A COMPUTER CODE FOR CALCULATING THE ATMOSPHERIC TRANSPORT OF RADIOACTIVE POLLUTANTS UNDER INHOMOGENEOUS AND INSTATIONARY CONDITIONS

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1. INTRODUCTION

For calculations of atmospheric dispersion of radioactive emissions from the nuclear industry under instationary and inhomogeneous conditions, numerical computer codes using the particle-in-cell method are developed by several groups for example by LLL (1) and 3S (2), and our group (3). This method simulates the pollutant dispersion in the atmosphere by the transport of Lagrangian particles in an Eulerian grid mesh and in a given wind field.

These programs can be successfully applied even when the turbulent and advection wind fields are varying so strong in time and space during the dispersion of the radioactive pollutant cloud, that calculations with the Gaussian plume model will fail. These particle diffusion programs have the advantage to eliminate the fictitious diffusion inherent in conventional finite-difference techniques in the case of inhomogeneous wind fields. Individual and multiple, instantaneous and continuous sources can be applied.
Besides these codes can handle rainout and washout, wet and dry deposition and surface roughness variable in space. Introducing a particle weight the codes are capable of considering the radioactive decay and potential chemical effects of the pollutant.

2. PARTICLE-IN-CELL METHOD

In these programs the Lagrangian particles are moved in the Eulerian grid according to a given time step and to a velocity linearly interpolated from the velocities at the eight cell corners to the position of the particle. The velocities at the cell corners are composed of the advection velocities $\vec{u}$ given from the wind field and by a net-diffusion velocity $\vec{w}$ calculated by a difference-scheme of the pollutant concentration c.

In a turbulent field a concentration gradient grad c causes a net-current density $\vec{j}$ in the opposite direction:

$$\vec{j} = - K \text{ grad } c = -K \cdot \nabla c$$

with the diffusion coefficient K.
Then a net-diffusion velocity can be defined:

$$\vec{w} = \frac{\vec{j}}{c} = -K \frac{1}{c} \text{ grad } c = -\frac{K}{c} \nabla c$$

So this model solves the nonlinear transport diffusion equation

$$\frac{\partial c}{\partial t} + \vec{u} \cdot \nabla c = \nabla (K \cdot \nabla c)$$

Under the assumption of incompressibility of the mass-consistent advection wind field the term $\vec{u} \cdot \nabla c$ can be replaced by $\nabla(c \cdot \vec{u})$ and with a so-called pseudovelocity $\vec{v} = \vec{u} + \vec{w}$ we can rewrite the equation:

$$\frac{\partial c}{\partial t} + \nabla c(\vec{u} - \frac{K}{c} c) = \frac{\partial c}{\partial t} + \nabla(c \cdot \vec{v}) = 0$$

That corresponds to a compressible pollutant gas, which can be simulated by an adequate distribution of pollutant particles.

3. PROGRAM XPIC

Based on the mentioned mathematical scheme we have developed the program XPIC, the flow-chart of which is shown in fig. 1. For practical use the code has been developed in two versions: one for handling single clouds over wide ranges with an expanding Eulerian grid, and the other for multiple sources in a limited area with a very large number of fixed cells.

Version A:
In the code version A the grid system follows the cloud path with cells stepwise expanding. Whenever the cloud border would begin to leave the grid system, the cell dimensions are enlarged in correspondence with changed time steps as mentioned later. Because of the limited memory capacity of our computer (CDC CYBER 73/76), at the moment the version A can handle about 26 000 particles in a grid system up to 10 000 cells. Fig. 2 shows the vertical concentration profile at distance 3 km from the source in the free atmosphere or with earth surface. In each case the dispersion is calculated by the Gaussian plume model or by XPIC. The difference of the concentration values in the lowest cell is probably caused by the different reflection mechanism of XPIC and the Gaussian model.

Version B:
For some problems as above-mentioned, the grid system of version A is too small. Because of the restricted memory capacity of our computer, we performed the calculations by tracking the particles group-wise and by handling the grid system in sections. Until now total grid systems of up to 100 000 cells can be handled by this way in version B, but the number of cells can be increased greatly by a not too difficult programming. In each version any desired number of particles can be transported, if the necessary computer time is available.

If there is no initial concentration distribution given by measurement or calculation, in both versions (single or multiple source) a cloud of Gaussian distributed particles may be injected at the beginning of each time step. The initial growth of the clouds is calculated by the common Gaussian plume model, until the curvature of the cloud can be reproduced by the PIC-method according to the desired accuracy.

To warrant a faultless dispersion of a pollutant cloud across the border of the grid system in the version B, special boundary conditions have to be observed, e.g. by linear extrapolating the diffusion velocities at the free-air boundaries of the grid system.

For evaluating the correct concentration on the earth surface, we had to introduce a special handling of the particles in the lowest layer of cells. Two different techniques, for assigning diffusion velocity to the particles in this layer seemed to be applicable:
a) linear interpolation according to the vertical position of the particle between the diffusion velocity value zero at the surface and the value on the upper border of the lowest cell layer calculated by the normal difference scheme,
b) statistically sampling between both values and assigning the diffusion velocity to the particle positions.
The case a) seems to agree with linear decrease of eddies whereas case b) seems to simulate a constant eddy spectrum in this layer. An option is installed for total reflection or a certain surface adsorption rate, e.g. by a Russian Roulette for killing the particles. Concerning the calculation of the diffusion coefficients used in this code, it is referred to Voelz at al., paper 161.

The concentration time integral at a reference point is got by adding all concentration values weighted by the time step during the time of interest. Assuming that a single cloud is unchanged during the passage along the reference point, it is possible in the code version A to calculate the concentration time integral by adding up all concentrations along the trajectory across this point.

4. ACCURACY

To avoid inaccuracies by using a difference scheme certain rules must be observed for proportioning the cell dimensions of the Eulerian grid system and the time intervall at the Lagrange step.
First the cell dimensions must be adjusted appropriately to the curvature of the Gaussian distribution at the beginning of the calculation. Therefore the diffusion velocities which are calculated by the difference scheme are compared with those of the differential solution by the Gaussian plume model. The relative deviation ß is given by

$$ß = 1 - \frac{1}{\bar{c}} \frac{\Delta c}{\Delta x_i} \Big/ \frac{1}{c} \frac{dc}{dx_i}$$

Under the assumption, that the mean concentration values in the cells are given by

$$c = c_o \cdot \exp(-x_i^2/2\sigma_i^2)$$

follows $\alpha = \frac{1}{1-ß} \; th\alpha$ with $\alpha = x_i \Delta x_i / 2\sigma_i^2$

Besides, normally the timestep has to be adjusted to the cell dimensions and must satisfy the following inequation:

$$\Delta t \leq f \cdot \Delta x_i / (v_i)_{max}$$

where f is a constant in the range between 0 and 1 and $(v_i)_{max}$ is the i-component of the maximum pseudo-velocity. Without advection velocity, the pseudo-velocity is equal to the

diffusion velocity w, with $(w_i)_{max} = 2\ K_i/\Delta x_i$ in XPIC. Without advection in XPIC therefore follows: $\Delta t \leq f \cdot \Delta x_i^2/2K_i$.

5. CONCLUSION

In the meantime the code was also used for investigations concerning different vertical distributions of the diffusion coefficient and the wind speed as prepared by Voelz et al.paper 16!. Further problems have to be solved concerning the evaluation of the wind field from meteorological data, the effect of surface structure, the optimization of the calculation process and the improvement of handling very large grid systems.
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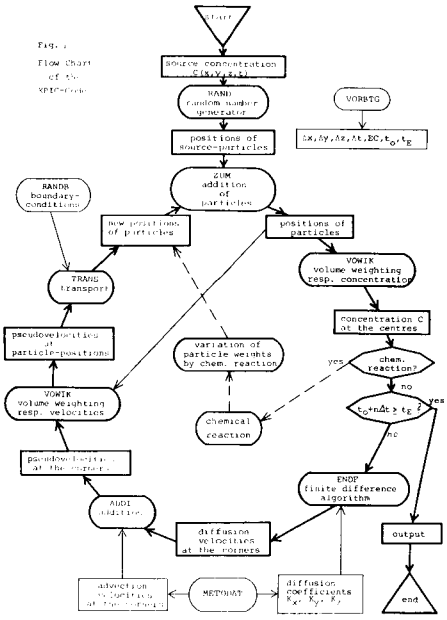

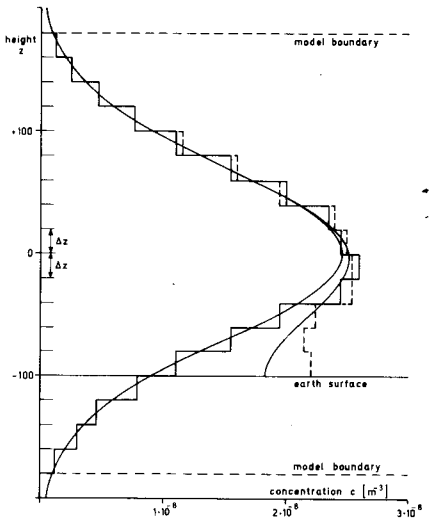

Fig. 2 Vertical concentration profile c(z) calculated by Gaussian model or XPIC, at the mass centre of the cloud, 3 km downwind from the source, height of emission: H_q = 100 m, Pasquill's turbulence type D, XPIC-calculations: step curves