

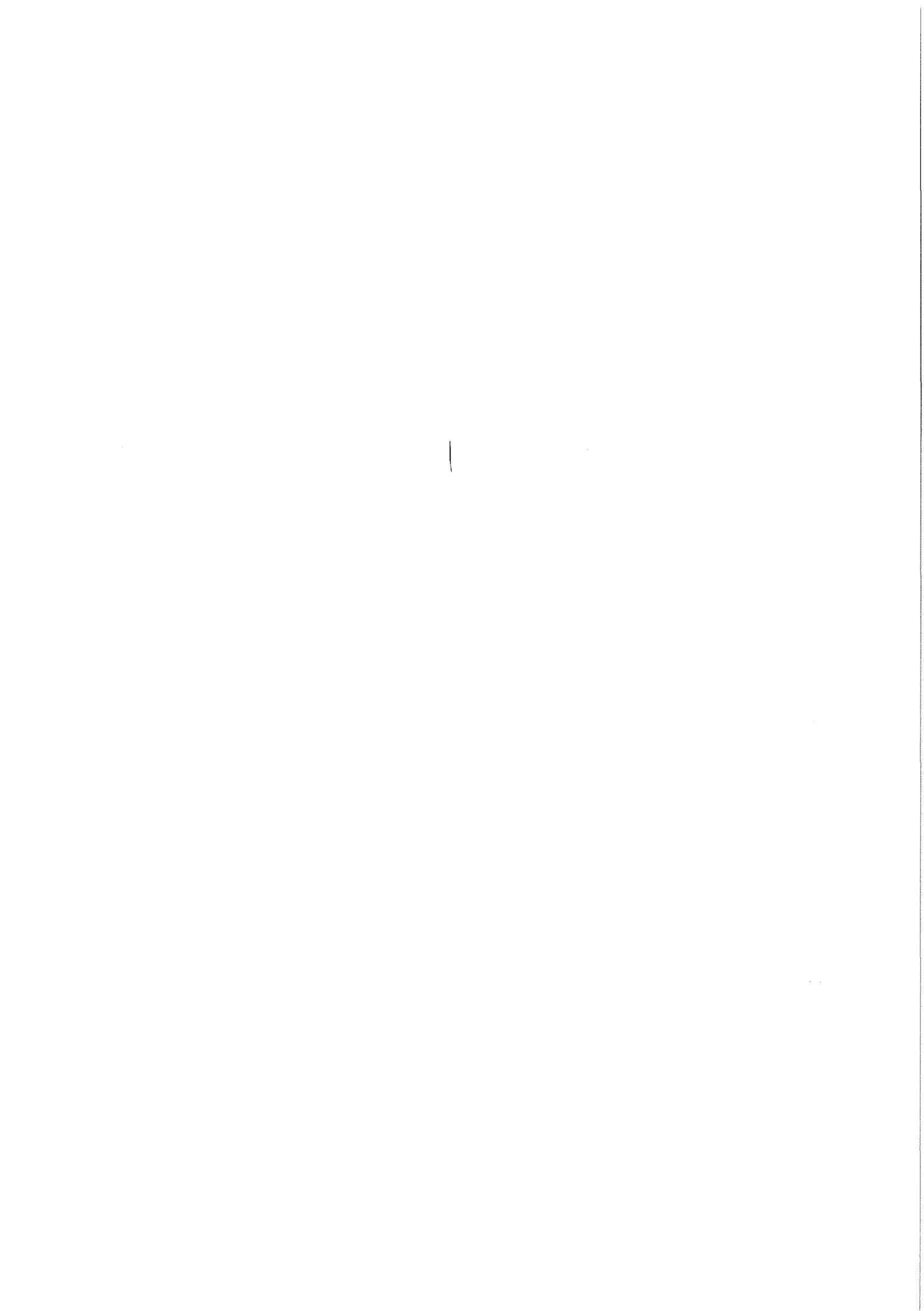
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# **The Lagrangian Particle Model Traveling Version 92/3**

## **Model Description and Users' Guide**

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**Energie- und Stoffumsetzungen in der Umwelt**

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KERNFORSCHUNGSZENTRUM KARLSRUHE

Institut für Meteorologie und Klimateforschung  
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**THE LAGRANGIAN PARTICLE MODEL TRAVELING  
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## **Abstract**

The report describes the standard version of the Lagrangian particle model TRAVELING to simulate the transport and dilution of airborne material in inhomogeneous terrain. The model is part of a mesoscale model system available at the Institute for Meteorology and Climatology of the Nuclear Research Centre Karlsruhe and the University of Karlsruhe to model the mesoscale atmospheric flow and dispersion over complex terrain.

In the report the well-known model fundamentals are repeated. The numerical procedures to calculate the concentration distributions and the meaning of each module of the model are described. The user's guide helps to understand the structure of the necessary meteorological input data, explains the user defined input data which control a specific simulation and describes the output data generated by the model.

In the Appendix the TRAVELING/COSYMA version is briefly described. This version has been developed to apply TRAVELING in connection with the accident consequence assessment code COSYMA.

## **Das Lagrange-Partikelmodell TRAVELING Version 92/3 Modellbeschreibung und Benutzeranleitung**

### **Zusammenfassung**

Der Bericht beschreibt die Standardversion des Lagrange-Partikelmodells TRAVELING. Das Modell simuliert den Transport und die Verdünnung von luftgetragenen Stoffen über inhomogenem Gelände. Das Modell ist Teil eines mesoskaligen Modellsystems, das am Institut für Meteorologie und Klimaforschung (IMK) des Kernforschungszentrums Karlsruhe (KfK) und der Universität Karlsruhe zur Verfügung steht, um mesoskalige Strömungen und Ausbreitungsprozesse über komplexem Gelände zu modellieren.

Im Bericht werden zunächst die bekannten Modellgrundlagen wiederholt. Numerische Methoden zur Berechnung der Konzentrationsverteilungen und die Inhalte der einzelnen Module des Modells werden beschrieben. Die Benutzeranleitung hilft die Struktur der meteorologischen Eingabedaten zu verstehen, erläutert die vom Benutzer zu spezifizierenden Eingabeparameter, die eine spezielle Simulation kontrollieren, und beschreibt die vom Modell erzeugten Ausgabedaten.

Im Anhang wird kurz die Modellversion TRAVELING/COSYMA beschrieben. Sie wurde entwickelt, um TRAVELING auch im Zusammenhang mit dem Unfallfolgenmodell COSYMA anwenden zu können.

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## 1. INTRODUCTION

Lagrangian particle modelling (or random walk modelling as it is also called) of atmospheric dispersion has been widely investigated and exploited during the last decade. The method is based on Taylor's theory [1] who studied the case of one-dimensional dispersion in stationary and homogeneous turbulence. The dispersion is described by tracking a number of individual particles each carrying an amount of mass of airborne pollutants. Each particle moves according to prescribed mean wind conditions and to turbulent motion by random velocity fluctuations. The turbulent fluctuations can be generated by a Markov chain relation if the timestep,  $\Delta t$ , is chosen to be much less than the Lagrangian time scale,  $T_L$ , [2]. The Markov chain model is based on the assumption that the turbulent velocities at successive timesteps are correlated.

$$v(t + \Delta t) = R(\Delta t) v(t) + r(t)$$

The correlation is described by the Lagrangian autocorrelation function,  $R(\Delta t)$ .  $r(t)$  is a random variable with mean zero and standard deviation  $\sigma_r$ . For example, Hall [2] showed that the correlation function can be approximated by

$$R(\Delta t) = \exp(-\Delta t/T_L)$$

If it is assumed that the velocity at any time depends only on the velocity during the previous step, and if  $\Delta t \ll T_L$ , a form which has also been adopted by Taylor in his original work [1]. Applying this model, Hall [2] simulated observational concentration profiles and cloud heights under neutral and unstable conditions with reasonable agreement.

Already Smith [3] suggested the linear Markov chain model to investigate theoretically the conditioned particle motion in a homogeneous turbulent field. He tested the validity of the Markov assumption using a particular data set of geostrophic trajectories in the mid-latitude troposphere. His analysis also suggested a method for obtaining the Lagrangian time scale from measurements of diffusion.

Similar to Hall, Reid [4] modelled the vertical dispersion in the neutral surface layer treating elevated as well as surface releases. His results showed the importance of the Lagrangian time scale and its vertical variation.

Gifford [5] derived a Lagrangian-dynamical theory of horizontal diffusion in the atmosphere and he demonstrated an excellent fit of his solution for the mean square particle displacement to atmospheric horizontal diffusion data. This fit was not only good for diffusion times very much less and very much larger than the Lagrangian time scale but also through the broad middle range of times corresponding to distances from a few hundred meters to several hundred kilometers.

Wilson et al. [6], [7], [8] and Legg and Raupach [9] extended the random walk modelling of atmospheric dispersion to inhomogeneous flows. In addition to vertical variations of the time scale, they also considered changes of the vertical velocity variance with height,  $\sigma_w = \sigma_w(z)$ , which happens, for example, within vegetation canopies or in an unstable

stratified surface layer. Wilson et al. employed a coordinate transformation which converted a trajectory in inhomogeneous turbulence to a corresponding trajectory in homogeneous turbulence [6]. To avoid physically unrealistic concentration distribution in the case of a height dependent vertical velocity variance they added a vertical bias velocity which is proportional to the gradient of  $\sigma_w$ . The procedure was successful for slowly varying gradients in  $\sigma_w$  but failed if  $\sigma_w$  changed rapidly, for example within a corn canopy ([7]). Legg and Raupach [9] showed that if  $\sigma_w$  is not constant with height there exists an associated pressure gradient which appears as a force-like term in the Markov equation. A simulation using the modified equation demonstrated that a uniform concentration profile is preserved.

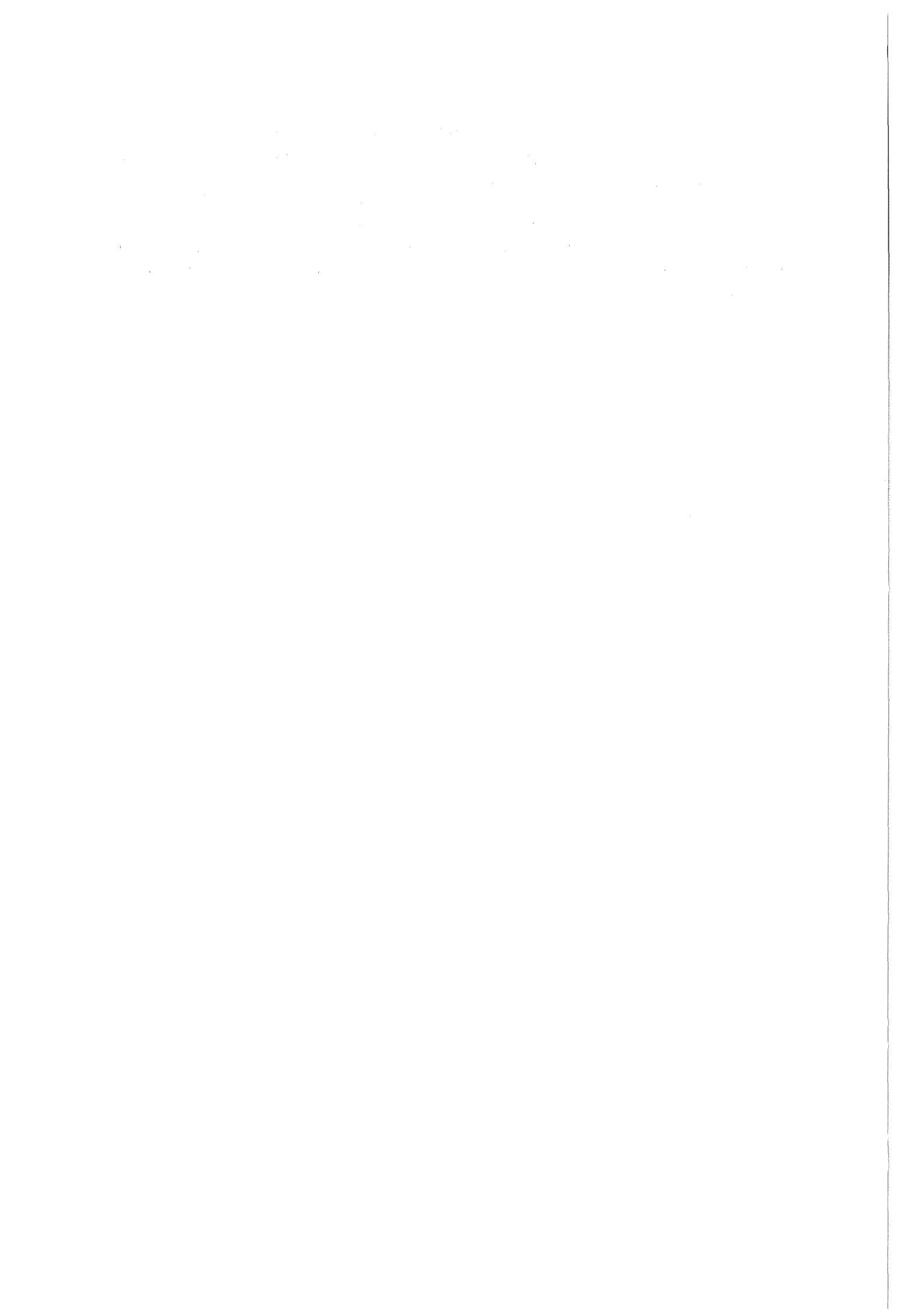
The model TRAVELING (TRAnsport und VErdünnung von Luftbeimengungen in INhomogenem Gelände; in Engl.: Transport and Dilution of Airborne Material in Inhomogeneous Terrain) which is presented in this report uses the same fundamental concepts and equations as Legg and Raupach [9] in their model. It has been developed by H. Vogel [10] to study concentration distributions in the presence of a mesoscale flow over irregular terrain. Although the model equations have been already derived in [10] and [11], they are repeated in Chapter 2 of this report for reasons of completeness. The user's guide starts with Chapter 3 which describes the numerical procedures to calculate the concentrations. Chapter 4 describes each module of the model, the necessary meteorological and user defined input data and the output generated by the model. In addition, an example of a complete lineprinter output is given.

TRAVELING is part of a mesoscale model system available at the Institut für Meteorologie and Klimaforschung (IMK) of the Nuclear Research Centre Karlsruhe (KfK) and the University of Karlsruhe to simulate the atmospheric flow and dispersion over complex terrain. The system consists of the non-hydrostatic mesoscale flow model KAMM (Karlsruhe Atmospheric Mesoscale Model) [12], [13], the Eulerian dispersion model DRAIS (Dreidimensionales Regionales Ausbreitungs- und Immissions-Simulationsmodell) and the TRAVELING model.

Both dispersion models use the wind and turbulence fields generated by the mesoscale flow model KAMM as input data. By this procedure they are working with three-dimensional atmospheric data which are varying in space and time and which are inherently consistent at any point in space and at any time. In contrast to this, most Lagrangian particle models developed and published recently use three-dimensional mass-consistent wind fields and derive the turbulence parameters from empirical formulas, e.g. those summarized by Hanna [14]. With such a procedure spatial and temporal consistency of the meteorological data is not guaranteed.

The model system mentioned above has been applied successfully in a variety of atmospheric dispersion studies. Vogel et al. [15] and Nester et al. [16] compared simulated and measured concentration and dry deposition fields of SO<sub>2</sub> over the state of Baden-Württemberg (F.R.G.) using DRAIS and TRAVELING. Applying the TRAVELING model the transport and the dispersion of airborne releases after the SANDOZ accident have been simulated [17]. Nester and Vogel [18] calculated the dispersion of radioactive

material over structured terrain with the TRAVELING model and demonstrated the applicability of a Lagrangian particle model under meteorological conditions as they can prevail over inhomogeneous and complex terrain. Panitz and Nester [19] performed a validation study using the hydrodynamic model KAMM and the particle model TRAVELING. The comparison between simulated and measured observations showed, in general, a good agreement. But the study also demonstrated that the quality of a numerical dispersion experiment strongly depends on the quality of the simulated flow and turbulence fields which are the necessary input for the dispersion model.



## 2. MODEL FUNDAMENTALS

The present model is similar to that of Legg and Raupach [9]. For reason of completeness the derivation of the governing equations is repeated.

The Lagrangian dispersion model TRAVELING calculates the three-dimensional concentration distributions after a release by tracking a large number of particles. The location of an individual particle at time  $t + \Delta t$  is given by

$$\vec{r}_i(t + \Delta t) = \vec{r}_i(t) + \vec{v}_i(t)\Delta t \quad (2.1)$$

where  $\vec{r}_i$  is the location of the  $i$ -th particle,  $\vec{v}_i$  is its velocity, and  $\Delta t$  is the timestep.

The velocity is splitted into a mean part  $\vec{\bar{v}}_i$  and a fluctuating part  $\vec{v}'_i$ :

$$\vec{v}_i = \vec{\bar{v}}_i + \vec{v}'_i \quad (2.2)$$

Assuming that the mean flow field is known from a wind field model or a mesoscale atmospheric model the remaining task is to determine the turbulent velocity field,  $\vec{v}'_i$ .

Without loss of generality, the following derivation will be restricted to the vertical velocity component,  $w = \bar{w} + w'$ . For convenience, the index  $i$  for the  $i$ -th particle will be omitted.

### 2.1 Integration of the Langevin Equation

Markov-chain simulations of particle trajectories are based on the Langevin equation of motion.

$$\frac{dw}{dt} = -\alpha w + \lambda \bar{x}_i(t) \quad (2.3)$$

$w(t)$  is the vertical velocity component of a particle and  $\alpha$  and  $\lambda$  are coefficients which will be specified below.  $x_i(t)$  is a Gaussian white noise which is a stationary stochastic process with a Gaussian probability density function, a mean of zero and a covariance of

$$\overline{x_i(s)x_i(t)} = \delta(t - s) \quad (2.4)$$

$\delta$  is the Dirac delta function and the overbar denotes an ensemble average over many realizations of the stochastic process. The Langevin equation Eq. (2.3) has been studied in connection with the Brownian motion. It describes the motion of a particle which experiences a viscous resistance proportional to the relative velocity of fluid and particle (first term on the right hand side of the equation), and a random acceleration due to turbulent fluctuations of the fluid (second term on the right hand side).

Eq. (2.3) is a stochastic differential equation which can be solved like an ordinary first-order linear differential equation applying the method of variation of constants (see for example [20]).

The solution of the homogeneous equation

$$\frac{dw}{dt} + \alpha w = 0$$

is

$$w(t) = Ce^{-\alpha t}, \quad C = \text{const.}$$

A general solution of the inhomogeneous equation can be found in the following manner: substitution of constant  $C$  of the solution of the homogeneous equation by function  $C = C(t)$ , so that  $C(t) e^{-\alpha t}$  solves the inhomogeneous equation.

$$\frac{dw}{dt} + \alpha w = \left( \frac{dC}{dt} - \alpha C(t) + \alpha C(t) \right) e^{-\alpha t} = \frac{dC}{dt} e^{-\alpha t} = \lambda x_i(t)$$

Integration yields

$$C(t) = \lambda \int_0^t e^{\alpha s} x_i(s) ds + C_0$$

Substitution into the solution of the homogeneous equation with  $C = C(t)$  gives the general solution of Eq. (2.3)

$$w(t) = w(0)e^{-\alpha t} + \lambda \int_0^t e^{\alpha(s-t)} x_i(s) ds \quad (2.5)$$

with  $w(t=0) = w(0) = C_0$ . Eq. (2.5) defines the velocity  $w(t)$  of a particle as a random process.  $w(t)$  consists of two parts. The first part on the right hand side of Eq. (2.5) depends on the random initial velocity  $w(0)$ . It vanishes if  $t\alpha \gg 1$ , the particle has forgotten its initial state. The second component in Eq. (2.5) results in a large number of random impulses due to the turbulence. It is independent of  $w(0)$  because the random acceleration is independent of velocity.

The mean of  $w(t)$  is calculated as the ensemble average of Eq. (2.5)

$$\overline{w(t)} = \overline{w(0)}e^{-\alpha t}. \quad (2.6)$$

The fluctuation about this mean ( $w' = w - \overline{w}$ ) is

$$w'(t) = w'(0)e^{-\alpha t} + \lambda \int_0^t e^{\alpha(s-t)} x_i(s) ds \quad (2.7)$$

Now the variance  $\overline{w'^2(t)}$  and the covariance  $\overline{w'(0)w'(t)}$  of  $w(t)$  can be determined. Because  $x_i$  and  $w'$  are uncorrelated the variance is

$$\overline{w'^2(t)} = \overline{w'^2(0)e^{-2\alpha t}} + \lambda^2 \int_0^t \int_0^t e^{\alpha(s-t)} e^{\alpha(u-t)} \overline{x_i(s)x_i(u)} ds du \quad (2.8)$$

which can be written, using Eq. (2.4) as

$$\overline{w'^2(t)} = \overline{w'^2(0)e^{-2\alpha t}} + \lambda^2 \int_0^t e^{2\alpha(s-t)} ds$$

Evaluation of the integral gives

$$\overline{w'^2(t)} = \overline{w'^2(0)e^{-2\alpha t}} + \frac{\lambda^2}{2\alpha} (1 - e^{-2\alpha t}) \quad (2.9)$$

The covariance follows directly from Eq. (2.7)

$$\overline{w'(0)w'(t)} = \overline{w'^2(0)e^{-\alpha t}} \quad (2.10)$$

The coefficients  $\alpha$  and  $\lambda$  can now be expressed in terms of measurable velocity statistics of the particle. If the Lagrangian time scale,  $T_L$ , for the particle's velocity is defined as

$$T_L = \frac{\int_0^\infty \overline{w'(0)w'(t)} dt}{\overline{w'^2(0)}}$$

then it follows from Eq. (2.10)

$$\alpha = \frac{1}{T_L} \quad (2.11)$$

Assuming that  $w(t)$  is a random stationary process, then  $\overline{w'^2(t)} = \overline{w'^2(0)} = \sigma_w^2$ , and from Eq. (2.9) one obtains

$$\lambda = \sigma_w \sqrt{2\alpha} = \sigma_w \sqrt{\frac{2}{T_L}} \quad (2.12)$$

Knowing now the velocity statistics  $\sigma_w$  und  $T_L$ , Eq. (2.7) determines the velocity fluctuations of an ensemble of particles with a prescribed distribution of initial fluctuations  $w'(0)$ . This ensemble constitutes a Markov process which is a stochastic process  $w(t)$  whose behaviour at times subsequent to some time  $t_0$  depends only on  $w(t_0)$  and not on  $w(t)$  at times prior to  $t_0$  [9]. A Markov process is continuous but not differentiable. Therefore, the particle velocities in a turbulent flow can not be exactly represented by a Markov process because infinite accelerations would occur. Hence, it is necessary to consider the particle velocities at discrete times  $t_0, t_1 \dots t_n$ , whose interval  $\Delta t = t_{n+1} - t_n$  is

very much larger than the time scale over which the particle acceleration remains correlated. Considering the particle velocity fluctuations at discrete times transforms the Markov process Eq. (2.7) into a discrete Markov sequence. Formally, this can be done by substituting the continuous time  $t$  in Eq. (2.7) by the discrete time  $t + \Delta t$ . After some manipulations this leads to

$$w'(t + \Delta t) = e^{-\alpha \Delta t} \left( w'(t) + \lambda \int_t^{t + \Delta t} e^{\alpha(s - t)} x_i(s) ds \right) \quad (2.13)$$

Taking the square of both sides of the integral

$$I = \int_t^{t + \Delta t} e^{\alpha(s - t)} x_i(s) ds$$

leads to

$$I^2 = \int_t^{t + \Delta t} \int_t^{t + \Delta t} e^{\alpha(s - t)} e^{\alpha(u - t)} x_i(s) x_i(u) ds du.$$

During a timestep from  $t$  to  $t + \Delta t$  the following equation is valid:

$$x_i(s) x_i(u) = x_i^2(t) \delta(s - u) \quad (2.14)$$

Taking into account the properties of the  $\delta$ -function one obtains

$$I^2 = x_i^2(t) \int_t^{t + \Delta t} e^{2\alpha(s - t)} ds.$$

This integral can easily be solved. Taking the square-root of both sides of the solution gives

$$I = x_i(t) \frac{\sqrt{e^{2\alpha \Delta t} - 1}}{\sqrt{2\alpha}}.$$

Successive terms in the Markov sequence are then given by

$$w'(t + \Delta t) = w'(t) e^{-\alpha \Delta t} + \frac{\lambda}{\sqrt{2\alpha}} \sqrt{1 - e^{-2\alpha \Delta t}} x_i(t) \quad (2.15)$$

The coefficients  $\lambda$  and  $\alpha$  can be determined by calculating the variance  $w'^2(t + \Delta t)$  and the covariance  $w'(t + \Delta t)w'(t)$  of  $w(t + \Delta t)$ . Using the stationarity condition

$$\sigma_w^2(t + \Delta t) = \sigma_w^2(t),$$

then

$$\sigma_w = \frac{\lambda}{\sqrt{2\alpha}} \quad (2.16)$$

follows from the variance calculation. Calculation of the covariance leads to the expression of the Lagrangian autocorrelation function  $R(\Delta t)$  as it has been defined for example by Hall [2]:

$$R(\Delta t) = e^{-\alpha \Delta t} = e^{-\Delta t/T_L} = \frac{\overline{w'(t + \Delta t)w'(t)}}{\overline{w'^2(t)}} \quad (2.17)$$

with

$$\alpha = \frac{1}{T_L}$$

Thus, the equation for the vertical velocity fluctuation can be written as

$$w'(t + \Delta t) = e^{-\Delta t/T_{Lz}} w'(t) + \sqrt{1 - e^{-2\Delta t/T_{Lz}}} \sigma_w x_i(t) \quad (2.18)$$

where  $x_i(t)$  is a random number from a Gaussian distribution with zero mean and unit variance.

In analogy, to get a three-dimensional particle distribution the horizontal velocity fluctuations are given by

$$u'(t + \Delta t) = e^{-\Delta t/T_{Lx}} u'(t) + \sqrt{1 - e^{-2\Delta t/T_{Lx}}} \sigma_u x_i(t) \quad (2.19)$$

$$v'(t + \Delta t) = e^{-\Delta t/T_{Ly}} v'(t) + \sqrt{1 - e^{-2\Delta t/T_{Ly}}} \sigma_v x_i(t) \quad (2.20)$$

Strictly speaking, the equations derived above are only valid if the turbulence is homogeneous, i.e. that both  $T_{Lz}$  and  $\sigma_w$  are independent of particle position. When  $T_{Lz}$  varies with position and  $\sigma_w$  is constant as in the case of a neutral surface layer, Eq. (2.18) can be solved numerically using a timestep  $\Delta t$  which is much less than  $T_{Lz}$ . Then it can be assumed that  $T_{Lz}$  does not vary strongly over a single step (see for example [2], [4]). Wilson et al. [7] showed that an application of the model when  $\sigma_w$  varies with position leads to an unrealistic accumulation of particles in regions with weak turbulence. Legg and Raupach [9] derived that in a stationary and only horizontally homogeneous turbulent flow a vertical gradient of  $\sigma_w$  is always associated with a mean pressure gradient. Therefore, the Langevin equation Eq. (2.3) must include a mean force due to the action of the mean pressure gradient on a particle.

$$\frac{dw}{dt} = -\alpha w + \lambda x_i(t) + F \quad (2.21)$$

with

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

where  $\rho$  is the air density and  $p$  the pressure.

Repeating formally the above procedure to solve Eq. (2.21) and transforming the resulting Markov process into a Markov sequence of discrete timesteps, leads to the same coefficients  $a$  and  $b$  as in Eq. (2.14) and Eq. (2.15) and to an additional term

$$c = F T_{Lz} \left(1 - e^{-\Delta t / T_{Lz}}\right)$$

$F T_{Lz}$  represents a mean vertical drift velocity of the particle in the case of varying  $\sigma_w$ . Commonly, the additional term  $c$  will be added to the equation for vertical velocity fluctuation. Therefore, when the turbulence is inhomogeneous, Eq. (2.18) has to be changed to

$$w'(t + \Delta t) = e^{-\Delta t / T_{Lz}} w'(t) + \sqrt{1 - e^{-2\Delta t / T_{Lz}}} \sigma_w x_i(t) + \left(1 - e^{-\Delta t / T_{Lz}}\right) T_{Lz} \frac{\partial \sigma_w^2}{\partial z} \quad (2.22)$$

## 2.2 Determination of Turbulence Parameters

To calculate the particle trajectories it is necessary to know the three-dimensional velocity field (see Eq. (2.1) and Eq. (2.2)). In the case of TRAVELING the mean wind field is calculated with the non-hydrostatic mesoscale model KAMM [13]. Besides the wind field the model also delivers the spatial distributions of mean potential temperature,  $\bar{\Theta}$ , and vertical diffusion coefficients for momentum,  $K_{mz}$ , and heat,  $K_{hz}$ , in topographically structured terrain. With the aid of these parameters the three-dimensional distributions of  $\sigma_u$ ,  $\sigma_v$ ,  $\sigma_w$ ,  $T_{Lx}$ ,  $T_{Ly}$  and  $T_{Lz}$  can be derived.

### 2.2.1 Calculation of Velocity Standard Deviations

The standard deviations  $\sigma_u$ ,  $\sigma_v$ ,  $\sigma_w$  which appear in the equations Eq. (2.19), Eq. (2.20) and Eq. (2.22) represent a Lagrangian statistics of a particle following air motion. Assuming stationary and homogeneous turbulence over the time interval  $\Delta t$  the Lagrangian statistics are equated to Eulerian statistics (see e.g. Panofsky and Dutton, [21]). The velocity standard deviations are calculated from the mean turbulent kinetic energy,  $E$ , which itself is derived in a Eulerian framework. The corresponding equations are:

$$E = 0.5 (\sigma_u^2 + \sigma_v^2 + \sigma_w^2) = 0.5 q^2 \quad (2.23)$$

(see for example [22]), and

$$\begin{aligned}\sigma_u &= \sqrt{2m_1 E} \\ \sigma_v &= \sqrt{2m_2 E} \\ \sigma_w &= \sqrt{2m_3 E}\end{aligned}\quad (2.24)$$

The weighting factors  $m_i$ ,  $i = 1, 2, 3$ , define the contributions of  $E$  to the turbulence and account for the nonisotropy of turbulence. From Eq. (2.23) and Eq. (2.24) it becomes evident that  $m_1 + m_2 + m_3 = 1$ , and that

$$m_j = \frac{\sigma_j^2}{\sum_{i=1}^3 \sigma_i^2}, \quad j = 1, 2, 3$$

	unstable	neutral	stable
$m_1$	0.40	0.54	0.54
$m_2$	0.30	0.30	0.37
$m_3$	0.30	0.16	0.09

Table 1. Values of weighting factors  $m_i$  [10]

The factors, which depend on thermal stratification, have been derived by Vogel [10] who analyzed various parametrizations of  $\sigma_u$ ,  $\sigma_v$ , and  $\sigma_w$  published in the literature (Table 1).

Unstable, neutral, and stable thermal stratification are distinguished through the gradient of potential temperature.

$$\begin{aligned}\text{unstable} : \frac{\partial \bar{\Theta}}{\partial z} &\leq -0.5K/100m \\ \text{neutral} : -0.5K/100m &< \frac{\partial \bar{\Theta}}{\partial z} < 0.5K/100m \\ \text{stable} : \frac{\partial \bar{\Theta}}{\partial z} &\geq 0.5K/100m\end{aligned}$$

Presently, the velocity standard deviations are calculated in the TRAVELING program itself using Eq. (2.24). Therefore, it is necessary to provide three-dimensional fields of turbulent kinetic energy,  $E$ , as input data. This is done by the application of the Level 2 model of Mellor and Yamada [23], [24], which provides a simplified equation for the turbulent kinetic energy. Assuming that the atmospheric flow is horizontally homogeneous and that subsidence can be neglected, applying the Boussinesq approximation, and further assuming a steady state for the eddy kinetic energy without advection and diffusion, a balance between shear production,  $P_s$ , buoyancy production,  $P_b$ , and viscous dissipation,  $\varepsilon$ , can be derived.

$$0 = P_s + P_b - \varepsilon \quad (2.25)$$

With:

$$P_s = -\overline{u'w'} \frac{\partial \bar{u}}{\partial z} - \overline{v'w'} \frac{\partial \bar{v}}{\partial z} \quad (2.26)$$

$$P_b = \frac{g}{\bar{\Theta}} \overline{w'\Theta'} \quad (2.27)$$

$$\varepsilon = \frac{q^3}{\Lambda} = \frac{(2E)^{3/2}}{\Lambda} \quad (2.28)$$

The energy dissipation,  $\varepsilon$ , is expressed as a function of turbulent kinetic energy and characteristic dissipation length,  $\Lambda$ .  $\Lambda$  is related to the adiabatic mixing length,  $l_a$ , by

$$\Lambda = 16.6 l_a \Phi^{-1} = 16.6 l_d, \quad l_d = l_a \Phi^{-1} \quad (2.29)$$

where  $\Phi = \Phi(z/L_*)$  is a stability function depending on the height,  $z$ , and the Monin-Oubukhov-length,  $L_*$ .

The constant value 16.6 is taken from [24].

In the equations above, primed characters denote the turbulent parts of the corresponding physical parameter and the bar denotes a Reynolds average.

The correlation terms  $\overline{u'w'}$ ,  $\overline{v'w'}$ , and  $\overline{w'\Theta'}$ , which physically represent the vertical kinematic fluxes of  $u$ -momentum,  $v$ -momentum, and heat, respectively, are parameterized according to the gradient transport theory ( K-theory ) [22].

$$\begin{aligned} -\overline{u'w'} &= K_{mz} \frac{\partial \bar{u}}{\partial z} \\ -\overline{v'w'} &= K_{mz} \frac{\partial \bar{v}}{\partial z} \\ -\overline{w'\Theta'} &= K_{hz} \frac{\partial \bar{\Theta}}{\partial z} \end{aligned} \quad (2.30)$$

Using these expressions the following equation can be derived:

$$q^3 = \Lambda \varepsilon = 16.6 l_d \left[ K_{mz} S^2 - K_{hz} \frac{g}{\bar{\Theta}} \frac{\partial \bar{\Theta}}{\partial z} \right] \quad (2.31)$$

In this equation  $S^2$  denotes the square of the magnitude of the vertical shear vector of horizontal wind.

$$S^2 = \left[ \left( \frac{\partial \bar{u}}{\partial z} \right)^2 + \left( \frac{\partial \bar{v}}{\partial z} \right)^2 \right] \quad (2.32)$$

Applying the definition of the gradient Richardson number,  $R_i$ ,

$$R_i = \frac{\frac{g}{\bar{\Theta}} \frac{\partial \bar{\Theta}}{\partial z}}{S^2} \quad (2.33)$$

one, finally, arrives at an equation for the mean turbulent kinetic energy.

$$E = 0.5 q^2 = 0.5 (\Lambda \varepsilon)^{2/3} = 3.25 \left\{ I_d K_{hz} S^2 \left[ \frac{K_{mz}}{K_{hz}} - R_i \right] \right\}^{2/3} \quad (2.34)$$

The parametrization of the diffusion coefficients  $K_{mz}$  and  $K_{hz}$  depends on the thermal stratification.

In the cases of neutral and stable conditions the diffusion coefficients are calculated according to

$$\begin{aligned} K_{mz} &= \frac{\kappa z u_*}{\Phi_m} = I_d u_* \\ K_{hz} &= K_{mz} \frac{\Phi_m}{\Phi_h} \end{aligned} \quad (2.35)$$

The dimensionless wind shear  $\Phi = \Phi_m = \Phi_m(z/L_*)$  and the dimensionless lapse rate  $\Phi_h = \Phi_h(z/L_*)$ , are chosen according to Businger et al. [25].

For convective conditions a parametrization of Degrazia [27] is used to determine the diffusion coefficient of heat,  $K_{hz}$ .

$$K_{hz} = 0.15 w_* z_i \left( \frac{\Psi}{q_i^4} \right)^{1/3} \quad (2.36)$$

with:

$$\Psi = \left( \frac{136 z}{z_i} \right)^{-1} \left[ (1 - z/z_i)^2 + 0.75 (136 z/z_i)^{2/3} \right]^{3/2}$$

and

$$q_i = [1 - \exp(-4z/z_i) - 0.0003 \exp(8z/z_i)]^{-1}$$

In these equations  $z_i$  denotes the height of the convective boundary layer and  $w_*$  is referred to as the convective velocity scale defined as

$$w_* = \left( \frac{g}{\Theta} \overline{w' \Theta'} z_i \right)^{1/3}$$

The second equation in Eq. (2.35) is then used to calculate  $K_{mz}$

### 2.2.1.1 Surface layer

Inside the surface layer it is assumed that the adiabatic length scale,  $I_a$ , is linear dependent on the height,

$$l_a = \kappa z \quad (2.37)$$

where  $\kappa$  is the von Karman constant which takes a value of 0.4. Thus, the diabatic length scale,  $l_d$ , (see Eq. (2.29) ) can be written as

$$l_d = \frac{l_a}{\Phi} = \frac{l_a}{\Phi_m} = \frac{\kappa z}{\Phi_m} \quad (2.38)$$

The square of the wind shear,  $S^2$ , can be expressed by

$$S^2 = \frac{\Phi_m^2}{l_a^2} u_*^2 = \frac{u_*^2}{l_d^2} \quad (2.39)$$

where  $u_*$  is the friction velocity.

Now, Eq. (2.34) can be rewritten as

$$E = 3.25 u_*^2 \left( 1 - R_i \frac{K_{hz}}{K_{mz}} \right)^{2/3} \quad (2.40)$$

Inside the surface layer the Richardson number is calculated according to [25]:

$$\begin{aligned} R_i &= \frac{z}{L_*}, && (\text{unstable stratification}) \\ R_i &= \frac{z}{L_*} \frac{\Phi_h}{\Phi_m^2}, && (\text{stable stratification}) \\ R_i &= 0, && (\text{neutral stratification}) \end{aligned} \quad (2.41)$$

### 2.2.1.2 Ekman layer

In the Ekman layer above the surface layer the mixing length  $l_a$  is calculated using Blackadar's equation [26].

$$l_a = \frac{\kappa z}{1 + \frac{\kappa z}{\lambda}} \quad (2.42)$$

Here  $\lambda = 0.009u_*/f$  is the maximum possible mixing length and  $f$  is the Coriolis parameter.

The turbulent kinetic energy is calculated using Eq. (2.34). But in the Ekman layer the square of the wind shear,  $S^2$ , is substituted by the deformation term,  $D^2$ . This deformation term, which is also available from the KAMM model, represents the three-dimensional mean wind shear and it can be expressed as [13]:

$$D^2 = \sum_{i=1}^3 \sum_{j=1}^3 \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)^2 \quad (2.43)$$

$D^2$  is also used to determine the gradient Richardson number in the Ekman layer.

## 2.2.2 Calculation of Lagrangian Time Scales

The way how to determine the Lagrangian time scales will be outlined only for the vertical time scale,  $T_{Lz}$ . The horizontal time scales,  $T_{Lx}$  and  $T_{Ly}$ , are calculated analogously.

Assuming an exponential Lagrangian autocorrelation function, Taylor's theorem [1] can be integrated to give

$$\sigma_z^2 = 2 \sigma_w^2 T_{Lz} \left( t - T_{Lz} (1 - \exp(-\frac{t}{T_{Lz}})) \right) \quad (2.44)$$

where  $t$  is the travel time.

If  $t \gg T_{Lz}$  then Eq. (2.44) can be approximated by

$$\sigma_z^2 = 2 T_{Lz} \sigma_w^2 t \quad (2.45)$$

Combining Eq. (2.45) with the equation

$$\sigma_z^2 = 2 K_{cz} t, \quad (2.46)$$

where  $K_{cz}$  is the vertical diffusion coefficient for mass, leads to an expression for  $T_{Lz}$ .

$$T_{Lz} = \frac{K_{cz}}{\sigma_w^2} \quad (2.47)$$

The time scales are calculated using Eq. (2.47) and Eq. (2.24) assuming that  $K_{cz}$  is equal to  $K_{hz}$ , the diffusion coefficient of heat which is available from the mesoscale model KAMM.

With Eq. (2.24) and Eq. (2.47) all statistical parameters are determined which are necessary to calculate the three-dimensional velocity fluctuations.

## 2.3 Coordinate System, Coordinate Transformations and Particle Trajectory

To determine the trajectory of an individual particle according to Eq. (2.1) using Eq. (2.2) it is necessary to know the mean windfield,  $\bar{v}$ , and the fluctuating part,  $v'$ . The mean windfield is available from the mesoscale model KAMM on a three-dimensional meteorological grid spanning the whole simulation area. The turbulent components are calculated in TRAVELING according to the Markov sequences described in Section 2.1 (Eq. (2.19), Eq. (2.20), Eq. (2.22)). The 3-D meteorological grid is related to a terrain following coordinate system. Therefore, in TRAVELING a similar system is used as in KAMM [13].

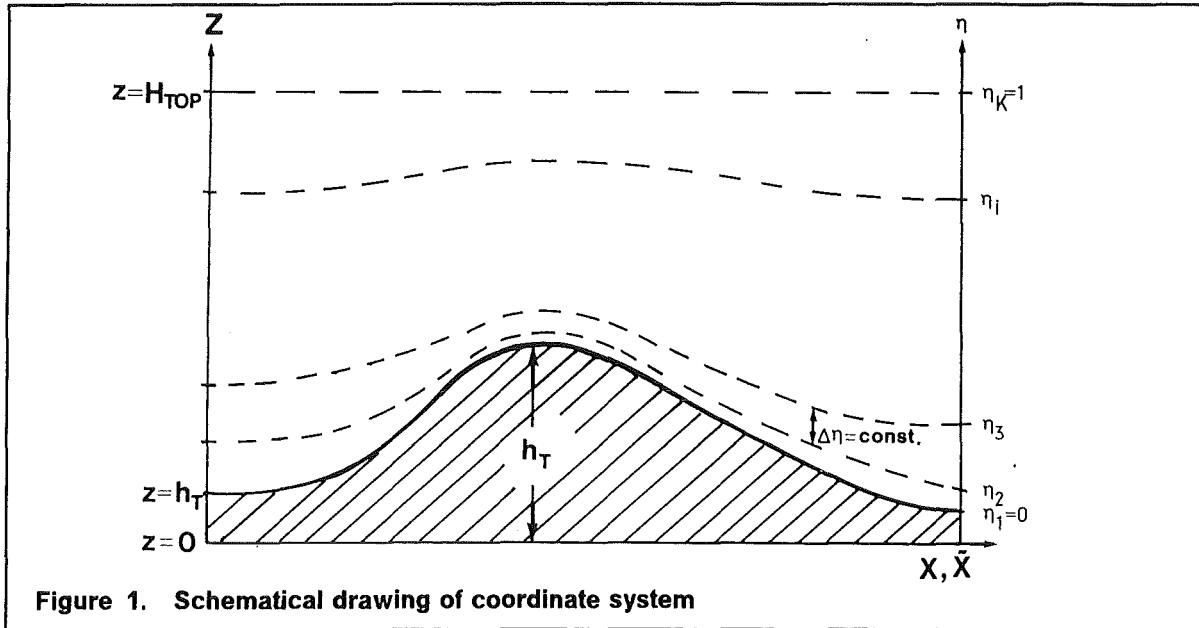
The coordinates  $x$ ,  $y$ , and  $z$  of an Eulerian frame of reference are related to the coordinates  $\tilde{x}$ ,  $\tilde{y}$ , and  $\eta$  of the terrain following  $\eta$ -system by

$$\begin{aligned}\tilde{x} &= x \\ \tilde{y} &= y \\ a\eta^2 + b\eta &= \frac{z(x, y) - h_t(x, y)}{H_{top} - h_t(x, y)}\end{aligned}\quad (2.48)$$

with:

$h_t(x, y)$	height of topography above sea level (m)
$H_{top} = \text{const.}$	upper boundary of simulation (model) area (m)
$x, y, z$	rectangular coordinates of a cartesian frame of reference
$\tilde{x}, \tilde{y}$	horizontal coordinates of the terrain following frame of reference
$\eta$	vertical coordinate of the terrain following frame of reference

The quadratic transformation relation for the vertical coordinate in Eq. (2.48) has the advantage that the vertical resolution inside the boundary layer can be chosen higher than outside the boundary layer. This is illustrated in Figure 1.



The parameters  $a$  and  $b$  are determined by

$$a = \frac{p-1}{p+1}, \quad b = 1-a = \frac{2}{p+1} \quad (2.49)$$

The coefficient  $p$  is approximately the ratio between the vertical grid sizes at the top of the model domain ( $z = H_{top}$ ) and at the ground surface ( $z = h_t$ ).

The velocity fluctuations derived in Section 2.1 have to be transformed into the terrain following coordinate system. By taking the time derivative it follows from Eq. (2.48) that

$$\tilde{u}' = u' , \tilde{v}' = v'. \quad (2.50)$$

The vertical component,  $\omega'$ , is given by

$$\omega' = \frac{\partial \eta}{\partial z} \left\{ w' - \left( u' \frac{\partial h_t}{\partial x} + v' \frac{\partial h_t}{\partial y} \right) [1 - (a \eta^2 + b \eta)] \right\} \quad (2.51)$$

with:

$$\frac{\partial \eta}{\partial z} = \frac{1}{2a\eta + b} \frac{1}{H_{top} - h_t}$$

The trajectory of a particle in the terrain following coordinate system can now be calculated from

$$\begin{aligned} x(t + \Delta t) &= x(t) + (\bar{u}(t) + u'(t)) \Delta t \\ y(t + \Delta t) &= y(t) + (\bar{v}(t) + v'(t)) \Delta t \\ \eta(t + \Delta t) &= \eta(t) + (\bar{\omega}(t) + \omega'(t)) \Delta t \end{aligned} \quad (2.52)$$

But it has to be noted that this trajectory is determined in a Eulerian framework, whereas the velocity fluctuations which are calculated according to Eq. (2.19) and Eq. (2.20) are Lagrangian velocity components. They have been determined relative to a Lagrangian frame of reference which is moving with the mean flow and whose x-axis coincides with the direction of the mean flow (see Figure 2). Therefore, it is necessary to transform the horizontal Lagrangian components,  $u'_L, v'_L$ , from the Lagrangian system into the Eulerian system. This is accomplished by a rotation along the angle  $\alpha$  between the direction of the mean wind and the x-axis of the fixed Eulerian coordinate system (see Figure 2).

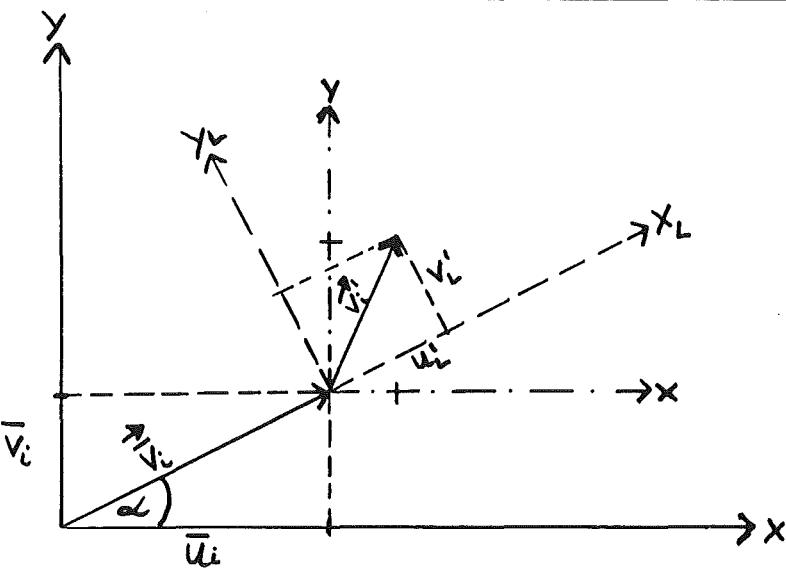
$$\begin{aligned} u' &= u'_L \cos \alpha - v'_L \sin \alpha \\ v' &= u'_L \sin \alpha + v'_L \cos \alpha \end{aligned} \quad (2.53)$$

The rotation angle is related to the horizontal components of the mean velocity,  $\bar{u}$  and  $\bar{v}$ , by:

$$\alpha = \tan^{-1} \left( \frac{\bar{v}}{\bar{u}} \right)$$

## 2.4 Boundary Conditions

The lower boundary of the simulation area is the ground surface which can not be penetrated by the particles. It is assumed that the particles are reflected perfectly at ground

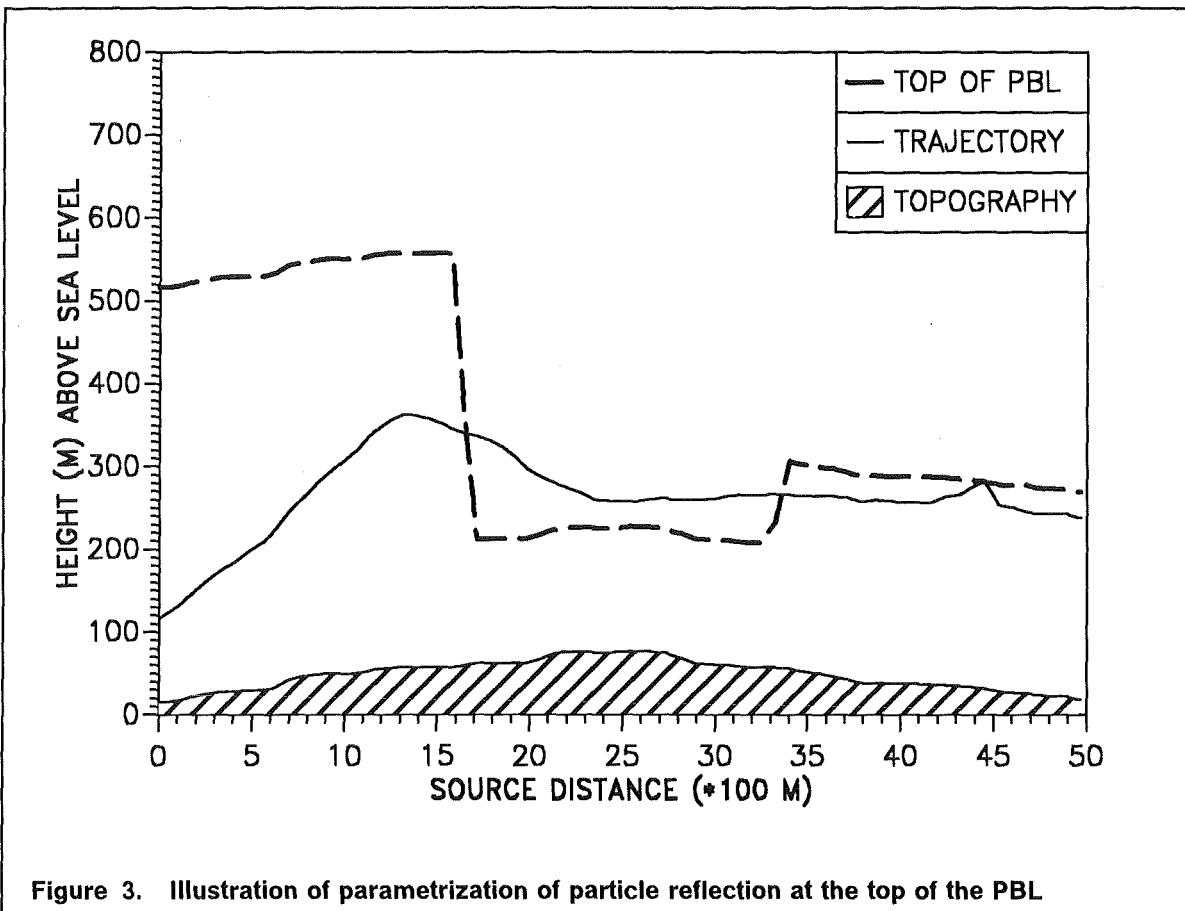


**Figure 2. Illustration of transformation of horizontal velocity components**

changing also the sign of the velocity. Thereby, the mass carried by a particle is reduced by the proportion of mass being deposited.

The top of the planetary boundary layer (PBL) which changes with daytime acts as an internal upper boundary. The parametrization of the behaviour of particles close to the top of the PBL is illustrated schematically in Figure 3, which shows the trajectory of a particle being released in 100 m height above the topography. In addition, the upper boundary of the mixing layer is shown. It should be noted that the situation shown is purely hypothetical and serves only for illustration.

A particle being far below the PBL is advected and dispersed according to the flow and turbulence conditions inside the boundary layer. If the height of the PBL descends a particle might escape into the free atmosphere if the "path" of the sinking PBL height intersects the particle's trajectory and if the vertical location of the particle at the end of the previous timestep lies above the new height of the boundary layer. If a particle impinges from below on a rising, sinking or constant upper boundary and if its vertical location at the end of the previous timestep is lower than the instantaneous height of the PBL, then it is reflected perfectly. Those particles which are above the PBL are mainly transported by the average wind prevailing in the free atmosphere. They are allowed to entrain into the PBL either due to downward motion or due to the deepening of the layer itself under convective conditions. Thus fumigation is accounted for. Figure 3 also illustrates that the upper internal boundary is usually not identical with the top of the model domain,  $H_{top}$  (see Sect. 2.3.1), which in this example has a value of 800 m above sea level.



**Figure 3.** Illustration of parametrization of particle reflection at the top of the PBL

## 2.5 Modelling of Deposition Processes

Depending on the physico-chemical form of the pollutant parts of its mass may be deposited on the ground either by dry and/or wet deposition. Thus, deposition is an important sink of airborne pollutants, resulting in contamination of the ground.

### 2.5.1 Dry deposition

The processes by which airborne pollutants are removed from the atmosphere without precipitation are called dry deposition.

Commonly, mass transfer to the surface is represented in terms of a dry deposition velocity,  $v_d$  (see for example the reviews on dry deposition of Underwood [28] and Sehmel [29]):

$$v_d(z_d) = \frac{F(z_d)}{C(z_d)}$$

where  $z_d$  denotes the height at which  $v_d$  is determined,  $F(z_d)$  the downward flux of pollutant towards the surface at height  $z_d$  and  $C(z_d)$  the concentration of pollutant at  $z_d$ . The deposition velocity depends not only on the height  $z_d$  but also on the physico-chemical properties of the pollutant represented by the Lagrangian particles, the characteristics of the underlying surface, and the atmospheric turbulence conditions.

In the context of TRAVELING dry deposition is included by introducing a deposition probability  $W_d$ . The deposition probability determines the deposited fraction of mass of a particle being below a deposition height  $z_d$ . Accordingly, the mass reduction for a particle is taken into account by a depletion factor  $f_d = 1 - W_d$ . The method has been adopted from Axenfeld et al. [32]. They assume that, near to the ground, the distribution of the vertical velocity can be approximated by a Maxwell distribution, which can be distorted by a settling velocity  $v_g$  if gravitational settling is taken into account.

Let  $\sigma_0 = \sigma_w(z = 0)$ , then the distribution for particles impinging on the ground can be written as

$$f_-(w) = A_- \exp\left(-\frac{(w + v_g)^2}{2\sigma_0^2}\right) \text{ for } w < 0 \quad (2.54)$$

The mirror distribution for the reflected particles is

$$f_+(w) = A_+ \exp\left(-\frac{(w - v_g)^2}{2\sigma_0^2}\right) \text{ for } w > 0 \quad (2.55)$$

where the amplitude is reduced by the deposition probability  $W_d$ :

$$A_+ = (1 - W_d) A_- \quad (2.56)$$

The particle density is given by

$$\begin{aligned} N &= \int_{-\infty}^0 f_-(w) dw + \int_0^\infty f_+(w) dw \\ &= \sqrt{\frac{\pi}{2}} \sigma_0 (A_+ + A_-) \{1 + \operatorname{erf}(\gamma)\} \end{aligned} \quad (2.57)$$

with

$$\gamma = \frac{v_g}{\sqrt{2} \sigma_0}$$

and

$$\operatorname{erf}(\gamma) = \frac{2}{\sqrt{\pi}} \int_0^\gamma \exp(-s^2) ds \quad \text{error function}$$

The deposition flux  $M_d$  can be calculated from

$$\begin{aligned}
M_d &= - \int_{-\infty}^0 w f_-(w) dw - \int_0^\infty w f_+(w) dw \\
&= \sigma_0 (A_- - A_+) \left\{ \sigma_0 \exp(-\gamma^2) + v_g \sqrt{\frac{\pi}{2}} [1 + \operatorname{erf}(\gamma)] \right\}
\end{aligned} \tag{2.58}$$

On the other hand,  $M_d$  is given as  $M_d = v_d N$ . Substituting Eq. (2.56 - 2.58) leads to the following general expression for  $W_d$  which includes also gravitational settling of heavy particles.

$$W_d = \frac{\sqrt{2\pi} \frac{v_d}{\sigma_0}}{F_g + \sqrt{\frac{\pi}{2}} \frac{v_d}{\sigma_0}} \tag{2.59}$$

with

$$F_g = \sqrt{\frac{\pi}{2}} \frac{v_g}{\sigma_0} + \frac{\exp(-\gamma^2)}{1 + \operatorname{erf}(\gamma)}$$

If only small particles are considered or if gravitational settling is ignored ( $v_g = 0$ ) (this is presently the case in TRAVELING),  $F_g$  equals unity.

Depending on the ratio between  $v_d$  and  $\sigma_0$  it is possible, from a pure mathematical point of view, that  $W_d$  becomes greater than one. Assuming that  $F_g = 1$ , it can be derived from Eq. (2.58) that  $W_d \geq 1$ , if  $v_d/\sigma_0 \geq 0.8$ .

But the following assessment demonstrates that, from the physical point of view, this situation is very unlikely.

From Eq. (2.24) and Eq. (2.40) it can be derived (for  $z = 0$ ) that

$$\sigma_0 = 2.5 u_* \sqrt{m_3} .$$

Using typical values of  $u_*$  which range from about 0.1 m/s to about 0.5 m/s,  $\sigma_0$  covers a range from about 0.08 m/s to 0.38 m/s under stable thermal conditions.

Dry deposition velocities for different gases can range four orders of magnitude [29]. A typical maximum deposition velocity is that for  $\text{SO}_2$  which might take a value of about 0.04 m/s. Using these values the ratio between  $v_d$  and  $\sigma_0$  typically ranges from about 0.11 to about 0.5.

To determine the deposition velocity it is either necessary to model  $v_d$  (see [31]) or to use values measured during field or wind tunnel experiments.

### 2.5.2 Wet deposition

The removal of pollutants from the atmosphere due to precipitation processes (e.g. due to rain, snowfall, hail etc.) is referred to as wet deposition or precipitation scavenging.

A reliable modelling of wet deposition is difficult and complex because it depends on the physico-chemical properties of the pollutant and the spatial and temporal variations of precipitation and its intensity. Comprehensive reviews on precipitation scavenging are given for example by Underwood [33] and Slinn [34].

Presently, wet deposition in TRAVELING is described by a washout coefficient,  $\lambda$ , which has the dimension [ $s^{-1}$ ]. It describes the amount of precipitation scavenging and the rate of wet deposition on the ground. This coefficient may vary in space and time. The reduction of the fraction of mass carried by each particle after a timestep  $\Delta t$  is given by the depletion factor

$$f_w = \exp(-\lambda \Delta t) \quad (2.60)$$

The probability for wet deposition of a particle is then given by

$$W_w = 1 - \exp(-\lambda \Delta t) \quad (2.61)$$

### 3. NUMERICAL PROCEDURES

#### 3.1 *Interpolation of Meteorological Data*

As already mentioned all data necessary to calculate the time-dependent trajectory of an individual particle are available at fixed grid-points of a three-dimensional meteorological grid. These data have to be interpolated to the particle location which changes from timestep to timestep.

In the present version of TRAVELING a linear interpolation procedure has been chosen for horizontal (2-D, e.g. topography) and three-dimensional interpolations (e.g. the mean flow components,  $\bar{u}$ ,  $\bar{v}$ ,  $\bar{\omega}$ ).

##### 3.1.1 Two-dimensional interpolation

The procedure is illustrated in Figure 4.

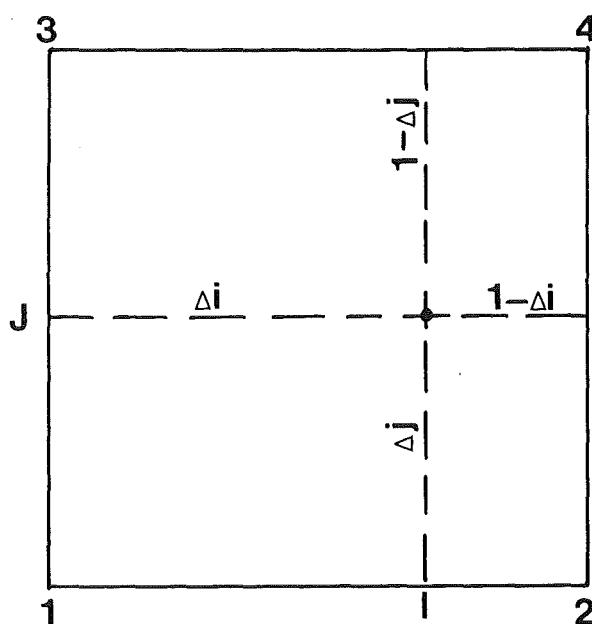


Figure 4. Illustration of 2-D linear interpolation

The values of a variable  $f$  are given at four gridpoints (1, 2, 3, 4) surrounding the particle location ( $I, J$ ). It is assumed that the distance between two neighbouring grid points is normalized to unity.

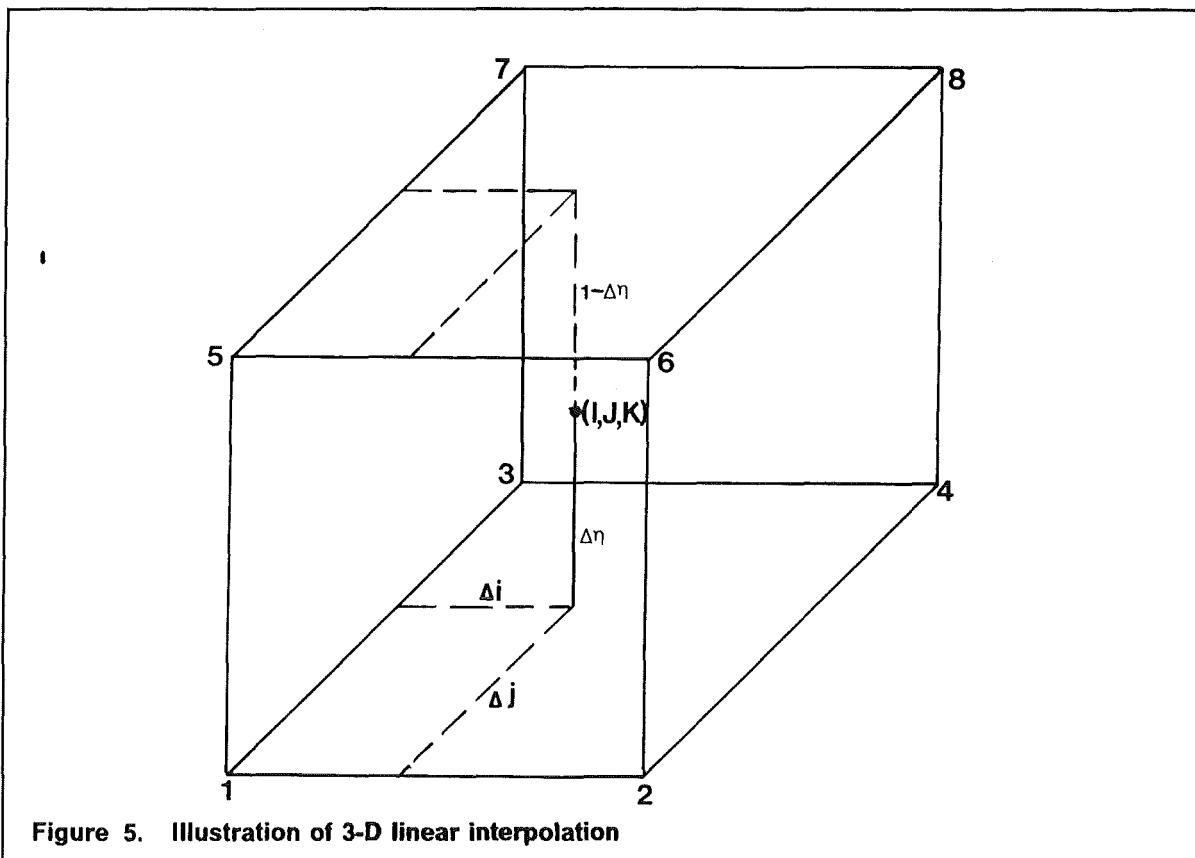
Then, the interpolated value is calculated according to

$$f_{I,J} = \{f_1(1 - \Delta i) + f_2 \Delta i\}(1 - \Delta j) + \{f_3(1 - \Delta i) + f_4 \Delta i\} \Delta j \quad (3.1)$$

The distances  $\Delta i$  and  $\Delta j$  between the particle location and the lower-left grid point can be calculated in grid-units ( $0 \leq \Delta i \leq 1$ ,  $0 \leq \Delta j \leq 1$ ) from the knowledge of the particle location and the resolution of the meteorological grid.

### 3.1.2 Three-dimensional interpolation

To find the value of a variable at the location  $(I, J, K)$  using the values at the eight neighbouring grid-points a method analogous to the two-dimensional case is applied. The method is illustrated in Figure 5.



The interpolated value is then given according to

$$f_{I,J,K} = \{[f_1(1 - \Delta i) + f_2 \Delta i](1 - \Delta j) + [f_3(1 - \Delta i) + f_4 \Delta i]\Delta j\}(1 - \Delta \eta) + \\ \{[f_5(1 - \Delta i) + f_6 \Delta i](1 - \Delta j) + [f_7(1 - \Delta i) + f_8 \Delta i]\Delta j\}\Delta \eta \quad (3.2)$$

## 3.2 Concentration Grid and Calculation of Concentrations

To determine the concentration distributions in the air and on the ground it is necessary to divide the simulation area into volume elements using a three-dimensional terrain following concentration grid. The horizontal size of this grid is independent of the size of

the meteorological grid mentioned in Section 3.1 but the vertical resolution of both grids should be identical.

If the horizontal resolution of the concentration grid is different from that of the meteorological grid the topography has to be interpolated from the latter grid into the former one. This is accomplished by a simple two-dimensional linear interpolation method.

Initially, when being released, each particle carries a fraction of mass of the airborne material. This fraction is given by

$$M^p = \frac{Q \Delta t}{N} \quad (3.3)$$

with:

$Q$	source strength (e.g. in mass units / s)
$\Delta t$	timestep (s)
$N$	number of particles released per timestep

Note that  $M^p$  can be reduced from timestep to timestep if deposition is taken into account.

After each timestep the location of each particle is known. Summing up all fractions of mass,  $M_{i,j,k}^p$ , carried by the particles which are located in volume element ( $i, j, k$ ) gives the concentration in this box.

$$C_{i,j,k} = \frac{\sum_{p=1}^{n_{i,j,k}} M_{i,j,k}^p}{\Delta V_{i,j,k}} \quad (3.4)$$

Here  $n_{i,j,k}$  denotes the number of particles in the gridbox ( $i, j, k$ ) of volume  $\Delta V_{i,j,k}$ .

To calculate the deposition flux onto the ground it is distinguished between dry and wet deposition. If ( $i, j$ ) denotes an area element of size  $\Delta x \Delta y$  then the deposition flux due to dry deposition is determined by

$$F_{i,j,(d)} = \frac{\sum_{p=1}^{n_{i,j,(d)}} M_{i,j,(d)}^p}{\Delta x \Delta y \Delta t} \quad (3.5)$$

In this case  $M_{i,j,(d)}^p$  denotes the fraction of mass of particle  $p$  being deposited by dry deposition on the area element ( $i, j$ ).  $n_{i,j,(d)}$  denotes the number of particles which are below a deposition height  $z_d$  (see Section 2.5.1), but only those particles contribute to deposition which penetrate the deposition level from above.

Similarly, the wet deposition flux is determined.

$$F_{i,j,(w)} = \frac{\sum_{p=1}^{n_{i,j,(w)}} M_{i,j,(w)}^p}{\Delta x \Delta y \Delta t} \quad (3.6)$$

$M_{i,j,(w)}^p$  is the proportion of mass of particle p being affected by precipitation scavenging and  $n_{i,j,(w)}$  gives the number of particles in the whole vertical column over the area element (i, j).

Counting the particles - this is equivalent to the summation of the corresponding proportions of mass - is carried out in a staggered grid which is shifted horizontally by  $\Delta x/2$ ,  $\Delta y/2$  relative to the concentration grid. This is illustrated schematically in Figure 6. The bullets show the grid points of the concentration grid, the crosses the grid-points of the staggered counting grid. The resulting concentrations are assigned to the concentration grid points in the centre of each staggered grid cell.

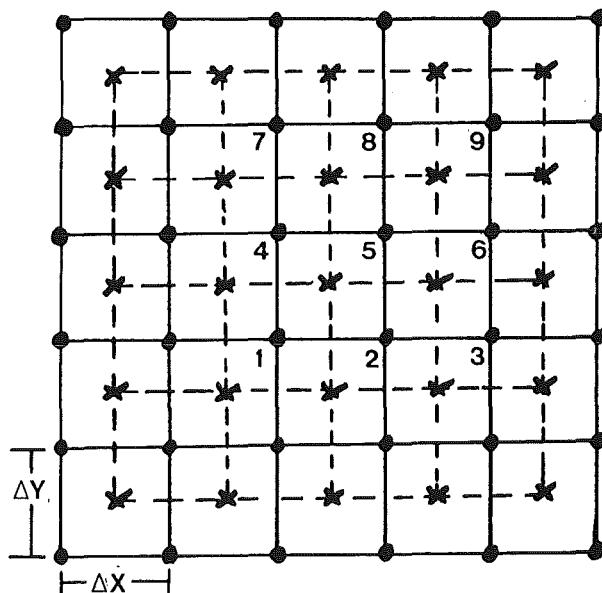


Figure 6. Schematical drawing of concentration and counting grids

To determine the volume  $\Delta V$  of a three-dimensional concentration grid cell the vertical distance  $\Delta z$  (in meter) of two  $\eta$ -levels,  $\eta_{k+1}$  and  $\eta_k$ , has to be calculated. Since the  $\eta$ -system follows the terrain, an average value for  $\bar{\Delta z}_k$  has to be calculated for each box. Applying formally the vertical transformation equation of Eq. (2.48) the following formula can be derived:

$$\bar{\Delta z}_k = (H_{top} - \bar{h}_t) (a (\eta_{k+1}^2 - \eta_k^2) + b \Delta \eta) \quad (3.7)$$

The interpolated topography value  $\bar{h}_t$  is calculated from the topography value at the concentration grid point itself and the values of the eight neighbouring grid points (see also Figure 6).

$$\bar{h}_t = \frac{1}{16} (4f_5 + 2f_2 + 2f_4 + 2f_6 + 2f_8 + f_1 + f_3 + f_7 + f_9) \quad (3.8)$$

where  $f_i, i = 1, \dots, 9$  denotes the values of topography at the nine concentration grid points.

### **3.3 Source configuration and modes of application**

In TRAVELING it is possible to consider the dispersion of pollutants emitted from a single source or from multiple sources. In the latter case the particles considered per timestep are distributed equally among all sources.

TRAVELING can be applied under stationary as well as under unstationary atmospheric conditions. It is also possible to treat unstationary sources with emission rates changing in time.

Under stationary conditions one ensemble with a large number of particles (e.g. 20000 particles) is released only during the first timestep. It is assumed that subsequent ensembles with the same number of particles which would be released during subsequent timesteps would give concentration distributions which are statistically identical to the distribution of the the first ensemble. Therefore, it is sufficient to track only one particle cloud. The simulation stops when all particles have left the simulation area.

Under unstationary conditions new particles have to be released and tracked individually for each timestep. Therefore, to achieve statistical reliable results, a considerable larger amount of particles has to be considered than in the stationary mode. To decrease the CPU-time and storage capacity required those particles which have left the simulation area are not lost. They will be emitted again with reinitialized source conditions. Therefore, the number of flying particles will be less than the number of particles which effectively contribute to the concentration distribution. In the unstationary mode the simulation stops at the end of a predefined simulation period (predefined by the number of timesteps) or after the end of the release when all flying particles are outside of the simulation domain.

### **3.4 Choice of timestep**

The timestep  $\Delta t$ , which is not a varying quantity in the present version of TRAVELING, must fulfill two conditions. At first, it is necessary that the timestep is much less than the Lagrangian time scale. Wilson and Zhuang [35] showed that there exist no physical lower limit of a timestep for a Lagrangian model; such a lower limit might be given by the capacity of the used computer system. However, they suggest as an upper limit

$$\Delta t = 0.1 \min(T_{Lx}, T_{Ly}, T_{Lz}).$$

In the inhomogeneous case they suppose that the timestep must be even smaller than in the homogeneous case. But commonly, the condition above is used.

Secondly, the timestep must be chosen small enough so that the trajectory segment of a particle during a timestep is less than the smallest side-length of a box of the concentration grid.

### 3.5 *Random number generator*

To calculate the turbulent velocity components the model requires for each timestep three ensembles of Gaussian random numbers with zero mean and unit variance. The generation of these random numbers, even if vectorized subroutines from appropriate system libraries (e.g. SSL II) are used, is a very time consuming procedure. Therefore, a very large ensemble of Gaussian random numbers is created only once. From this single ensemble three subensembles are drawn randomly during each timestep using a uniform random number generator because it is very much quicker than the Gaussian random number generator. The subensembles are also Gaussian with zero mean and unit variance and they are mutually independent.

## 4. USERS' GUIDE

### 4.1 Structure of the Model TRAVELING

It has been tried to give the program a modular structure. This makes it more readable for users and simplifies the substitution of modules by other ones.

The main program has only steering functions. It calls different subroutines and decides whether a simulation has to be stopped. The connection between the main program and the different subroutines is illustrated in Figure 7.

Mostly, the model variables are transferred between the different program units by named COMMON-blocks. All these COMMON-blocks are inserted into the program using the INCLUDE-statement. Therefore, changes in the COMMON-blocks have to be performed only once. In the current version the name of the source library member to be included is **COMINST**.

In the COMMON-blocks dimensions are assigned to all arrays. The dimensions are upper boundaries of the array sizes allowed. The program checks whether these boundaries are exceeded. The dimensions are defined in one PARAMETER-statement which is read from the source library member **PARANEU** using the INCLUDE statement.

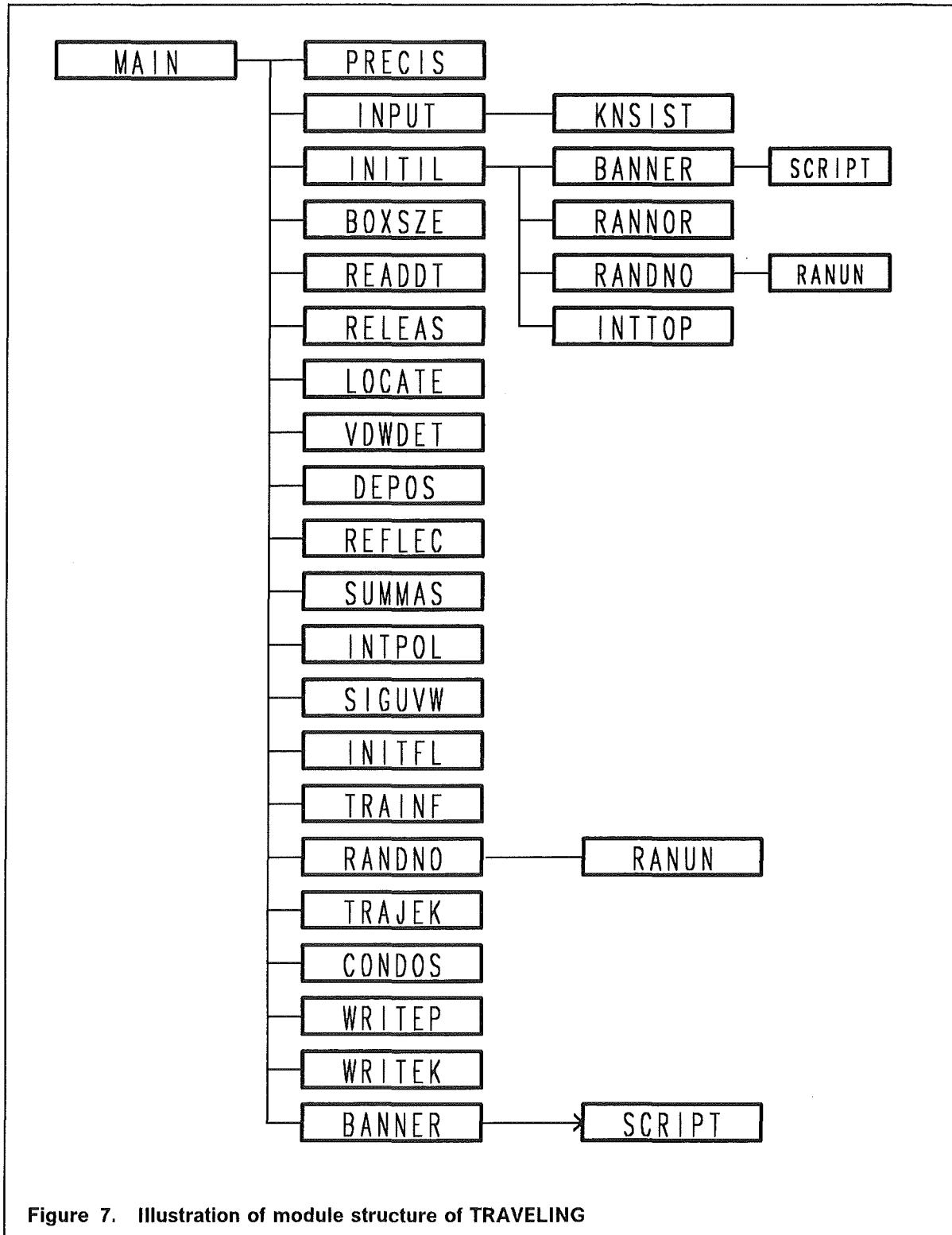
This PARAMETER-statement is listed below with some arbitrary values for the particular parameters.

```
PARAMETER (NRMAX=20000,NXMAX=51,NYMAX=51,NETAMX=25,NEQMAX=1)
```

with:

<b>NRMAX</b>	maximum number of flying particles
<b>NXMAX</b>	maximum number of grid points of concentration grid in x-direction
<b>NYMAX</b>	maximum number of grid points of concentration grid in y-direction
<b>NETAMX</b>	maximum number of vertical levels in $\eta$ -system
<b>NEQMAX</b>	maximum number of sources

In the following, the function of each subroutine is briefly described.



**Figure 7. Illustration of module structure of TRAVELING**

## **SUBROUTINE INPUT**

is called by the main program and reads grid parameters of the meteorological grid from logical unit 30 and the user-defined input data from standard input unit (commonly, logical unit 5). In addition, it calls the subroutine KNSIST.

## **SUBROUTINE KNSIST**

is called by the subroutine INPUT and checks the consistency of the most important user-defined input variables.

The program stops with an appropriate message on the printer if:

- the maximum dimensions defined in the PARAMETER-statement explained above are exceeded;
- the source parameters are meaningless under unstationary conditions (e.g. if release stops before it starts);
- sampling intervals and chosen timestep are inconsistent
- TRAVELING grid parameters and grid parameters of the meteorological grid are inconsistent.

## **SUBROUTINE INITIL**

is called by the main program and initializes all arrays and variables. All particles are located in an imaginary "pool" outside of the simulation area. It reads the topography data from input unit 30 and calls the

## **SUBROUTINE INTTOP**

which performs a linear interpolation of the topography data from meteorological grid into the concentration grid.

Further, INITIL calls the

## **SUBROUTINE RANNOR**

which creates a large number ( $5 \times \text{NRMAX}$ ) of Gaussian random numbers with zero mean and unit variance. The algorithm used to generate the random numbers is independent of the computer system used (see for example [36]), but it can be substituted easily by any other subroutine available in a system library.

From the ensemble of Gaussian random numbers subensembles are drawn randomly using a uniform random number generator to initialize the turbulent velocity fluctuations.

It is evident that such subensembles of Gaussian random numbers are also Gaussian with zero mean and unit variance. This is done in the

### **SUBROUTINE RANDNO.**

Subroutine RANDNO is also called by the main program for each timestep.

The routine itself calls the

### **SUBROUTINE RANUN**

three times to generate three independent sets of uniform distributed random numbers. The algorithm used in RANUN is the congruence method of Lehmer. It can be applied on every computer system if the intrinsic function **IAND(IA,IB)** is available which returns the bitwise logical sum of the INTEGER variables IA and IB. This subroutine can also be substituted easily by another appropriate subroutine available in a system library.

### **SUBROUTINE BANNER**

together with

### **SUBROUTINE SCRIPT**

are called twice. Firstly, in INITIL, they print a leading header with date and start-time of the simulation run. Secondly, they are called in the main program at the end of the simulation to print a trailer with date and stop-time of the simulation run.

### **SUBROUTINE BOXSZE**

is called by the main program and calculates, basically, the average volume of each box of the concentration grid using Eq. (3.7). TRAVELING calculates concentration distributions which are averaged over a sampling interval DTSMPL. Therefore, the average volumes are multiplied by the number of averaging intervals which is needed to calculate average concentration distributions. Then the reciprocal of the resulting product is assigned to a three-dimensional array called **VOLUME**.

## SUBROUTINE READDT

is called by the main program and reads the meteorological data from logical input unit 30 during the first timestep, and latter timesteps if unstationary atmospheric conditions are considered. In this case, the program allows for a shift between the time for which the first meteorological data are available and the start of the release which is identical with the beginning of the simulation. This temporal shift might be less than the sampling interval of the meteorological data (see Figure 8 as an illustration).

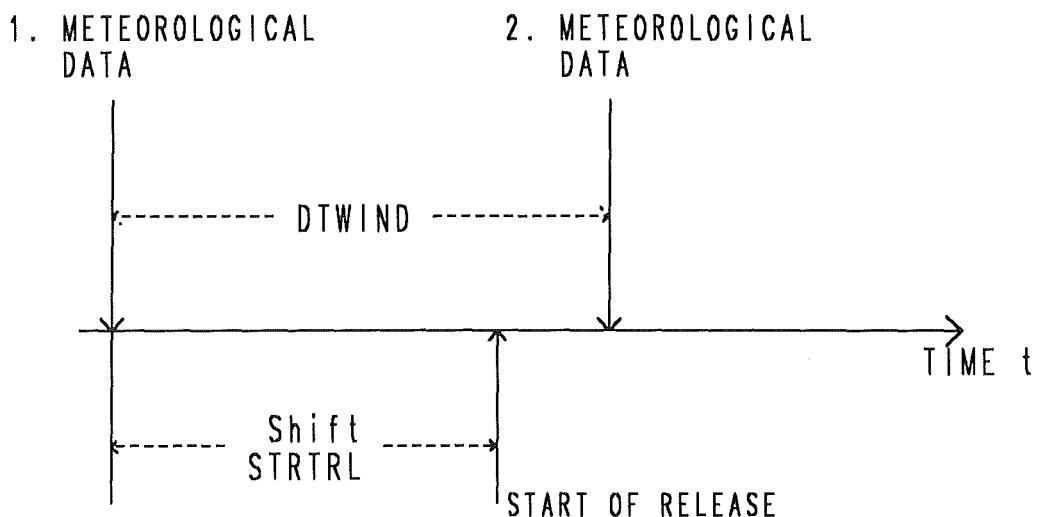


Figure 8. Illustration of relationship between begin of meteorological data and start of release

## SUBROUTINE RELEASE

is called by the main program and controls the release of the particles per timestep.

In the stationary mode this subroutine will be performed only once and all particles will be taken out of an imaginary particle "pool" outside of the simulation area and released from the source during the first timestep.

In the unstationary mode NR particles will be taken out of the pool during each timestep and emitted as long as neither of particles already flying has left the simulation area. If particles are outside the simulation domain they will be reemitted with reinitialized source conditions. Then the number of particles drawn out of the particle pool will be decreased appropriately. Thus, the number of particles released from one or several sources will never exceed the value NR. If the number of particles in the pool is chosen too small the program stops with a message printed on the line printer.

### **SUBROUTINE LOCATE**

is called by the main program. It finds the location of each flying particle and checks whether a particle has left the simulation domain. A flying particle being outside the simulation area is marked. It is not deleted and the number of flying particles is not reduced because TRAVELING has been designed for a vector processor which works more effectively with long particle vectors. Such a particle is put back into the center of the simulation domain and its fraction of mass is set to zero. Thus, the particle does not contribute to the air and ground concentrations.

### **SUBROUTINE VDWDET**

is called by the main program and interpolates the deposition parameters (dry deposition velocity, washout coefficient, deposition height) and the height of the mixing layer (PBL) from the meteorological grid-points to the location of each flying particle.

### **SUBROUTINE DEPOS**

called by the main program, calculates the probabilities for dry and wet deposition and reduces the fraction of mass carried by each particle in the case of deposition.

### **SUBROUTINE REFLEC**

which is called by the main program fulfills the boundary condition of perfect reflection at the ground and parametrizes the behaviour of the particles at the top of the PBL. If a particle is reflected either at the ground surface or at the upper boundary a new vertical index in the meteorological grid is calculated corresponding to the new  $\eta$ -coordinate of the particle.

### **SUBROUTINE SUMMAS**

is called by the main program. From the known particle positions the corresponding indices of the concentration grid are calculated. The proportions of mass of all particles inside a gridbox are summed. In addition, the deposition on the surface is calculated.

### **SUBROUTINE INTPOL**

is called by the main program and performs the 2-D and 3-D linear interpolations of several parameters from the meteorological grid points to the location of each particle. In addition, parts of the vertical drift velocity according to [9] are calculated.

### **SUBROUTINE SIGUVW**

is called by the main program and determines the standard deviations of the velocity fluctuations, the Lagrangian autocorrelation functions, and the vertical drift velocity under inhomogeneous conditions.

### **SUBROUTINE TRAINF**

is called by the main program and prints, if desired, trajectory informations of a selected particle and a few other useful informations. Printing stops when the selected particle has left the simulation area.

### **SUBROUTINE INITFL**

is called by the main program and initializes the fluctuating velocity components for all particles at the time of their emission and reemission.

### **SUBROUTINE TRAJEK**

is called by the main program and calculates the new position of each particle in the terrain following coordinate system at the end of a timestep. For this purpose the transformations of the vertical velocity fluctuations into the  $\eta$ -system and of the Lagrangian velocity components into the Eulerian frame of reference are carried out.

### **SUBROUTINE CONDOS**

is called by the main program and calculates the time-averaged air and ground concentrations

### **SUBROUTINE WRITEP**

is called by the main program and creates, if desired, printer dumps of the concentration and deposition fields, the number of independent particles in a gridbox, and the heights above sea level of the lower and upper boundaries of a selected vertical layer.

#### **SUBROUTINE WRITEK**

is called by the main program and stores heights above sea level, concentration fields, deposition fields and other informations on logical output unit MOUT:

#### **SUBROUTINE PRECIS**

called at first by the main program determines the smallest positive number on the computer system used which, if it is added to one, gives a value different from 1. This number is referred to as the machine accuracy or rounding error ([37]).

### **4.2 The Input Data**

TRAVELING requires two different kinds of input data.

1. The meteorological data and all informations related to the meteorological grid are expected in  
*binary code*  
*on logical input unit 30*
2. User-defined input data to set-up a specific simulation run are expected on the  
*standard logical input unit*  
of the computer system which commonly is the logical unit 5.

#### **4.2.1 Meteorological data and structure of input data-file**

As already mentioned several times, TRAVELING needs the three dimensional flow and turbulence fields as input parameters which are provided by the non-hydrostatic mesoscale model KAMM with respect to the terrain following coordinate system which is referred to as the  $\eta$ -system.

Before the meteorological data are read, informations on the meteorological grid and the topography data are expected. They are read only once in any case.

Particularly, all necessary parameters and variables are, in the sequence as they are read:

1. number of horizontal grid points, NXKA, NYKA;

2. number of vertical  $\eta$ -levels, NETAKA;
3. horizontal grid resolutions in meter, DXKA, DYKA;
4. transformation parameter p, PARAKA.
5. the topography H (in meter)
6. the components  $\bar{u}$  (m/s),  $\bar{v}$  (m/s),  $\bar{\omega}$  (1/s) of the mean wind field;
7. the potential temperature  $\Theta$  (K);
8. the turbulent kinetic energy E ( $m^2/s^2$ );
9. the Lagrangian time scales  $T_{Lx}$ ,  $T_{Ly}$ ,  $T_{Lz}$  (in seconds);
10. the dry deposition velocity (m/s);
11. the height of the planetary boundary layer  $H_{mix}$  (in meter above topography).

In the stationary mode of application these data will be read only once. In the unstationary mode the atmospheric conditions change and the meteorological parameters defined above have to be available several times (e.g. 24 times if a complete diurnal variation is simulated with a meteorological sampling interval of one hour).

The program expects that the data are available ***in binary code*** on the

***logical input-unit 30.***

The following FORTRAN statements show how all the data are read in the TRAVELING subroutines INPUT, INITIL, and READDT, respectively.

```

C*****
C      READ OF KAMM GRID PARAMETERS (ONLY ONCE)          *
C      IN SUBROUTINE INPUT                            *
C*****
C
C      READ (30) NXKA,NYKA,NETAKA,DXKA,DYKA,PARAKA

C
C*****
C      READ OF TOPOGRAPHY (ONLY ONCE)          *
C      IN SUBROUTINE INITIL                      *
C*****
C
C      DO 110 J=1,NYKA
C             READ(30) (H(I,J),I=1,NXKA)
110    CONTINUE

C
C*****INPUT OF METEOROLOGICAL AND TURBULENCE DATA,      *
C*****CALCULATED WITH KAMM, FROM UNIT 30                  *
C*****IN SUBROUTINE READDT                            *
C*****MEAN ZONAL WIND COMPONENT (X-DIRECTION)
C
C      DO 10 K = 1,NETA
C             DO 20 J = 1,NYKA
C                   READ(30) (U(I,J,K),I=1,NXKA)
20      CONTINUE
10      CONTINUE

C
C      MEAN LATERAL WIND COMPONENT (Y-DIRECTION)
C
C      DO 11 K = 1,NETA
C             DO 21 J = 1,NYKA
C                   READ(30) (V(I,J,K),I=1,NXKA)
21      CONTINUE
11      CONTINUE

C
C      MEAN VERTICAL WIND COMPONENT (OMEGA IN ETA-SYSTEM)
C
C      DO 12 K = 1,NETA
C             DO 22 J = 1,NYKA
C                   READ(30) (W(I,J,K),I=1,NXKA)
22      CONTINUE
12      CONTINUE

```

```

C
C      POTENTIAL TEMPERATURE
C
DO 13 K = 1,NETA
    DO 23 J = 1,NYKA
        READ(30) (T(I,J,K),I=1,NXKA)
23    CONTINUE
13    CONTINUE
C
C      TURBULENT KINETIC ENERGY
C
DO 14 K = 1,NETA
    DO 24 J = 1,NYKA
        READ(30) (TE(I,J,K),I=1,NXKA)
24    CONTINUE
14    CONTINUE
C
C      LAGRANGIAN TIME SCALE X-DIRECTION
C
DO 15 K = 1,NETA
    DO 25 J = 1,NYKA
        READ(30) (TLX(I,J,K),I=1,NXKA)
25    CONTINUE
15    CONTINUE
C
C      LAGRANGIAN TIME SCALE Y-DIRECTION
C
DO 16 K = 1,NETA
    DO 26 J = 1,NYKA
        READ(30) (TLY(I,J,K),I=1,NXKA)
26    CONTINUE
16    CONTINUE
C
C      LAGRANGIAN TIME SCALE VERTICAL DIRECTION
C
DO 17 K = 1,NETA
    DO 27 J = 1,NYKA
        READ(30) (TLZ(I,J,K),I=1,NXKA)
27    CONTINUE
17    CONTINUE
C
C      DRY DEPOSITION VELOCITY (M/S)
C
DO 28 J = 1,NYKA
    READ(30) (ETAMIX(I,J),I=1,NXKA)
28    CONTINUE

```

```
C  
C      HEIGHT OF PBL (IN METER)  
C  
DO 29 J = 1,NYKA  
    READ(30) (ETAMIX(I,J),I=1,NXKA)  
29    CONTINUE
```

#### 4.2.2 User-defined input data

User-defined input data are necessary to set-up a specific simulation run. They are expected on the

*standard logical input-unit*

of the computer system which commonly is the logical unit 5.

The input variables define the following model parameters:

- mode of application
- the size of the TRAVELING (concentration) grid
- the timestep and the number of timesteps
- the number of particles per timestep
- the sampling interval of meteorological data
- the source and deposition parameters
- parameters steering the lineprinter output and the storage of results

The data are read by list-directed read statements in the subroutine INPUT; the type of the variables (REAL or INTEGER) is according to the FORTRAN convention. If several variables are read in one line they have to be separated by a blank or a comma.

The following variables must be assigned to a value or a logical expression:

<b>STATNY</b>	<b>LOGICAL</b>	= .TRUE.      stationary mode = .FALSE.     unstationary mode
<b>NXTR</b>	<b>INTEGER</b>	number of grid points in the x-direction of TRAVELING (concentration) grid
<b>NYTR</b>	<b>INTEGER</b>	number of grid points in the y-direction of TRAVELING (concentration) grid
<b>NETA</b>	<b>INTEGER</b>	number of vertical levels of $\eta$ -system; • must be identical to NETAKA (see Sect. 4.2.1)
<b>DXTR</b>	<b>REAL</b>	resolution (in meter) of concentration grid (x-direction) • $DXTR \leq DXKA$ (see Sect. 4.2.1) • $DXKA$ must be an integer multiple of $DXTR$
<b>DYTR</b>	<b>REAL</b>	resolution (in meter) of concentration grid (y-direction) • $DYTR \leq DYKA$ (see Sect. 4.2.1) • $DYKA$ must be an integer multiple of $DYTR$

<b>PARAF</b>	<b>REAL</b>	transformation parameter p; • must be identical to PARAKA
<b>DT</b>	<b>REAL</b>	duration of timestep (s)
<b>NDT</b>	<b>INTEGER</b>	number of timesteps • should be a large number in stationary mode • defines the end of simulation in unstationary mode
<b>NR</b>	<b>INTEGER</b>	number of particles per timestep
<b>DTWIND</b>	<b>REAL</b>	sampling interval (s) of meteorological data • must be an integer multiple of DT • only relevant for unstationary mode • will be set to DTWIND = 1.E+06 by the program for stationary mode
<b>STRTRL</b>	<b>REAL</b>	time of start of release (s); • has to be given relative to time of the first meteorological data available • only relevant for unstationary mode • will be set to STRTRL = 0. by the program for stationary mode
<b>STOPRL</b>	<b>REAL</b>	duration of release (s); • only relevant for unstationary mode • will be set to STOPRL = DT by the program for stationary mode
<b>STRTSP</b>	<b>REAL</b>	time of beginning of sampling (s) after the start of the release • must be an integer multiple of DT • only relevant for unstationary mode • will be set to STRTSP = 0. by the program for stationary mode
<b>DTSMPL</b>	<b>REAL</b>	sampling interval (s) • must be an integer multiple of DT • only relevant for unstationary mode • will be set to STSMPL = DT by the program for stationary mode
<b>NEQ</b>	<b>INTEGER</b>	number of sources considered

the following group of 4 source parameters has to be defined in one line;  
 for each source (NEQ-times) one input line must appear;

<b>SPX</b>	<b>REAL</b>	x-component of source position (in meter) relative to the lower-left edge of the concentration grid
<b>SPY</b>	<b>REAL</b>	y-component of source position (in meter) relative to the lower-left edge of the concentration grid
<b>SPZ</b>	<b>REAL</b>	height of source (in meter) above topography
<b>Q</b>	<b>REAL</b>	source strength (in mass units per second, e.g. kg/s)

end of variables defining the source parameters

<b>DEPOSI</b>	<b>LOGICAL</b>	= .TRUE. deposition is considered = .FALSE. deposition is not considered
<b>WSHLAM</b>	<b>REAL</b>	washout coefficient (1/s)
<b>DEPHGT</b>	<b>REAL</b>	deposition height (in meter above topography); <ul style="list-style-type: none"> <li>• defines the height below which dry deposition will be considered</li> <li>• commonly, DEPHGT = 1. is used</li> </ul>
<b>UPBND</b>	<b>REAL</b>	top of the model domain (in meter above mean sea level) <ul style="list-style-type: none"> <li>• must not necessarily be identical with the height of the PBL</li> <li>• must be the same value as used in the mesoscale model KAMM</li> </ul>
<b>KZLEV</b>	<b>INTEGER</b>	air concentrations are only calculated and stored for the vertical layers 1, ..., KZLEV $1 \leq KZLEV \leq (NETA-1)$
<b>OUTPRT</b>	<b>LOGICAL</b>	= .TRUE. extended lineprinter output is desired = .FALSE. only a few informations are printed
<b>IXDMP</b>	<b>INTEGER</b>	if an extended printer output is desired, the output for the height (in meter) of vertical levels KZDMP (see be- low) and KZDMP+1, the air and ground concen- trations, and the number of independent particles per volume element begins at grid point IXDMP in the x- direction $1 \leq IXDMP \leq NXTR$

<b>IYDMP</b>	<b>INTEGER</b>	if an extended printer output is desired, the output for the height (in meter) of vertical levels KZDMP (see below) and KZDMP+1, the air and ground concentrations, and the number of independent particles per volume element begins at grid point IYDMP in the y-direction $1 \leq IYDMP \leq NYTR$
<b>KZDMP</b>	<b>INTEGER</b>	if an extended printer output is desired, the output for air concentrations is given for vertical level KZDMP $1 \leq KZDMP \leq (NETA-1)$
<b>OUTTRJ</b>	<b>LOGICAL</b>	= .TRUE.      trajectory informations are printed = .FALSE.     no trajectory informations are printed
<b>NOUT</b>	<b>INTEGER</b>	number of a single particle for which trajectory information is printed
<b>OUTDSK</b>	<b>LOGICAL</b>	= .TRUE.      results are stored = .FALSE.     results are not stored
<b>MOUT</b>	<b>INTEGER</b>	number of logical output unit to store the results

The user is led through the user-defined input section by some descriptive informations.

An example how this input could look like for a stationary simulation is given below.

In this example the size of the concentration grid is (51\*51\*25) gridpoints with a horizontal resolution of 100 meters in both horizontal directions. The highest  $\eta$ -level corresponds to the top of the model domain which in this case is 800 m above sea level.

The timestep is 5 s and 18000 particles are released.

The source is located at  $x=0$  m and  $y=2500$  m. The emission height is 100 m and the source strength 1 kg/s.

The time parameters, except the timestep, are irrelevant in this stationary case. They will be set to fixed default values in the program itself.

Deposition is not considered.

Extended lineprinter output, trajectory informations for particle number one, and storage of all results are desired. The air concentrations are calculated in 15 levels although the whole simulation domain has been divided into 25 ( $\eta$ -) levels. The printout of concentrations for vertical level 1 (concentrations near the ground) begins at gridpoint 2 in the x, and at gridpoint 21 in the y direction.

' INPUT OF MODEL VARIABLES TO DETERMINE '
   
 '- THE GRID SIZE '
   
 '- THE timestep AND THE NUMBER OF timesteps '
   
 '- THE NUMBER OF PARTICLES PER timestep '
   
 '- THE SAMPLING INTERVAL OF METEOROLOGICAL DATA '
   
 '- THE SOURCE AND DEPOSITION PARAMETERS '
   
 '- THE STEERING OF OUTPUT '
   
  
 'THE DATA ARE READ BY LIST-DIRECTED READ STATEMENTS; THE TYP OF '
   
 'VARIABLES (REAL OR INTEGER) IS ACCORDING TO THE FORTRAN STANDARD '
   
 'IF SEVERAL VARIABLES ARE READ IN ONE LINE THEY HAVE TO SEPERATED '
   
 'BY A BLANK OR A COMMA '
   
  
 '0) MODE OF SIMULATION'
   
 ' STATNY = .TRUE. : STATIONARY        STATNY = .FALSE. : UNSTATIONARY '
   
 ' STATNY '
   
 '.TRUE.'
   
 '1) GRID VARIABLES'
   
 'NUMBER IN X-DIRECT.    NUMBER IN Y-DIRECT.    NUMBER OF VERTICEL LEVELS'
   
 '                        NXTR                        NYTR                        NETA
   
 '                        51                            51                            25
   
 'GRID SIZES (X UND Y) IN M    SCALE PARAMETER FOR ETA-TRANSFORM.
   
 '                        DXTR                        DYTR                        PARAF
   
 '                        100.                        100.                        5.887
   
 'TIMESTEP (S)    NUMBER OF TIMESTEPS    NUMBER PARTICLES/TIMESTEP
   
 '                        DT                        NDT                        NR
   
 '                        5.                        10000                        18000
   
 'SAMPLING INTERVAL OF METTEOROLOGICAL DATA
   
 '                        DTWIND
   
 '                        36000.
   
 '2) SOURCE, RELEASE AND SAMPLING PARAMETER'
   
 'START RELEASE (s)                                STOP RELEASE (s)
   
 '                        STRTRL                        STOPRL
   
 '                        0.                            100000.
   
 'START SAMPLING (s)                                SAMPLING-INTERVAL (s)
   
 '                        STRTSP                        DTSMPL
   
 '                        1800.                        600.
   
 'NUMBER OF SOURCES'
   
 '                        NEQ
   
 '                        1

'SOURCE COORDINATES X, Y, AND Z (M) SOURCE STRENGTH (MASS UNITS/S) '  
 SPX SPY SPZ Q  
 FOLLOWING LINE MUST APPEAR NEQ TIMES  
 0. 2500. 100. 1.  
 '3) DEPOSITION PARAMETER'  
 'DEPOSITION FLAG WASHOUT (1/S) DEPOSITION HEIGHT (M) '  
 DEPOSI WSHLAM DEPHGT  
 .FALSE. 0.0 1.0  
 '4) MODEL BOUNDARY '  
 'UPBND'  
 800.  
 '5) CALCUALTION OF CONCENTRATION'  
 'AIR CONCENTRATIONS ARE DETERMINED IN THE LOWEST KZLEV LEVELS '  
 KZLEV '  
 15  
 '6) STEERING OF OUTPUT'  
 'EXTENDED PRINTEROUTPUT (CONCENTRATIONS) DESIRED? '  
 OUTPRT '  
 .TRUE.  
 'AT WHICH GRID POINTS (X AND Y) THE PRINTER OUTPUT SHOULD BEGIN '  
 'AND FOR WHICH VERTICAL LEVEL  
 IXDMP JYDMP KZDMP  
 2 21 1  
 'TRAJECORY INFORMATIONS FOR A SPECIFIED PARTICLE DESIRED?  
 OUTTRJ '  
 .TRUE.  
 'FOR WHICH PARTICLE?  
 NOUT '  
 1  
 'STORAGE OF RESULTS DESIRED?  
 OUTDSK '  
 .TRUE.  
 'ON WHICH LOGICAL UNIT?  
 MOUT '  
 20

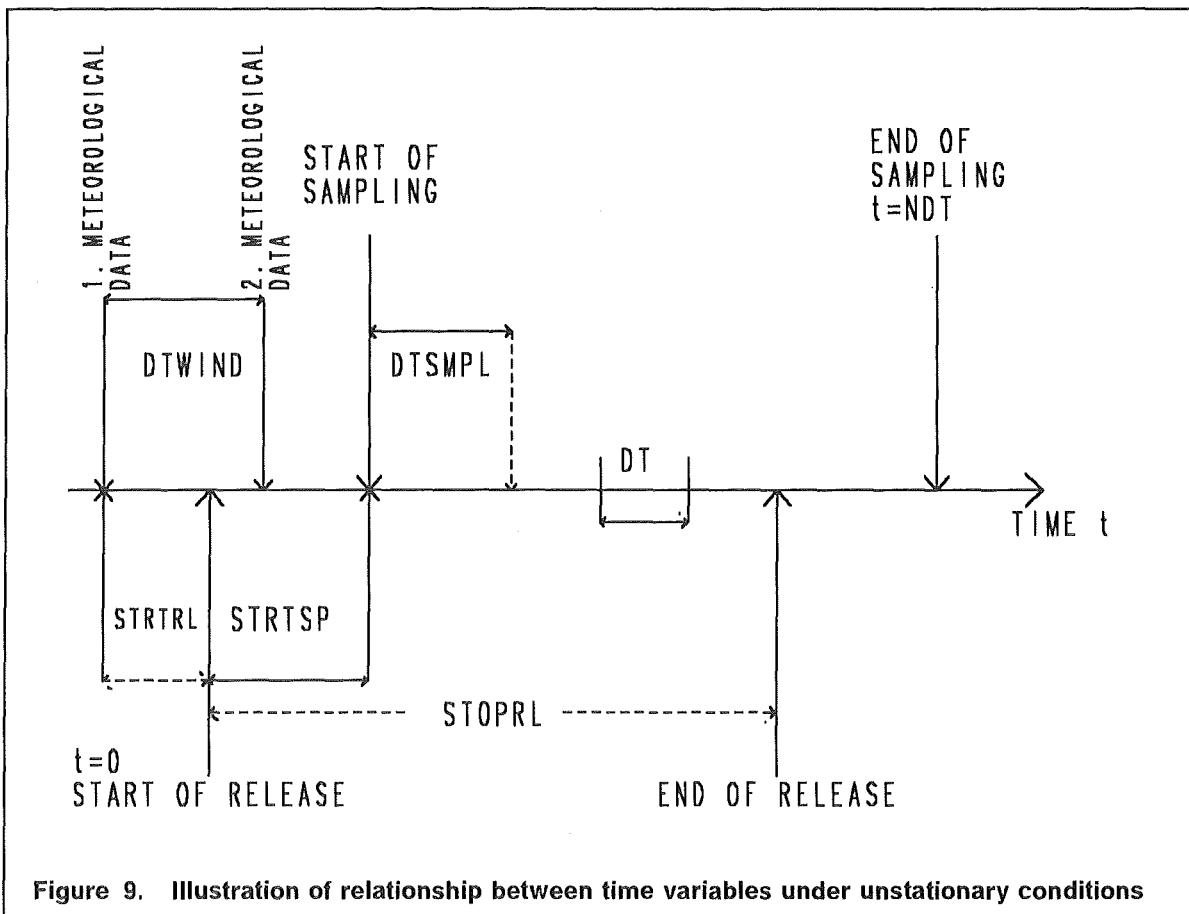


Figure 9. Illustration of relationship between time variables under unstationary conditions

All time variables and their relationships are illustrated in Figure 9.

The first timestep and thus tracking of particles begins at the time of the release. Despite of this, the first "observation" time of meteorological data might lie before the release. This possibility is taken into account by the variable STRTRL. The time interval between two meteorological "observations" is DTWIND. STRTSP seconds after the release the sampling of pollutants, i.e. the calculation of concentrations, begins. The release stops STOPRL seconds after it began. The simulation and thus the sampling stops after NDT timesteps. The diagram demonstrates the possibility that the whole sampling period exceeds the duration of the release. The sampling period might be divided into intervals of length DTSMPL. After each interval average concentration distributions are calculated and stored (if desired). The model timestep DT is also indicated.

## **4.3 The Output Data**

TRAVELING produces two different kinds of output data.

1. The results of the model can be stored unformatted in  
*binary code*  
*on logical output unit MOUT*
2. Informations on the specific simulation run are printed on the lineprinter. The standard output unit corresponding to the lineprinter is commonly the logical unit 6.

### **4.3.1 Storage of results**

Storage of the results is optional. The following data can be stored:

1. geometric heights (in meters) of KZLEV  $\eta$ -levels above mean sea level;  
will be stored only once;  
Dimension of each level: (NXTR \* NYTR)
2. three-dimensional distributions of air concentrations;  
Dimension: (NXTR \* NYTR \* KZLEV)
3. three-dimensional distribution of number of independent particles;  
Dimension: (NXTR \* NYTR \* KZLEV)
4. two-dimensional distribution of dry deposition flux;  
Dimension: (NXTR \* NYTR)
5. two-dimensional distribution of wet deposition flux;  
Dimension: (NXTR \* NYTR)

Each of these fields is preceded by a header. At the beginning of the whole storage file, informations on the concentration grid, the simulation domain, the source configuration, and the length of the headings are stored once.

For a stationary run the whole data described above are stored only once.

In the unstationary case the data explained under points 2.), ..., 5.) of the list above are stored after each sampling interval.

The FORTRAN program below shows, as an example, a possible interface to read for further evaluation the results stored during an unstationary simulation with five sampling intervals.

```

C
PARAMETER (NXMAX=100,NYMAX=100,NZMAX=81,NQMAX=10)
PARAMETER (IRUN=5)
*****
*
* FUNCTION.: INTERFACE TO READ THE STORED RESULTS
* FROM UNIT 20
*
*
*
*
*
* PARAMETER:
*      NXMAX = MAXIMUM DIMENSION X_DIRECTION
*      NYMAX = MAXIMUM DIMENSION Y_DIRECTION
*      NZMAX = MAXIMUM DIMENSION Z_DIRECTION
*      NQMAX = MAXIMUM NUMBER OF SOURCES
* STATIONARY SIMULATION : IRUN = 1
* UNSTATIONARY SIMULATION : IRUN = NUMBER OF AVERAGING INTERVALS
*
*
*
*
*
* PARAMETER READ FROM UNIT 20:
*
*      NXTR      GRIDPOINTS IN X-DIRECTION
*      NYTR      GRIDPOINTS IN Y-DIRECTION
*      NETATTR   GRIDPOINTS IN Z-DIRECTION
*              UP TO THE MODEL BOUNDARY
*      KZLEV     CONCENTRATIONS ARE STORED UP
*              TO KZLEV LAYERS
*      DXTR      GRID RESOLUTION X DIRECTION
*      DYTR      GRID RESOLUTION Y DIRECTION
*      PARAF     TRANSFORMATION PARAMETER
*      NEQ       NO. OF SOURCES
*      UPBND    UPPER BOUNDARY OF MODEL DOMAIN
*      SPX       X LOCATION (M) OF SOURCES
*      SPY       Y LOCATION (M) OF SOURCES
*      SPZ       HEIGHT (M) OF SOURCES
*      LENTDM   LENGTH OF HEADING STRINGS
*
*      HZ        GEOMETRICAL HEIGHT MATRIX
*      CK        AIR-CONCENTRATION MATRIX
*      FP        NO. OF INDEPENDENT PARTICLES
*      CD        DRY DEPOSITION MATRIX
*      CW        WET DEPOSITION MATRIX
*
*
*****

```

```

C
DIMENSION CK(NXMAX,NYMAX,NZMAX),HZ(NXMAX,NYMAX,NZMAX)
DIMENSION FP(NXMAX,NYMAX,NZMAX)
DIMENSION CD(NXMAX,NYMAX)
DIMENSION CW(NXMAX,NYMAX)
DIMENSION LENTDM(5)
DIMENSION SPX(NQMAX),SPY(NQMAX),SPZ(NQMAX)

C
      READ (20) NXTR,NYTR,NETATTR,KZLEV,
+          DXTR,DYTR,NEQ,PARAF,UPBND
      WRITE(6,*) NXTR,NYTR,NETATTR,KZLEV,
+          DXTR,DYTR,NEQ,PARAF,UPBND
      READ (20) LENTDM

C
      DO 300 NQ=1,NEQ
      READ (20) SPX(NQ),SPY(NQ),SPZ(NQ)
300    CONTINUE

C
      CALL READK(1,HZ,NXMAX,NYMAX,NZMAX,LENTDM)

C
      DO 9000 MM=1,IRUN

C
      DO 9005 KZ=1,NZMAX
      DO 9004 JY=1,NYMAX
      DO 9003 JX=1,NXMAX
      CK(JX,JY,KZ)=-999.9
9003    CONTINUE
9004    CONTINUE
9005    CONTINUE

C
      CALL READK(2,CK,NXMAX,NYMAX,NZMAX,LENTDM)
      CALL READK(3,FP,NXMAX,NYMAX,NZMAX,LENTDM)
      CALL READK(4,CD,NXMAX,NYMAX,     1,LENTDM)
      CALL READK(5,CW,NXMAX,NYMAX,     1,LENTDM)

C
*
*
*
* further data evaluation by the user
*
*
C
9000  CONTINUE
C
      STOP
      END

```

```
SUBROUTINE READK(ITYPE,VALUES,NXMAX,NYMAX,NZMAX,LENTDM)
```

```
*****
*      FUNCTION.: INPUT      OF HEIGHT, CONCENTRATION, AND DEPOSITION      *
*                  FIELDS FROM UNIT 20                                     *
*      INPUT....: ITYPE    = SWITCH FOR THE ARRAYS ABOVE (1,2,3,4,5)      *
*                  NXMAX    = MAXIMUM DIMENSION X_DIRECTION                 *
*                  NYMAX    = MAXIMUM DIMENSION Y_DIRECTION                 *
*                  NZMAX    = MAXIMUM DIMENSION Z_DIRECTION                 *
*                  VALUES   = VALUES TO BE PRINTED                      *
*                  LENTDM  = LENGTHS OF TEXTS IN TDIM                     *
*      THE FOLLOWING RELATIONS ARE VALID:                                *
*      ITYPE   VALUES   NDIM3   CONTENTS                               *
*      -----  -----  -----  -----
*      1       HZ      NETAB   GEOMETRICAL HEIGHT MATRIX             *
*      2       CK      NETAB   AIR CONCENTRATION MATRIX              *
*      3       FP      NETAB   NO OF INDEPENDENT PARTICLES           *
*      4       CD      1       DRY DEPOSITION MATRIX                 *
*      5       CW      1       WET DEPOSITION MATRIX                 *
*      LOCAL VAR: IX      = LOOP INDEX (1,...,NXMAX)                *
*                  JX      = LOOP INDEX (1,...,NYMAX)                *
*                  NZB     = LOOP INDEX (1,...,NZMAX)                *
*                  TDIM   = TEXT ARRAY FOR PRINT OF PHYS. DIMENSIONS  *
*      CALLS....: REAL    R*4-FUNCT.  FORTRAN                         *
*                  MIN     INT-FUNCT.  FORTRAN                         *
*      ****
```

```
C      REAL VALUES(NXMAX,NYMAX,NZMAX)
```

```
C      ****
*      DATAAREA: LOCAL ARRAYS AND CONSTANTS                         *
*      ****
```

```
C      CHARACTER*40 TDIM(5)
C      CHARACTER*40 BLANK
```

```
C      INTEGER LENTDM(5)
```

```
C      DATA BLANK '/'          '/'
```

```
*****
```

```

*      END OF DATAAREA
*****
C
      TDIM(ITYPE)=BLANK
C
      DO 300 NZ=1,NZMAX
         DO 290 JY=1,NYMAX
            DO 280 IX=1,NXMAX
               VALUES(IX,JY,NZ)=0.0
280      CONTINUE
290      CONTINUE
300      CONTINUE
C
      READ (20) TDIM(ITYPE)(:LENTDM(ITYPE))
      WRITE(6,6000) TDIM(ITYPE)(:LENTDM(ITYPE))
6000    FORMAT(1X,A)
100     CONTINUE
C
      READ (20) IX,JY,NZK
      IF (IX.GT.-1) THEN
         READ (20) NNXMAX,(VALUES(IX+II,JY,NZK),II=0,NNXMAX)
      ELSE
         GOTO 200
      END IF
C
      GOTO 100
C
200     CONTINUE
C
      IF (IX.GT.-2) THEN
         GOTO 100
      ELSE
         RETURN
      END IF
C
      E N D

```

### 4.3.2 Lineprinter output

To explain the lineprinter output an example is shown corresponding to a run of the model according to the input example in Section 4.2.2.

The meteorological data for the example will not further be described because they are purely hypothetical.

Most of the printed informations are self-explaining, perhaps with the exception of the trajectory informations. Therefore, the meanings of the particular columns are explained below:

<b>T(S)</b>	time of travel of selected particle
<b>X(KM)</b>	X-position of selected particle in km from the lower-left edge of the grid
<b>Y(KM)</b>	Y-position of selected particle in km from the lower-left edge of the grid
<b>ETA</b>	vertical position of selected particle with respect to the terrain following coordinate system ( $\eta$ -system)
<b>Z(M)</b>	vertical position of selected particle in meter above topography
<b>UX</b>	zonal turbulent (random) velocity component (m/s)
<b>VY</b>	lateral turbulent (random) velocity component (m/s)
<b>WZ</b>	vertical turbulent (random) velocity component (m/s)
<b>REST</b>	percentage of remaining fraction of mass carried by the specific particle after dry and/or wet deposition
<b>DEMA</b>	fraction of mass carried by the particle
<b>I, J, K</b>	lower-left corner of volume element where the particle is located in grid-units
<b>NOUT</b>	particles outside of the simulation area; includes also the particle in the "pool"
<b>NDRY</b>	number of particles deposited by dry deposition during a timestep
<b>NWET</b>	number of particles deposited by wet deposition during a timestep
<b>NRFLY</b>	number of flying particles

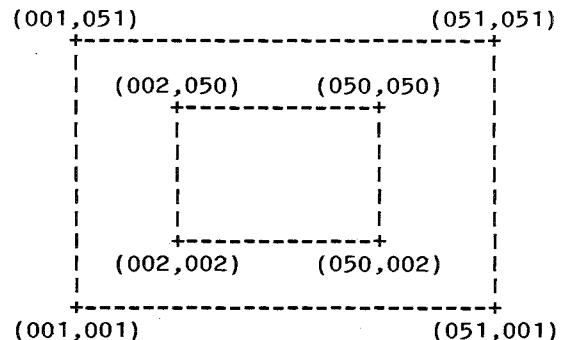
**NEFF**

number of particles contributing effectively to the concentration distribution

ISEED= 36178110

TTTTTTTTTTTTT	RRRRRRRRRRR	AAAAAAA	VV	VV	EEEEEEEEE	LL		NN	NN	GGGGGGGGGGG
TTTTTTTTTTTTT	RRRRRRRRRRR	AAAAAAAAAA	VV	VV	EEEEEEEEE	LL		NNN	NN	GGGGGGGGGGGG
TT	RR RRR	AAA AA	VV	VV	EE	LL		NNNN	NN	GG GGG
TT	RR RR	AA AA	VV	VV	EE	LL		NNNN	NN	GG
TT	RR RRR	AA AA	VV	VV	EE	LL		NN NNN	NN	GG
TT	RRRRRRRRRRR	AAAAAAAAAA	VV	VV	EEEEEEEEE	LL		NN NNN	NN	GG GGGGGGG
TT	RRRRRRRRRRR	AAAAAAAAAA	VV	VV	EEEEEEEEE	LL		NN NNN	NN	GG GGGGGGG
TT	RRRR	AA AA	VV	VV	EE	LL		NN NNN NN	GG GGG	
TT	RR RRR	AA AA	VV	VV	EE	LL		NN NNNNN	GG GG	
TT	RR RRR	AA AA	VV	VV	EE	LL		NN NNNNN	GG GGG	
TT	RR RRR	AA AA	VVVV	VVVV	EEEEEEEEE	LLLLLLLLLL		NN	NNN	GGGGGGGGGGGG
TT	RR RRR	AA AA	VV	VV	EEEEEEEEE	LLLLLLLLLL		NN	NN	GGGGGGGGGGGG
SSSSSSSSSSS	TTTTTTTTTTTT	AAAAAAA	TTTTTTTTTTTT		0000000000	NN	NN			
SSSSSSSSSSS	TTTTTTTTTTTT	AAAAAAAAAA	TTTTTTTTTTTT		000000000000	NNN	NN			
SSS	TT	AAA AA	TT		000	000	NNNN	NN		
SS	TT	AA AA	TT		00	00	NNNNN	NN		
SSS	TT	AA AA	TT		00	00	NN NNN	NN		
SSSSSSSSSSS	TT	AAAAAAAAAA	TT		00	00	NN NNN	NN		
SSSSSSSSSSS	TT	AAAAAAAAAA	TT		00	00	NN NNN	NN		
SSS	TT	AA AA	TT		00	00	NN NNN	NN		
SS	TT	AA AA	TT		00	00	NN NNNNN	NN		
SSS	TT	AA AA	TT		000	000	NN NNNNN	NNNN	XXXXXX	
SSSSSSSSSSS	TT	AA AA	TT		000000000000	NN	NNN	XXXXXX		
SSSSSSSSSSS	TT	AA AA	TT		000000000000	NN	NN	XXXXXX		
000000000000	777777777777		000000000000	44		999999999999	2222222222			
000000000000	777777777777		000000000000	44		999999999999	222222222222			
00	00	777	00	00	44	999	999	222	222	
00	00	777	00	00	44 44	99	99	22	222	
00	00	777	00	00	44 44	999	99		222	
00	00	777	00	00	444444444444	999999999999			222	
00	00	777	00	00	444444444444	999999999999			222	
00	00	777	00	00	44	99		222		
00	00	777	00	00	44	99		222		
00	00	777	XXXXXX	00	44	XXXXXX	999			
00000000000000	777	XXXXXX	000000000000	44	XXXXXX	999999999999	222222222222			
000000000000	777	XXXXXX	000000000000	44	XXXXXX	999999999999	222222222222			
111	000000000000		000000000000	111		44		33333333333		
1111	0000000000000		0000000000000	1111		44		333333333333		
11111	00 00	XXXXXX	00 00	11111		44		333	333	
111 11	00 00	XXXXXX	00 00	111 11		44 44		33		
111 11	00 00	XXXXXX	00 00	111 11		44 44		333		
11	00 00	00	00	11		444444444444		3333333333		
11	00 00	00	00	11		444444444444		3333333333		
11	00 00	XXXXXX	00 00	11		XXXXXX	44		333	
11	00 00	XXXXXX	00 00	11		XXXXXX	44		33	
11	00 00	XXXXXX	00 00	11		XXXXXX	44	333	333	
111111111111	0000000000000		000000000000	111111111111		44		333333333333		
111111111111	000000000000		000000000000	111111111111		44		333333333333		

AREA TO CALCULATE TRAJECTORIES  
AND CONCENTRATIONS ( IN GRID UNITS (GU) ) : :



+-----+  
| SOURCE DATA AND GRID DATA |  
+-----+

SOURCE NO.	X /GU/	Y /GU/	DX /M/	DY /M/	DT /S/	STRENGTH /G/S/	Z-HEIGHT /M/	STARHEIGHT ETA-SYSTEM	NETA	PARAF	NUMBER PARTICLE
1	1.00	26.00	100.00	100.00	5.00	1.000E+00	100.00	0.266	25	5.887	18000

+-----+  
| RELEASE AND SAMPLING TIMES (SEC) |  
+-----+

RELEASE	DURATION	START	SAMPLING	SAMPLING INTERVAL
	5.00		0.00	5.0000

+-----+  
| DEPOSITION PARAMETERS |  
+-----+

DEPOSITION F WASHOUT COEFFICIENT (1/S) DEPOSITION HEIGHT (M)  
0.00E+00 1.00







60 TRAVELING

740.00	4.82	2.21	0.356	147.87	0.37	-0.57	-0.53	1.000	2.778E-04	49	23	9	1233	0	0	18000	18000
745.00	4.85	2.21	0.351	144.88	0.74	-0.86	-0.50	1.000	2.778E-04	50	23	9	1422	0	0	18000	18000
750.00	4.89	2.21	0.345	141.48	0.19	-0.52	-0.62	1.000	2.778E-04	50	23	9	1614	0	0	18000	18000
755.00	4.92	2.20	0.339	137.69	0.51	-0.70	-0.67	1.000	2.778E-04	50	23	9	1836	0	0	18000	18000
760.00	4.95	2.20	0.334	134.73	0.67	-0.45	-0.52	1.000	2.778E-04	51	23	9	2070	0	0	18000	18000
765.00	4.99	2.20	0.333	133.87	0.59	-0.43	-0.11	1.000	2.778E-04	51	23	8	2328	0	0	18000	18000

AFTER 270 TIME STEPS 17803 PARTICLES OF 18000 HAVE LEFT THE AREA

CPU TIME ELAPSED 0.26199E+06









\*\*\*\*\* DRY DEPOSITION \*\*\*\*\* / \*\*\*\*\* CONCENTRATION (MASS UNITS/S/M\*\*2) \*\*\*\*\*  
=====

X(KM)	Y(KM)	2.00	2.10	2.20	2.30	2.40	2.50	2.60	2.70	2.80	2.90	3.00	3.10	3.20
0.10														

0.20 | THE WHOLE MATRIX CONTAINS ZEROS BECAUSE DEPOSITION IS NOT CONSIDERED  
0.30 |

\*\*\*\*\* WET DEPOSITION \*\*\*\*\* / \*\*\*\*\* CONCENTRATION (MASS UNITS/S/M\*\*2) \*\*\*\*\*  
=====

X(KM)	Y(KM)	2.00	2.10	2.20	2.30	2.40	2.50	2.60	2.70	2.80	2.90	3.00	3.10	3.20
0.10														

0.20 | THE WHOLE MATRIX CONTAINS ZEROS BECAUSE DEPOSITION IS NOT CONSIDERED  
0.30 |

HEIGHT OF ETA-PLANES (M) STORED ON UNIT 20

AIR CONCENTRATION (MASS UNITS/M\*\*3) STORED ON UNIT 20

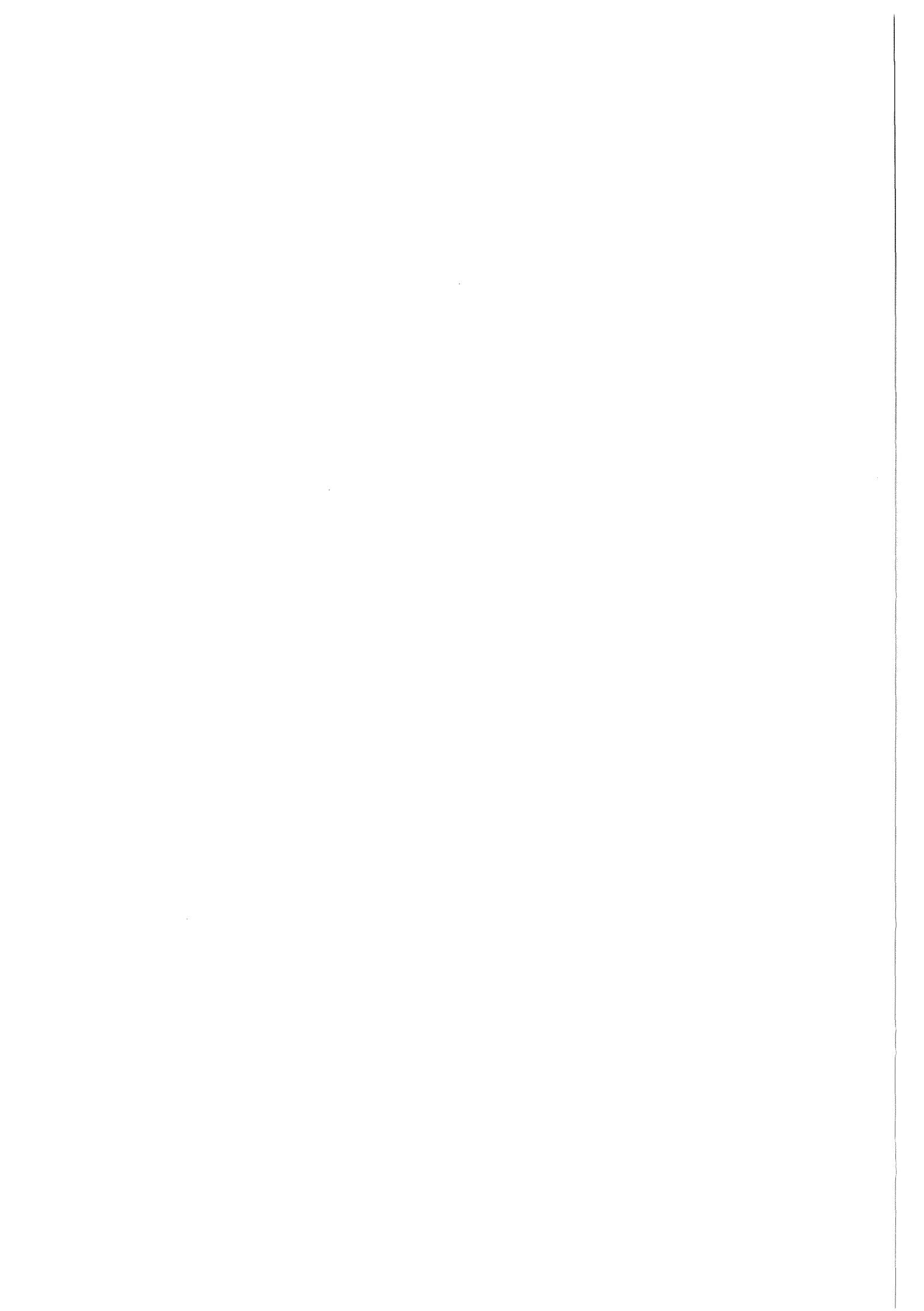
NO. OF INDEPENDENT PARTICLES STORED ON UNIT 20

DRY DEPOSITION (MASS UNITS/S/M\*\*2) STORED ON UNIT 20

WET DEPOSITION (MASS UNITS/S/M\*\*2) STORED ON UNIT 20

TTTTTTTTTTTTT	RRRRRRRRRRR	AAAAAAA	VV	VV	EEEEEEEEE	LL		NN	NN	GGGGGGGGGG
TTTTTTTTTTTTT	RRRRRRRRRRRR	AAAAAAAAAA	VV	VV	EEEEEEEEE	LL		NNN	NN	GGGGGGGGGGGG
TT	RR	RR	AAA	AA	VV	EE		NNNN	NN	GGG GGG
TT	RR	RR	AA	AA	VV	EE		NNNNN	NN	GG
TT	RR	RRR	AA	AA	VV	EE		NN NNN	NN	GG GGGGGGG
TT	RRRR	AA	AA	VV	VV	EE		NN NNN	NN	GG GGGGGGG
TT	RR RRR	AA	AA	VV	VV	EE		NN NNNN	NN	GG CG
TT	RR RRR	AA	AA	VV	VV	EE		NN NNNN	NN	GG GGG
TT	RR RRR	AA	AA	VVVV	EEEEEEEEE	LLLLL		NN	NNN	GGGGGGGGGGGG
TT	RR RRR	AA	AA	VV	EEEEEEEEE	LLLLL		NN	NN	GGGGGGGGGGGG
					EEEEEEEEE	NN	NN	DDDDDDDDDDDD		
					EEEEEEEEE	NNN	NN	DDDDDDDDDDDD		
					EE	NNNN	NN	DD DDD		
					EE	NNNNN	NN	DD DD		
					EE	NN NNN	NN	DD DD		
					EEEEEEEEE	NN NNN	NN	DD DD		
					EEEEEEEEE	NN NNN	NN	DD DD		
					EE	NN NNN NN	NN	DD DD		
					EE	NN NNNNN	DD	DD		
					EE	NN NNNN	DD	DD		
					EEEEEEEEE	NN NNN	DDDDDDDDDDDD			
					EEEEEEEEE	NN	NN	DDDDDDDDDDDD		
000000000000	777777777777			000000000000	44		999999999999	2222222222		
000000000000	777777777777			000000000000	44		999999999999	222222222222		
00	00	777		00	00	44	999	999	222	222
00	00	777		00	00	44 44	99	99	22	222
00	00	777		00	00	44 44	999	99	22	222
00	00	777		00	00	444444444444	999999999999	222		
00	00	777		00	00	444444444444	999999999999		222	
00	00	777		00	00	44		99	222	
00	00	777		00	00	44		99	222	
000000000000	777	XXXXXX		00	00	44	XXXXXX	999	222	
000000000000	777	XXXXXX		000000000000	44	XXXXXX	999999999999	222222222222		
000000000000	777	XXXXXX		000000000000	44	XXXXXX	999999999999	222222222222		
111	000000000000			000000000000	8888888888		44	44		
1111	0000000000000			000000000000	888888888888		44	44		
11111	00 00	XXXXXX		00 00	888 888	XXXXXX	44	44		
111 11	00 00	XXXXXX		00 00	88 88	XXXXXX	44 44	44 44		
111 11	00 00	XXXXXX		00 00	888 888	XXXXXX	44 44	44 44		
11	00 00	00		00 00	8888888888		444444444444	444444444444		
11	00 00	00		00 00	8888888888		444444444444	444444444444		
11	00 00	00		00 00	888 888	XXXXXX	44	44		
11	00 00	00		00 00	88 88	XXXXXX	44	44		
11	00 00	00		00 00	888 888	XXXXXX	44	44		
111111111111	000000000000			000000000000	888888888888		44	44		
111111111111	000000000000			000000000000	888888888888		44	44		





## 5. APPENDIX - THE TRAVELING/COSYMA VERSION

### 5.1 General features

TRAVELING can also be applied in the context of the probabilistic accident consequence assessment model COSYMA (**C**Ode **S**ystem from **M**Aria, where MARIA stands for "Methods for Assessing the Radiological Impact of Accidents") [38], [39], [40]. This version is denoted as TRAVELING/COSYMA.

The major changes compared to the standard version described in the previous chapters are:

- concentrations are time-integrals;
- the variables **STRTSP** and **DTSMPL** denote the beginning and the length of the integration interval (see Sect. 4.2.2);
- a new user-input variable **CONMIN** has been introduced which defines a cut-off value for low air concentrations;
- the arrival time of the plume at each grid point is calculated. It is defined as the time passed from the beginning of an integration interval until the value **CONMIN** is exceeded for the first time at a receptor point.

Simulation of building wake effects, lift-off out of a turbulent building wake, and plume rise are not yet included in the model.

Also,  $\gamma$ -radiation from the radioactive cloud passing overhead is not modelled. Since the COSYMA model expects data to calculate the  $\gamma$ -doses the time-integrated air concentrations of the first layer above the ground are transferred to the ACA codes in an appropriate manner.

It has to be noted that only one species of pollutant, e.g. one species of radioactive material, can be considered.

Only one weather sequence can be taken into account. A division of the dispersion simulation into successive release phases can be accomplished by applying the TRAVELING/COSYMA version in the unstationary mode with a predefined number of timesteps and a predefined length of the integration interval.

## 5.2 The Input Data

### 5.2.1 Meteorological data

The meteorological input part for TRAVELING/COSYMA is completely identical to that described in Sect. 4.2.1.

### 5.2.2 User-defined input data for TRAVELING/COSYMA

The user-defined input data are almost identical to those described in Section 4.2.2. For reasons of completeness also the unchanged input parameters are repeated here.

The data are expected on the

***standard logical input-unit***

of the computer system which commonly is the logical unit 5.

The input variables define the following model parameters:

- mode of application
- the size of the TRAVELING (concentration) grid
- the timestep and the number of timesteps
- the number of particles per timestep
- the sampling interval of meteorological data
- the temporal integration interval for the concentrations
- the source and deposition parameters
- parameters steering the lineprinter output and the storage of results

The data are read by list-directed read statements in the subroutine INPUT; the type of the variables (REAL or INTEGER) is according to the FORTRAN convention. If several variables are read in one line they have to be separated by a blank or a comma.

The following variables must be assigned to a value or a logical expression:

<b>STATNY</b>	<b>LOGICAL</b>	= .TRUE.      stationary mode = .FALSE.   unstationary mode
<b>NXTR</b>	<b>INTEGER</b>	number of grid points in the x-direction of TRAVELING (concentration) grid
<b>NYTR</b>	<b>INTEGER</b>	number of grid points in the y-direction of TRAVELING (concentration) grid
<b>NETA</b>	<b>INTEGER</b>	number of vertical levels of $\eta$ -system; • must be identical to NETAKA

<b>DXTR</b>	<b>REAL</b>	resolution (in meter) of concentration grid (x-direction) <ul style="list-style-type: none"> <li>• <math>DXTR \leq DXKA</math></li> <li>• <math>DXKA</math> must be an integer multiple of <math>DXTR</math></li> </ul>
<b>DYTR</b>	<b>REAL</b>	resolution (in meter) of concentration grid (y-direction) <ul style="list-style-type: none"> <li>• <math>DYTR \leq DYKA</math></li> <li>• <math>DYKA</math> must be an integer multiple of <math>DYTR</math></li> </ul>
<b>PARAF</b>	<b>REAL</b>	transformation parameter p; <ul style="list-style-type: none"> <li>• must be identical to PARAKA</li> </ul>
<b>DT</b>	<b>REAL</b>	duration of timestep (s)
<b>NDT</b>	<b>INTEGER</b>	number of timesteps <ul style="list-style-type: none"> <li>• should be a large number in stationary mode</li> <li>• defines the end of simulation in unstationary mode</li> </ul>
<b>NR</b>	<b>INTEGER</b>	number of particles per timestep
<b>DTWIND</b>	<b>REAL</b>	sampling interval (s) of meteorological data <ul style="list-style-type: none"> <li>• must be an integer multiple of DT</li> <li>• only relevant for unstationary mode</li> <li>• will be set to <math>DTWIND = 1.E+06</math> by the program for stationary mode</li> </ul>
<b>STRTRL</b>	<b>REAL</b>	time of start of release (s); <ul style="list-style-type: none"> <li>• has to be given relative to time of the first meteorological data available</li> <li>• only relevant for unstationary mode</li> <li>• will be set to <math>STRTRL = 0.</math> by the program for stationary mode</li> </ul>
<b>STOPRL</b>	<b>REAL</b>	duration of release (s); <ul style="list-style-type: none"> <li>• only relevant for unstationary mode</li> <li>• will be set to <math>STOPRL = DT</math> by the program for stationary mode</li> </ul>
<b>STRTSP</b>	<b>REAL</b>	time of beginning of integration (s) after the start of the release <ul style="list-style-type: none"> <li>• must be an integer multiple of DT</li> </ul>
<b>DTSMPL</b>	<b>REAL</b>	integration interval (s) <ul style="list-style-type: none"> <li>• must be an integer multiple of DT</li> </ul>
<b>CONMIN</b>	<b>REAL</b>	cut-off value for low concentrations (mass units * s / m**3)
<b>NEQ</b>	<b>INTEGER</b>	number of sources considered

the following group of 4 source parameters has to be defined in one line;  
 for each source (NEQ-times) one input line must appear;

<b>SPX</b>	<b>REAL</b>	x-component of source position (in meter) relative to the lower-left edge of the concentration grid
<b>SPY</b>	<b>REAL</b>	y-component of source position (in meter) relative to the lower-left edge of the concentration grid
<b>SPZ</b>	<b>REAL</b>	height of source (in meter) above topography
<b>Q</b>	<b>REAL</b>	source strength (in mass units per second, e.g. kg/s) <ul style="list-style-type: none"> <li>• <math>Q * DTSMP = 1</math> (mass units) is required, since the ACA codes expect normalized time-integrals</li> </ul>

end of variables defining the source parameters

<b>DEPOSI</b>	<b>LOGICAL</b>	= .TRUE. deposition is considered = .FALSE. deposition is not considered
<b>WSHLAM</b>	<b>REAL</b>	washout coefficient (1/s)
<b>DEPHGT</b>	<b>REAL</b>	deposition height (in meter above topography); <ul style="list-style-type: none"> <li>• defines the height below which dry deposition will be considered</li> <li>• commonly, DEPHGT = 1. is used</li> </ul>
<b>UPBND</b>	<b>REAL</b>	top of the model domain (in meter above mean sea level) <ul style="list-style-type: none"> <li>• must not necessarily be identical with the height of the PBL</li> <li>• must be the same value as used in the mesoscale model KAMM</li> </ul>
<b>KZLEV</b>	<b>INTEGER</b>	air concentrations are only calculated and stored for the vertical layers 1, ..., KZLEV $1 \leq KZLEV \leq (NETA-1)$
<b>OUTPRT</b>	<b>LOGICAL</b>	= .TRUE. extended lineprinter output is desired = .FALSE. only a few informations are printed
<b>IXDMP</b>	<b>INTEGER</b>	if an extended printer output is desired, the output for the height (in meter) of vertical levels KZDMP (see below) and KZDMP+1, the air and ground concentrations, and the number of independent particles per volume element begins at grid point IXdmp in the x-direction

$1 \leq IXDMP \leq NXTR$

<b>IYDMP</b>	<b>INTEGER</b>	if an extended printer output is desired, the output for the height (in meter) of vertical levels KZDMP (see below) and KZDMP+1, the air and ground concentrations, and the number of independent particles per volume element begins at grid point IYDMP in the y-direction $1 \leq IYDMP \leq NYTR$
<b>KZDMP</b>	<b>INTEGER</b>	if an extended printer output is desired, the output for air concentrations is given for vertical level KZDMP $1 \leq KZDMP \leq (NETA-1)$
<b>OUTTRJ</b>	<b>LOGICAL</b>	= .TRUE. trajectory informations are printed = .FALSE. no trajectory informations are printed
<b>NOUT</b>	<b>INTEGER</b>	number of a single particle for which trajectory information is printed
<b>OUTDSK</b>	<b>LOGICAL</b>	= .TRUE. results are stored = .FALSE. results are not stored
<b>MOUT</b>	<b>INTEGER</b>	number of logical output unit to store the results

The user is led through the user-defined input section by some descriptive informations.

An example how this input could look like for an unstationary simulation is given below.

In this example the size of the concentration grid is (51\*51\*25) gridpoints with a horizontal resolution of 100 meters in both horizontal directions. The highest  $\eta$ -level corresponds the top of the model domain which in this case is 800 m above sea level.

The timestep is 10 s and 100 particles are released per timestep.

The source is located at  $x=0$  m and  $y=2500$  m. The emission height is 100 m and the source strength 1.66E-3 (mass units/s).

Integration starts 1800 s after the beginning of the release and the integration interval is 600 s. Altogether, ten integration phases are calculated.

Deposition is considered with a deposition velocity of 1.E-2 m/s.

Extended lineprinter output, trajectory informations for particle number one, and storage of all results are desired. The air concentrations are calculated in 15 levels although the whole simulation domain has been divided into 25 ( $\eta$ -) levels. The printout of concentrations for vertical level 1 (concentrations near the ground) begins at gridpoint 2 in the x, and at gridpoint 21 in the y direction.

' INPUT OF MODEL VARIABLES TO DETERMINE '
   
 '- THE GRID SIZE '
   
 '- THE timestep AND THE NUMBER OF timesteps '
   
 '- THE NUMBER OF PARTICLES PER timestep '
   
 '- THE SAMPLING INTERVAL OF METEOROLOGICAL DATA '
   
 '- THE SOURCE AND DEPOSITION PARAMETERS '
   
 '- THE STEERING OF OUTPUT '
   
  
 'THE DATA ARE READ BY LIST-DIRECTED READ STATEMENTS; THE TYP OF '
   
 'VARIABLES (REAL OR INTEGER) IS ACCORDING TO THE FORTRAN STANDARD '
   
 'IF SEVERAL VARIABLES ARE READ IN ONE LINE THEY HAVE TO SEPERATED '
   
 'BY A BLANK OR A COMMA '
   
  
 '0) MODE OF SIMULATION'
   
 ' STATNY = .TRUE. : STATIONARY      STATNY = .FALSE. : UNSTATIONARY '
   
 ' STATNY '
   
 '.FALSE.'
   
 '1) GRID VARIABLES'
   
 'NUMBER IN X-DIRECT.    NUMBER IN Y-DIRECT.    NUMBER OF VERTICEL LEVELS'
   
 '       NXTR    NYTR                                  NETA
   
 '       51    51    25
   
 'GRID SIZES (X UND Y) IN M    SCALE PARAMETER FOR ETA-TRANSFORM.
   
 '       DXTR     DYTR    PARAF
   
 '       100.    100.    5.887
   
 'TIMESTEP (S)    NUMBER OF TIMESTEPS    NUMBER PARTICLES/TIMESTEP
   
 '       DT    NDT    NR
   
 '       10.    780    100
   
 'SAMPLING INTERVAL OF METEOROLOGICAL DATA
   
 '       DTWIND '
   
 '       36000.
   
 '2) SOURCE, RELEASE AND SAMPLING PARAMETER'
   
 'START RELEASE (s)                                       STOP RELEASE (s)
   
 '       STRTRL    STOPRL
   
 '       0.    100000.
   
 'START SAMPLING (s)                                      SAMPLING-INTERVAL (s)
   
 '       STRTSP    DTSMPL
   
 '       1800.    600.

'RELEVANT CONCENTRATION MINIMUM  
 'CONMIN  
 1.E-12

'NUMBER OF SOURCES'  
 'NEQ  
 1

'SOURCE COORDINATES X, Y, AND Z (M) SOURCE STRENGTH (MASS UNITS/S)'  
 'SPX SPY SPZ Q  
 'FOLLOWING LINE MUST APPEAR NEQ TIMES  
 0. 2500. 100. 1.66E-3

'3) DEPOSITION PARAMETER'  
 'DEPOSITION FLAG WASHOUT (1/S) DEPOSITION HEIGHT (M)  
 'DEPOSI WSHLAM DEPHGT  
 .FALSE. 0.0 1.0

'4) MODEL BOUNDARY  
 'UPBND'  
 800.

'5) CALCUALTION OF CONCENTRATION'  
 'AIR CONCENTRATIONS ARE DETERMINED IN THE LOWEST KZLEV LEVELS  
 'KZLEV  
 15

'6) STEERING OF OUTPUT'  
 'EXTENDED PRINTEROUTPUT (CONCENTRATIONS) DESIRED?'  
 'OUTPRT'  
 .TRUE.

'AT WHICH GRID POINTS (X AND Y) THE PRINTER OUTPUT SHOULD BEGIN  
 'AND FOR WHICH VERTICAL LEVEL  
 'IXDMP JYDMP KZDMP  
 2 21 1

'TRAJECORY INFORMATIONS FOR A SPECIFIED PARTICLE DESIRED?  
 'OUTTRJ'  
 .TRUE.

'FOR WHICH PARTICLE?  
 'NOUT  
 1

'STORAGE OF RESULTS DESIRED?  
 'OUTDSK'  
 .TRUE.

'ON WHICH LOGICAL UNIT?  
 'MOUT  
 20

### **5.3 The Output Data of TRAVELING/COSYMA**

TRAVELING/COSYMA produces two different kinds of output data.

1. The results of the model can be stored unformatted in  
*binary code*  
*on logical output unit MOUT*
2. Informations on the specific simulation run are printed on the lineprinter. The standard output unit corresponding to the lineprinter is commonly the logical unit 6.

Storage of the results is optional. The following data can be stored:

1. geometric heights (in meters) of KZLEV  $\eta$ -levels above mean sea level;  
will be stored only once;  
Dimension of each level: (NXTR \* NYTR)
2. three-dimensional distributions of air concentrations;  
Dimension: (NXTR \* NYTR \* KZLEV)
3. three-dimensional distribution of arrival times of the plume;  
Dimension: (NXTR \* NYTR \* KZLEV)
4. two-dimensional distribution of dry deposition flux;  
Dimension: (NXTR \* NYTR)
5. two-dimensional distribution of wet deposition flux;  
Dimension: (NXTR \* NYTR)

Each of these fields is preceded by a header. At the beginning of the whole data informations on the concentration grid, the simulation domain, the source configuration, and the length of the headings are stored once.

For a stationary run the whole data described above are stored only once.

In the unstationary case the data explained under points 2.), ..., 5.) of the list above are stored after each sampling interval.

### **5.4 The TRAVELING-COSYMA Interface**

COSYMA requires the time-integrated air and ground concentrations and the arrival times with respect to a polar grid system. Therefore, the TRAVELING results have to be interpolated into a polar grid. This is accomplished by a special interface program which reads the TRAVELING results, performs a quadratic interpolation of the data into a polar system which is defined by the radii and the azimuthal resolution, and stores the interpolated values according to the COSYMA loop structure.

### **5.4.1 The input-data**

The interface program requires two different kinds of input data.

1. The TRAVELING results are expected in

**binary code**

**on logical input unit 20.**

They are read using a program similar to that printed in Sect. 4.3.1.

2. User-defined input data to specify the polar grid and the number of release phases are expected on the

**standard logical input unit**

of the computer system which is commonly the logical unit 5.

The FORTRAN-NAMELIST is used to read the parameters.

The NAMELIST-name is **PARA**.

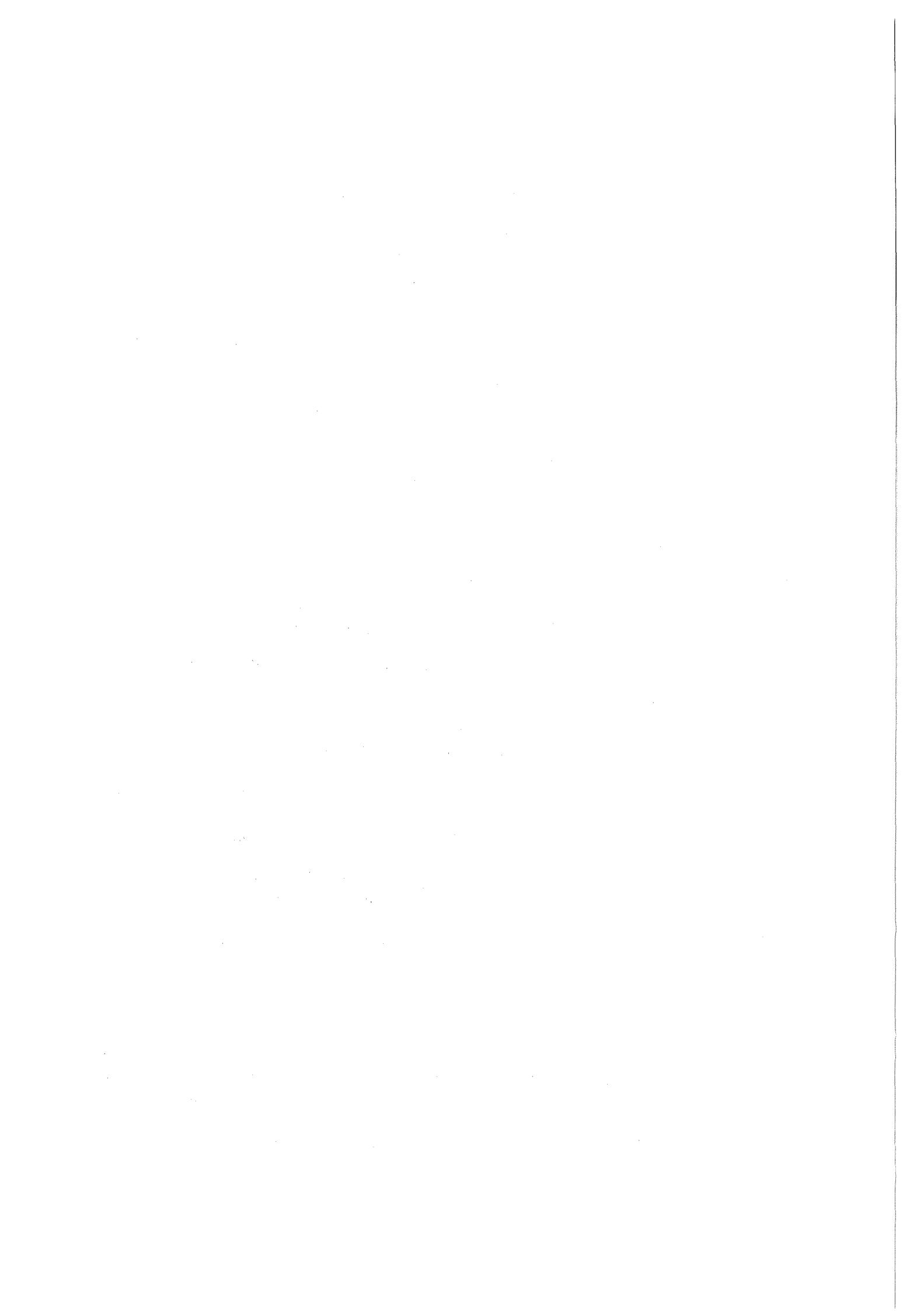
The variables and their meanings are described below.

The following variables and arrays must be assigned to values using the NAMELIST-statement:

<b>KOSYS</b>	<b>INTEGER</b>	defines orientation of polar system (Default: 0) • = 0 geographical polar system • = 1 mathematical polar system
<b>NRAD</b>	<b>INTEGER</b>	number of radii of polar system (Default: 20)
<b>NPHAS</b>	<b>INTEGER</b>	number of release phases = number of integration intervals (Default: 1) • maximum number allowed is 9
<b>DPHI</b>	<b>REAL</b>	azimuthal resolution of polar system in degree (Default: 5) • minimum resolution allowed is 5 degree
<b>R</b>	<b>REAL</b>	array containing the radii of the polar system in meter • maximum dimension allowed is 20
<b>REDGE</b>	<b>REAL</b>	concentrations less than REDGE are omitted

### **5.4.2 The output data**

The output of the interface program are time-integrated air concentrations in the first vertical layer above the ground, time-integrated ground concentrations due to deposition, concentrations of  $\gamma$ -radiation which are identical to the near-surface air concentrations, and the arrival times of the plume. They are available on a polar grid and are stored according to the COSYMA loop structure [38] on the **logical output unit 21**.



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