymbol{\Lambda} = O(u_0), \quad (24)$$

$$\mathbf{W} = O(\varepsilon u_0), \quad (25)$$

$$|\mathbf{u}| = O(u_0), \quad (26)$$

$$\bar{\mathbf{u}} = O(\varepsilon u_0). \quad (27)$$

Terms with spatial derivatives of the form  $\tau \mathbf{u} \cdot \nabla$  are also of order  $\varepsilon$ . Using in addition the abbreviation

$$\mathbf{S}^* = \mathbf{V} + \mathbf{S}, \quad (28)$$



the second moment of equation (18) reads to lowest order:

$$\int \mathbf{u} \mathbf{u} f(\mathbf{x}, \mathbf{u}, \tau) d^3 \mathbf{u} = n(\mathbf{x}, \tau) \overline{\mathbf{u}(\mathbf{x}, \tau) \mathbf{u}(\mathbf{x}, \tau)}, \quad (29)$$

$$= \int \mathbf{u} \mathbf{u} g(\hat{\mathbf{x}}, \hat{\mathbf{u}}, \mathbf{S}) \delta(\mathbf{x} - \hat{\mathbf{x}} - \tau[\mathbf{V} + \mathbf{u}]) \delta(\mathbf{u} - \mathbf{S}) d^3 \mathbf{S} d^3 \hat{\mathbf{u}} d^3 \hat{\mathbf{x}} d^3 \mathbf{u}, \quad (30)$$

$$= \int \mathbf{S} \mathbf{S} g(\hat{\mathbf{x}}, \hat{\mathbf{u}}, \mathbf{S}) \delta(\mathbf{x} - \hat{\mathbf{x}} - \tau \mathbf{S}^*) d^3 \mathbf{S} d^3 \hat{\mathbf{u}} d^3 \hat{\mathbf{x}}, \quad (31)$$

$$= \int \mathbf{S} \mathbf{S} g(\mathbf{x} - \tau \mathbf{S}^*, \hat{\mathbf{u}}, \mathbf{S}) d^3 \mathbf{S} d^3 \hat{\mathbf{u}}, \quad (32)$$

$$= \int \mathbf{S} \mathbf{S} g(\mathbf{x}, \hat{\mathbf{u}}, \mathbf{S}) d^3 \mathbf{S} d^3 \hat{\mathbf{u}} + O(\varepsilon u_0^2). \quad (33)$$

The mean value  $\overline{\mathbf{S} \mathbf{S}}$  is needed to lowest order only,

$$\overline{\mathbf{S} \mathbf{S}} = \overline{\Psi \cdot \mathbf{u} \Psi \cdot \mathbf{u}} + \overline{\Lambda \cdot \mathbf{R} \Lambda \cdot \mathbf{R}} + O(\varepsilon^2 u_0^2), \quad (34)$$

$$= \Psi \cdot \overline{\mathbf{u} \mathbf{u}} \cdot \Psi^\top + \Lambda \cdot \Lambda^\top, \quad (35)$$

and we get

$$n(\mathbf{x}, \tau) \overline{\mathbf{u}(\mathbf{x}, \tau) \mathbf{u}(\mathbf{x}, \tau)} = n(\mathbf{x}, 0) (\Psi \cdot \overline{\mathbf{u} \mathbf{u}} \cdot \Psi^\top + \Lambda \cdot \Lambda^\top). \quad (36)$$

For the steady state considered we assume that the velocity variance of the particles  $\overline{(\mathbf{u} - \overline{\mathbf{u}})(\mathbf{u} - \overline{\mathbf{u}})}$  equals the velocity variance of the atmospheric turbulence  $\Sigma$ . Then we have

$$\overline{\mathbf{u} \mathbf{u}} = \Sigma + \overline{\mathbf{u}} \overline{\mathbf{u}}, \quad (37)$$

$$= \Sigma + O(\varepsilon^2 u_0^2). \quad (38)$$

Furthermore, using  $\overline{\mathbf{u}(\mathbf{x}, \tau) \mathbf{u}(\mathbf{x}, \tau)} = \overline{\mathbf{u}(\mathbf{x}, 0) \mathbf{u}(\mathbf{x}, 0)}$  and  $n(\mathbf{x}, \tau) = n(\mathbf{x}, 0)$ , we get from equation (36)

$$\Sigma = \Psi \cdot \Sigma \cdot \Psi^\top + \Lambda \cdot \Lambda^\top. \quad (39)$$

If  $\Psi$  is known then  $\Lambda$  can be calculated from  $\Sigma - \Psi \cdot \Sigma \cdot \Psi^\top$  by a Cholesky decomposition.

Retaining only terms up to first order, the first moment of equation (18) yields:

$$\int \mathbf{u} f(\mathbf{x}, \mathbf{u}, \tau) d^3 \mathbf{u} = n(\mathbf{x}, \tau) \overline{\mathbf{u}(\mathbf{x}, \tau)}, \quad (40)$$

$$= \int \mathbf{S} g(\hat{\mathbf{x}}, \hat{\mathbf{u}}, \mathbf{S}) \delta(\mathbf{x} - \hat{\mathbf{x}} - \tau \mathbf{S}^*) d^3 \mathbf{S} d^3 \hat{\mathbf{u}} d^3 \hat{\mathbf{x}}, \quad (41)$$

$$= \int \mathbf{S} [g - \tau \mathbf{S}^* \cdot \nabla g] d^3 \mathbf{S} d^3 \hat{\mathbf{u}} + O(\varepsilon^2 u_0), \quad (42)$$

$$= n[\overline{\mathbf{S}} - \tau \nabla \cdot \overline{\mathbf{S}^* \mathbf{S}}], \quad (43)$$

$$= n[\overline{\mathbf{S}} - \tau \nabla \cdot \overline{\mathbf{S} \mathbf{S}}] + O(\varepsilon^2 u_0). \quad (44)$$

Using equations (17), (35), (38), and (39), we get

$$\overline{\mathbf{u}} = \Psi \cdot \overline{\mathbf{u}} + \mathbf{W} - \tau \nabla \cdot \Sigma. \quad (45)$$



It is not correct to assume that  $\bar{\mathbf{u}}$  vanishes, arguing for example that in a steady state no mean particle velocities are allowed, because they would disturb the uniform density, thereby introducing a time dependence into the system. Here, a steady state only means that at time  $t = \tau$  the system is in the same state as at time  $t = 0$ . Because all particles change their velocities at exactly these times — the random processes are synchronized — the density may change in between. Hence, the time derivative of the density may be different from zero and, as a consequence, the equation of continuity may yield a non vanishing flux.

Including terms up to second order, integrating equation (18) with respect to  $\mathbf{u}$  yields:

$$\int f(\mathbf{x}, \mathbf{u}, \tau) d^3\mathbf{u} = n(\mathbf{x}, \tau), \quad (46)$$

$$= \int g(\hat{\mathbf{x}}, \hat{\mathbf{u}}, \mathbf{S}) \delta(\mathbf{x} - \hat{\mathbf{x}} - \tau\mathbf{S}^*) d^3\mathbf{S} d^3\hat{\mathbf{u}} d^3\hat{\mathbf{x}}, \quad (47)$$

$$= \int [g - \tau\mathbf{S}^* \cdot \nabla g + \frac{1}{2}\tau^2(\mathbf{S}^* \cdot \nabla)^2 g] d^3\mathbf{S} d^3\hat{\mathbf{u}}, \quad (48)$$

$$= n(\mathbf{x}, 0) - \tau\nabla \cdot (n\overline{\mathbf{S}^*}) + \frac{1}{2}\tau^2\nabla\nabla \cdot (n\overline{\mathbf{S}^*\mathbf{S}^*}), \quad (49)$$

With  $n(\mathbf{x}, \tau) = n(\mathbf{x}, 0) = \text{const}$  we get

$$\nabla \cdot (\overline{\mathbf{S}^*} - \frac{1}{2}\tau\nabla \cdot \overline{\mathbf{S}^*\mathbf{S}^*}) = 0. \quad (50)$$

Using  $\nabla \cdot \mathbf{V} = 0$ , we have

$$\nabla \cdot \overline{\mathbf{S}^*} = \nabla \cdot (\mathbf{V} + \Psi \cdot \bar{\mathbf{u}} + \mathbf{W}), \quad (51)$$

$$= \nabla \cdot (\Psi \cdot \bar{\mathbf{u}} + \mathbf{W}), \quad (52)$$

$$= \nabla \cdot \overline{\mathbf{S}}, \quad (53)$$

$$\tau\nabla \cdot \overline{\mathbf{S}^*\mathbf{S}^*} = \tau\nabla \cdot (\mathbf{V}\mathbf{V} + \mathbf{V}\overline{\mathbf{S}} + \overline{\mathbf{S}}\mathbf{V} + \overline{\mathbf{S}\mathbf{S}}), \quad (54)$$

$$= \tau\nabla \cdot (\mathbf{V}\mathbf{V} + \Sigma) + O(\varepsilon^2 u_0). \quad (55)$$

Equation (50) can be satisfied if

$$\overline{\mathbf{S}} = \frac{1}{2}\tau\nabla \cdot \overline{\mathbf{S}^*\mathbf{S}^*} \quad (56)$$

or

$$\Psi \cdot \bar{\mathbf{u}} + \mathbf{W} = \frac{1}{2}\tau\nabla \cdot (\mathbf{V}\mathbf{V} + \Sigma). \quad (57)$$

By adding this equation to equation (45) we get

$$\bar{\mathbf{u}} = \frac{1}{2}\tau\nabla \cdot (\mathbf{V}\mathbf{V}) - \frac{1}{2}\tau\nabla \cdot \Sigma, \quad (58)$$

and inserting this into equation (57) yields

$$\mathbf{W} = \frac{1}{2}\tau(\mathbf{I} + \Psi) \cdot (\nabla \cdot \Sigma) + \frac{1}{2}\tau(\mathbf{I} - \Psi) \cdot (\mathbf{V} \cdot \nabla \mathbf{V}). \quad (59)$$

The second term on the right hand side has a special meaning, because it is retained even if the random walk of the particles is switched off. Its meaning becomes clear if we look



at the way the particle trajectory is calculated without any random walk ( $\Psi = 0$ ,  $\Lambda = 0$ ). Then the algorithm reads

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \tau[\mathbf{V}(\mathbf{x}_n) + \mathbf{W}(\mathbf{x}_n)]. \quad (60)$$

Each piece of the trajectory starts tangential to the local flow line. If the flow line is bent, the particle is displaced systematically away from the flow line. A more accurate way to follow the flow line would be to use a velocity averaged over the path of the particle during the time step instead of simply the value at the starting point  $\mathbf{x}_n$ . Alternatively, the velocity at the particle position in the middle of the time step can be used, i.e. at  $\mathbf{x}_n + \frac{1}{2}\tau\mathbf{V}$ . Using a Taylor expansion of  $\mathbf{V}(\mathbf{x})$  around the point  $\mathbf{x}_n$ ,

$$\mathbf{V}(\mathbf{x}_n + \frac{1}{2}\tau\mathbf{V}) = \mathbf{V}(\mathbf{x}_n) + \frac{1}{2}\tau\mathbf{V}\cdot\nabla\mathbf{V} + O(\varepsilon u_0), \quad (61)$$

we get to lowest order exactly the term calculated before for the drift velocity  $\mathbf{W}(\mathbf{x}_n)$ . Therefore, the second term in equation (59) may be omitted if the advection along  $\mathbf{V}(\mathbf{x})$  is calculated more accurate than to first order. For time steps small with respect to the Lagrangian correlation time, this term may also be dropped, because in this case we have  $\Psi \approx \mathbf{I}$  as will be shown later on.

## 5 The equation of diffusion

The parameters  $\Lambda$  and  $\mathbf{W}$  are given by equations (39) and (59). Only  $\Psi$  remains to be determined. For this purpose we consider a particle cloud after it has dispersed for a time period large with respect to the Lagrangian correlation time. Then it can be described by the equation of classical diffusion. We assume that the density gradients of the cloud are so small that the ordering scheme described before may be applied as well to the gradient of  $n(\mathbf{x})$ .

Again we use the momentum equations but now without the assumption of  $n$  being constant. The fluxes produced by the density gradients are small and from equation (33) we get as before to lowest order

$$\int \mathbf{u}\mathbf{u}f(\mathbf{x}, \mathbf{u}, \tau) d^3\mathbf{u} \approx n(\mathbf{x}, \tau) \Sigma(\mathbf{x}). \quad (62)$$

Equation (42) now reads

$$n(\mathbf{x}, \tau) \overline{\mathbf{u}(\mathbf{x}, \tau)} = \int \mathbf{S}[g - \tau\mathbf{S}^* \cdot \nabla g] d^3\mathbf{S} d^3\hat{\mathbf{u}}, \quad (63)$$

$$= n\Psi \cdot \bar{\mathbf{u}} + n\mathbf{W} - n\tau\nabla \cdot \Sigma - \tau\Sigma \cdot \nabla n + O(\varepsilon^2 u_0), \quad (64)$$

and we get for  $\bar{\mathbf{u}}$

$$n\bar{\mathbf{u}} = (\mathbf{I} - \Psi)^{-1} \cdot (n\mathbf{W} - n\tau\nabla \cdot \Sigma - \tau\Sigma \cdot \nabla n). \quad (65)$$

In equation (49), the particle density  $n$  no longer drops out. With

$$\frac{n(\mathbf{x}, \tau) - n(\mathbf{x}, 0)}{\tau} \approx \frac{\partial n(\mathbf{x}, t)}{\partial t} \quad (66)$$



we now get

$$\frac{\partial n}{\partial t} = \nabla \cdot \left[ -n\mathbf{V} - n\boldsymbol{\Psi} \cdot \bar{\mathbf{u}} - n\mathbf{W} + \frac{1}{2}n\tau \nabla \cdot (\mathbf{V}\mathbf{V} + \boldsymbol{\Sigma}) + \frac{1}{2}\tau(\mathbf{V}\mathbf{V} + \boldsymbol{\Sigma}) \cdot \nabla n \right]. \quad (67)$$

The drift velocity  $\mathbf{W}$  has been determined in such a way that the expression  $-n\boldsymbol{\Psi} \cdot \bar{\mathbf{u}} - n\mathbf{W} + \frac{1}{2}n\tau \nabla \cdot (\mathbf{V}\mathbf{V} + \boldsymbol{\Sigma})$  vanishes for constant  $n$ . Therefore, this expression reduces after inserting  $n\bar{\mathbf{u}}$  from equation (65) to the term containing the gradient of  $n$  and we get

$$\frac{\partial n}{\partial t} + \mathbf{V} \cdot \nabla n = \nabla \cdot \left[ \tau \boldsymbol{\Psi} \cdot (\mathbf{I} - \boldsymbol{\Psi})^{-1} \cdot \boldsymbol{\Sigma} \cdot \nabla n + \frac{1}{2}\tau(\mathbf{V}\mathbf{V} + \boldsymbol{\Sigma}) \cdot \nabla n \right], \quad (68)$$

$$= \nabla \cdot \left\{ \tau \left[ \boldsymbol{\Psi} \cdot (\mathbf{I} - \boldsymbol{\Psi})^{-1} + \frac{1}{2}\mathbf{I} \right] \cdot \boldsymbol{\Sigma} \cdot \nabla n \right\} + \frac{1}{2}\tau \nabla \cdot (\mathbf{V}\mathbf{V} \cdot \nabla n). \quad (69)$$

The last term represents again the error of a first order algorithm for the case of an inhomogeneous wind field and will not be considered further in the following. The remaining terms form a diffusion equation:

$$\frac{\partial n}{\partial t} + \mathbf{V} \cdot \nabla n = \nabla \cdot (\mathbf{K} \cdot \nabla n), \quad (70)$$

$$\mathbf{K} = \tau \left[ \boldsymbol{\Psi} \cdot (\mathbf{I} - \boldsymbol{\Psi})^{-1} + \frac{1}{2}\mathbf{I} \right] \cdot \boldsymbol{\Sigma}. \quad (71)$$

If the diffusion tensor  $\mathbf{K}$  is represented as

$$\mathbf{K} = \boldsymbol{\Phi}^{-1} \cdot \boldsymbol{\Sigma}, \quad (72)$$

then

$$\boldsymbol{\Phi}^{-1} = \tau \left[ \boldsymbol{\Psi} \cdot (\mathbf{I} - \boldsymbol{\Psi})^{-1} + \frac{1}{2}\mathbf{I} \right]. \quad (73)$$

Using the identity

$$\boldsymbol{\Psi} \cdot (\mathbf{I} - \boldsymbol{\Psi})^{-1} = -\mathbf{I} + (\mathbf{I} - \boldsymbol{\Psi})^{-1} \quad (74)$$

we get

$$\boldsymbol{\Psi} = (\mathbf{I} + \frac{1}{2}\tau\boldsymbol{\Phi})^{-1} \cdot (\mathbf{I} - \frac{1}{2}\tau\boldsymbol{\Phi}), \quad (75)$$

$$= (\mathbf{I} - \frac{1}{2}\tau\boldsymbol{\Phi}) \cdot (\mathbf{I} + \frac{1}{2}\tau\boldsymbol{\Phi})^{-1}, \quad (76)$$

$$= \frac{\mathbf{I} - \frac{1}{2}\tau\boldsymbol{\Phi}}{\mathbf{I} + \frac{1}{2}\tau\boldsymbol{\Phi}}. \quad (77)$$

The formulation in form of a fraction is possible, because it makes no difference whether the inverse term is multiplied from the left or from the right side.

For the one-dimensional case, we get the diffusion coefficient by multiplying the variance of the velocity fluctuations  $\sigma^2$  by the Lagrangian correlation time  $T$ ,

$$K = T\sigma^2. \quad (78)$$

Therefore, for the three-dimensional case, the tensor  $\boldsymbol{\Phi}$  represents the reciprocal of the Lagrangian correlation times. If the time step  $\tau$  is small with respect to the Lagrangian correlation times,  $\|\tau\boldsymbol{\Phi}\| \ll 1$ , equation (77) can be expanded with the result

$$\boldsymbol{\Psi} \approx \mathbf{I} - \tau\boldsymbol{\Phi} \quad \text{for} \quad \|\tau\boldsymbol{\Phi}\| \ll 1. \quad (79)$$

For the one-dimensional case, this reduces to

$$\Psi \approx 1 - \tau/T \quad \text{for} \quad \tau/T \ll 1. \quad (80)$$



## 6 Summary

If the mean wind field  $\mathbf{V}(\mathbf{x})$ , the tensor of the wind velocity fluctuations  $\mathbf{\Sigma}(\mathbf{x})$ , and the diffusion tensor  $\mathbf{K}(\mathbf{x})$  are given, then for constant time step  $\tau$  the parameters  $\mathbf{W}$ ,  $\mathbf{\Lambda}$  and  $\mathbf{\Psi}$  of the random walk model are given by

$$\mathbf{\Psi} = \frac{\mathbf{I} - \frac{1}{2}\tau\mathbf{\Phi}}{\mathbf{I} + \frac{1}{2}\tau\mathbf{\Phi}} \quad \text{with} \quad \mathbf{\Phi} = \mathbf{\Sigma} \cdot \mathbf{K}^{-1}, \quad (81)$$

$$\mathbf{W} = \frac{1}{2}\tau(\mathbf{I} + \mathbf{\Psi}) \cdot (\nabla \cdot \mathbf{\Sigma}), \quad (82)$$

$$\mathbf{\Lambda} \cdot \mathbf{\Lambda}^T = \mathbf{\Sigma} - \mathbf{\Psi} \cdot \mathbf{\Sigma} \cdot \mathbf{\Psi}^T. \quad (83)$$

A basic requirement for the derivation of these equations was the condition that the time step  $\tau$  did not vary in space. However, for some applications it is desirable to have a time step that can be adapted to spatially varying dispersion conditions. It is not difficult to replace the constant factor  $\tau$  by a function  $\tau(\mathbf{x})$  in equations (81) and (82). However, regarding equation (82) the question arises whether this function has to be differentiated together with the tensor  $\mathbf{\Sigma}$  or not.

Empirical results are available for two special cases:

- Small time step

If everywhere the time step  $\tau(\mathbf{x})$  is small with respect to the Lagrangian correlation times  $T_i$ , then  $\|\tau\mathbf{\Phi}\| \ll 1$  and therefore  $\mathbf{\Psi} \approx \mathbf{I}$ . Experiments show that the relation derived above for constant  $\tau$  also yields correct results in this case,

$$\mathbf{W}(\mathbf{x}) = \tau(\mathbf{x})\nabla \cdot \mathbf{\Sigma}(\mathbf{x}).$$

- Classical diffusion

We assume that all Lagrangian correlation times are equal and the tensor  $\mathbf{\Phi}$  is diagonal. Then  $\mathbf{\Phi}$  can be written as  $\mathbf{\Phi} = \frac{1}{T}\mathbf{I}$ . If the time step is set to twice the Lagrangian correlation time,  $\tau(\mathbf{x}) = 2T(\mathbf{x})$ , then  $\mathbf{\Psi} = 0$  and we get the algorithm for classical diffusion. Tests show that in this case  $\mathbf{W}(\mathbf{x})$  has to be chosen as

$$\mathbf{W}(\mathbf{x}) = \frac{1}{2}\nabla \cdot [\tau(\mathbf{x})\mathbf{\Sigma}(\mathbf{x})] = \nabla \cdot \mathbf{K}.$$

Both empirical findings are reproduced by the following relation:

$$\mathbf{W}(\mathbf{x}) = \frac{1}{2}[\mathbf{I} - \mathbf{\Psi}(\mathbf{x})] \cdot \{\nabla \cdot [\tau(\mathbf{x})\mathbf{\Sigma}(\mathbf{x})]\} + \tau(\mathbf{x})\mathbf{\Psi}(\mathbf{x}) \cdot [\nabla \cdot \mathbf{\Sigma}(\mathbf{x})]. \quad (84)$$

This relation is used in LASAT and has successfully been tested, but an exact theoretical derivation has not yet been found.