THE NEW GERMAN REGULATORY MODEL - A LAGRANGIAN PARTICLE DISPERSION MODEL

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INTRODUCTION

Following the demands from the EC directive concerning integrated pollution prevention control *(96/61/EC,* 24 September 1996) and the air quality framework directive (*96/62/EC*, 27 September 1996) the German Technical Instruction on Air Quality Control (*TA Luft,* 26/06/02) that governs the licensing of facilities in Germany has undergone a revision. Among others the first EC daughter directive (*99/30/EC*, 22 April 1999) refers to 24-hour mean values for SO_2 and PM10. These values cannot be calculated by methods based on the Gaussian plume model as it has been used in Germany until recently since the occurrence frequency of single situations is described by statistical probability. Thus, information is missing about in which chronological order one single situation is followed by the next one. To combine e.g. daytime and nighttime situations correctly a time series has to be calculated on an hourly basis. Despite its practical utility and its coverage of a wide range of relevant cases in regulatory practice, the Gaussian plume formulation does not explicitly consider phenomena such as: non-steady state emissions or dispersion conditions, wind shear with height, calm conditions, recirculating flows and spatial inhomogeneities in terrain.

CONCEPT

As a consequence, a concept has been developed that overcomes most of the above-mentioned restrictions and that fits with the requirements from the EC air quality directives. Furthermore the new approach should be state of the art, appropriate for practice and should have the potential for using e.g. complex meteorological pre-processors when they are ripe for routine applications.

Model Concept

During the last ten years, Lagrangian particle dispersion modelling has become common practice in air quality control in Germany. The German Association of Engineers has documented this development by formulating a model standard *VDI 3945 part 3* (2000). The guideline deals with the numerical calculation of trace species dispersion using a Lagrangian particle model. This type of model tracks point-like particles representing a trace species on their path through the atmosphere. The particles travel with the mean wind and are additionally subjected to the influence of turbulence. The effect of the turbulence is modelled by adding an additional random velocity to the mean motion for each particle. This random velocity, which is derived from a Markov process, is a function of the turbulence intensity and is different for each particle. The concentration distribution is determined by counting the particles in given sampling volumes and is expressed as mean values over the volume elements and time intervals.

The approach differs fundamentally from the majority of the established modelling techniques, which are founded on either a physical modelling in the wind tunnel, or the computed solution of the advection-diffusion equation.

The main advantages of the Lagrangian particle model, presented in this guideline, are that the model concept largely reflects the natural phenomena involved in turbulent diffusion and the method eliminates numerical diffusion. The method always yields non-negative mass densities and is mass-conserving. It can be applied to any source geometry desired for any temporal behaviour of a spatially variable source. The sedimentation of heavy dust, its resuspension as well as physical and linear chemical transformation processes can be accommodated. Complex obstacle geometries can likewise be accounted for. Depending on the spatial and temporal scale at which the meteorological input fields are provided, the Lagrangian particle model can be used for modelling regions ranging from 20 m to several 100 km and for time intervals of 10 minutes up to several years.

Required meteorological input information includes the fields (defined for certain time intervals) of the mean wind components, the wind fluctuations and the diffusion coefficients, which can be generated by meteorological pre-processors (*Schlünzen, K. H,* 1994). For time-dependent calculations, these input parameters must be made available as a chronological order of fields. Furthermore, emission data and, depending on the specific case, terrain data and a land use inventory will be required. The model output is a time sequence of the spatial distribution of the concentration of the emitted species, its transformation products and the amount deposited.

The accuracy of the result is affected by the sampling error associated with the particle count in the receptor volume. Increasing the number of particles emitted, although at the expense of a longer computation time, can reduce the sampling error.

DETAILS OF THE ALGORITHM

The path of the *i*-th particle in the sample, the trajectory $\boldsymbol{r}_i(t)$, is determined by

- start parameters (time t_i and position $\boldsymbol{r}_i(t_i)$),
- average wind field,
- atmospheric turbulence,
- external forces (e.g. gravitational settling).

The mass $m_i(t)$ represented by the *i*-th particle in the sample depends on

- the mass emitted by the source(s),
- transformation and removal processes (e.g. dry and wet deposition, interception).

Each of these topics is handled by an appropriate sub-model, e.g. the start parameters by an emission model and the removal processes by a deposition model. The most difficult part is the incorporation of atmospheric turbulence into the model.

The action of the turbulent wind field on a particle is simulated by a random process (random walk model). There are fast algorithms available for performing random walk processes on a computer and a lot of research has been done on this type of model within the last 20 years (*Wilson*, 1982; *Legg and Raupach*, 1982; *Janicke*, 1983; *van Dop et al.*, 1985, *Sawford*, 1986; *Thompson*, 1987; *Janicke*, 2000). For each particle the position **r** and a random velocity **v** are calculated in a sequence of time steps of size τ:

$$\mathbf{r}(t+\tau) = \mathbf{r}(t) + \tau[\overline{\mathbf{V}}(\mathbf{r}) + \mathbf{v}(t)] \tag{1}$$

$$\mathbf{v}(t+\tau) = \mathbf{A}(\mathbf{r},\tau)\cdot\mathbf{v}(t) + \mathbf{B}(\mathbf{r},\tau) \tag{2}$$

Here $\overline{\mathbf{V}}(\mathbf{r})$ is the mean wind field, $\mathbf{A}(\mathbf{r},\tau)$ is a function determined by the atmospheric turbulence and the time step and $\mathbf{B}(\mathbf{r},\tau)$ is a velocity randomly chosen with each time step. The physical quantities necessary to determine these parameters are (simplified):

$\overline{\mathbf{V}}(\mathbf{r})$	mean wind field
$\sigma_{u,v,w}(\mathbf{r})$	turbulent wind fluctuations
$K(\mathbf{r})$	diffusion coefficient

They are available from meteorological boundary layer models or from direct measurements. In any case, there are no calibration parameters in this model that have to be determined by dispersion experiments.

One important point in atmospheric diffusion is the fact that the random movement of a particle in a turbulent flow field is rather smooth, in contrast to the Brownian motion. A particle is moved by a turbulent eddy of typical size for some time, the Lagrangian correlation time T_L, before it is caught by another eddy. This is reflected by equation (2), where the simulation particle preserves its turbulent velocity to some part with each time step. The parameter **A** determines how long the particle remembers its velocity and therefore is strongly related to the Lagrangian correlation time T_L. Hence, the width σ_y of a plume generated by a stationary point source is proportional to the source distance *x* for travel times short with respect to T_L whereas classical diffusion would predict $\sigma_y \sim \sqrt{x}$. Atmospheric diffusion can only be described for larger distances from the source by the classical advection diffusion equation but only as a rough estimate in the near vicinity.

Set-up for regulatory purposes

The specific concept for use in regulatory purposes has been elaborated in close cooperation with representatives from the responsible Environmental Agencies in the German federal states (Bundesländer). The calculation method has been layed down in *TA Luft,* 26/06/02, Annex 3. It has been implemented in a computer programme called AUSTAL2000. AUSTAL2000 is available, together with the source code, on the World Wide Web at www.austal2000.de. The work in detail has been funded by the Federal Environmental Agency (UFOPLAN 200 43 256) and has been delivered by Ing.-Büro Janicke, 26427 Dunum, Germany. The complete documentation (until now in German only) can be downloaded as well.

Some of the main features of AUSTAL2000 are: Use of meteorological time series and of meteorological statistics as well, calculation of concentration and dry deposition (annual averages, highest daily or hourly values, time series), gravitational settling of coarse particles, 3-dimensional wind fields in complex terrain, point, line, area and volume sources, arbitrary number of sources, automatic estimation of the sampling error. The meteorological profiles used in AUSTAL2000 are taken from *VDI 3783 part 8-draft* (December 2001).

VALIDATION/ MODEL PERFORMANCE EVALUATION

Model validation is the assessment of how well the model performs. Typically, model predictions are compared to experimental results and the differences are documented. This procedure is difficult with atmospheric dispersion models because experimental results exhibit a large scatter due to the chaotic nature of turbulence. In addition, it is not possible to repeat an experiment exactly because the atmospheric conditions will always be at least slightly different. A lot of evaluation has been performed in this project (e.g. the comparison with the Prairie Grass data set). Here, a comparison with a wind tunnel experiment is presented. Experiments in the wind tunnel usually are restricted to neutral stratification, but they can precisely be evaluated and can be repeated exactly.

Wind tunnel Experiment

The comparison of the wind tunnel data (*Schatzmann et al.,* 2000) with the results calculated by the Lagrangian dispersion model AUSTAL2000 is shown in figure 1. The ground level concentration field c(x, y) generated by a stationary point source (stack) of height H at $x = 0$ and $y = 0$ with source strength Q over flat terrain with roughness length $z_0 = 0.007H$ is analysed. The atmospheric stratification is neutral with wind velocity U at height H. The upper part shows the maximum normalized concentration $UH^2Q^{-1}c(x, 0)$ as a function of the normalized source distance x/H. The part in the middle shows the normalized crosswind integrated concentration $UHQ^{-1} \int c(x, y)dy$ and the lower part the normalized horizontal plume width $\sigma_y(x)/H$. The results from calculation show fairly good agreement with the wind tunnel data.

Because of the free scaling of wind tunnel results the situation modelled can be interpreted e.g. as the plume of a stack with a height H = 100 m in flat terrain with roughness length z_0 = 0.7 m (industrial site) or with H = 10 m and z_0 = 0.07 m (agricultural site). When modelling the dispersion of coarse-grained dust it might be necessary to modify the diffusion coefficient used. The gravitational settling of heavy particles shortens the time these particles may spend within an eddy. Therefore, the Lagrangian correlation time decreases and so does the effective diffusion coefficient. This should become noticeable when the settling velocity v_s is comparable to the vertical velocity fluctuations σ_w of the turbulence. Usually this effect is neglected in dispersion models.

Verification tests

Another possibility to check the performance of a dispersion model is checking if the model behaves as it is expected to do for certain known solutions that are derived from theory. A number of such tests have been carried out for which the results are known from theory, such as:

- Homogeneity tests (homogeneous turbulence and constant time step; inhomogeneous turbulence and constant time step; inhomogeneous turbulence and variable time step
- Deposition tests (deposition without sedimentation and vice versa; deposition with sedimentation)
- Test of the Taylor's Theorem (*J.H. Seinfeld, S.N. Pandis*, 1998)
- Test of Berlyand's profile

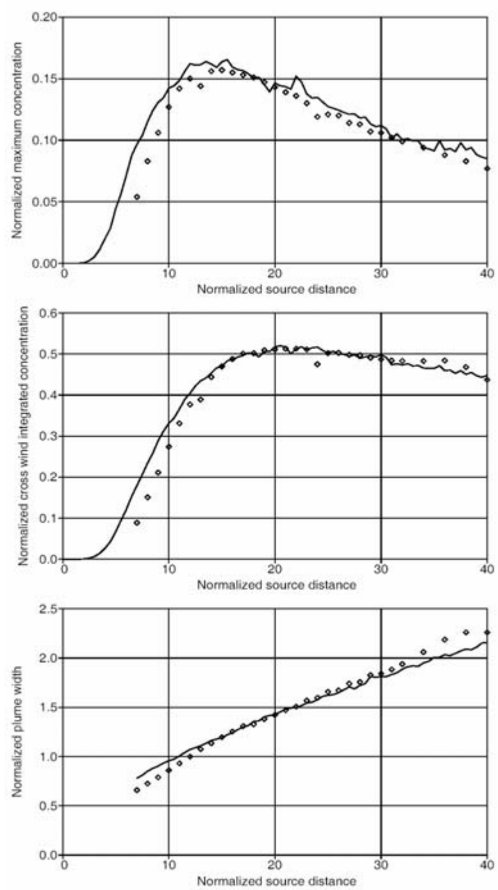

Fig.1 Comparison between results from wind tunnel (diamonds) and AUSTAL2000 (solid line)

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