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TURBULENT LAGRANGE PARTICLE TRAJECTORY MODEL FOR CHANGING ATMOSPHERIC CONDITIONS

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Abstract: The dispersion model ABR, developed at the Institute for Nuclear Technology and Energy Systems (IKE), has been designed to assess radiological situations in emergency cases. It is part of the Nuclear Power Plant Monitoring System (KFÜ) operated by the Ministry of the Environment Baden-Württemberg. This system collects and stores meteorological and radiological data such as dose rates and nuclide-specific activity in the vicinity of each nuclear power plant in Baden-Württemberg. Data from local weather stations and forecast weather data from the German Weather Service (DWD) are also stored in the KFÜ system. These data can be used as input of the ABR model. In cases of emergency an assessment for civil protection will be performed with the help of ABR.
The content of this paper is twofold: In the first part the dispersion model, presently used in ABR, is presented. The transport of particles is calculated using a Lagrangian particle model, which had been derived from measured plume data under constant atmospheric conditions. The dose calculation is based on dose factors mainly defined by the International Commission on Radiological Protection. In the second part an alternative turbulence model is discussed in order to improve the accuracy and to model particle transport under varying atmospheric conditions. This particle-dispersion turbulence model is based on a Markov-chain random-walk method to calculate the particle trajectories.

Key words: *Dispersion of radioactive particles, radiation exposure, turbulence kinetic energy, Markov-chain random-walk method, anisotropic turbulent velocity*

INTRODUCTION

On the 26th of April the eighteenth anniversary of the nuclear accident of the Chernobyl nuclear power plant in Ukrainian was remembered. This accident was the turning point in nuclear electricity generation since then excessive time has been invested every year for the development of civil protection systems. The Ministry of Environment of the state of Baden-Württemberg operates a Nuclear Power Plant Monitoring System to collect facility data, radiological data, weather measurements and weather forecast data. Measurements are provided and supported by the Agency of Environment, Measurement and Nature Protection (LUBW). This huge amount of data is stored in a data base and can be used as input for the atmospheric dispersion model (Ausbreitungsrechnung, ABR). The ABR is a modular system. In each module facility and weather data are used to simulate accidental nuclear releases and their impact on civil life.

The aim of the present work is to discuss alternative turbulence models for improving the Lagrangian particle trajectory description. These turbulence models should be able to be applied for varying atmospheric conditions, i.e. conditions which vary in space and time. Furthermore, non-isotropic velocity fluctuations from the sub-grid turbulence kinetic energy and atmospheric stability parameters have to be modelled.

ABR MODULES

Within the simulation system ABR the different modules represent the physical processes of release, meteorological conditions, particle transport, cloud shine and dose estimation. Due to the fact that the ABR is used in emergency situations, the calculation time is an important factor which influences the possible complexity of the physical models. But with increasing compute power the existing ABR models can be reviewed and the most relevant simplifications can be removed.

For the release and transport of the nuclides they are pooled in the nuclide groups: noble gas, aerosol, and the three iodine groups: elementary, organic, and aerosol. The module FREI estimates the release activity of these nuclide groups and the fraction of each nuclide within its group taking into account the changes of those fractions with the radioactive decay in the reactor.

To determine the meteorological conditions, in particular the wind speed and direction, two diagnostic wind-field models are available. They are based on either data from local weather stations or forecast wind data from the DWD. Both models start the calculation with interpolation of their input to the underlying surface-fitted grid for the horizontal wind components u_x and u_y. The wind field is modified taking into account the stability characteristics of the atmosphere and the terrain formation. Thereafter, the continuity equation is satisfied. The models differ in how the vertical wind profile is determined on the basis of measured values. The simpler model WINDO uses a power law whereas the model MCF additionally considers the shear in the Eckman layer, if data about the geostrophic wind are available. In addition, MCF uses a terrain-following coordinate system and can consider surface roughness.

A Lagrangian particle model (PAS) is used to calculate the transport of the radioactive particles. The dry deposition of particles on the ground is described by their sink speed, the washout by measured or forecast precipitation data. Each of these model particles represents a well-defined pollution concentration. The transport is calculated by solving the trajectory equation consisting of a convection part and a turbulence part. The particles are treated as tracers, which do not interact with each other. The turbulence part is described by a Monte Carlo Markov process on the basis of random displacements (Chino et al., 1991). As a result the particle model predicts the activity concentration in the cloud and close to the ground as well as the deposited concentration. Nobel gases are not deposited.

The cloud radiation is calculated by the module AIRDOS on the basis of adjoint fluxes. For each nuclide its gamma spectrum is divided into 30 energy groups. In a pre-processing step the adjoint fluxes have been determined for various distances between radiation source and the detector using the transport code DORT from Oak Ridge National Laboratory (Emmett et al., 1992). The concept of adjoint fluxes has been validated.

The doses, relevant for emergency countermeasures, result from cloud radiation, ground radiation, inhalation, and thyroid impact. These doses, as well as an effective dose, are calculated by using dose factors defined by the International Commission on Radiological Protection (ICRP). In addition, doses for different organs are estimated. These doses are provided for the current time as well as integrated over time. Inhalation and thyroid doses are estimated by considering exposure time and respiratory rate. The effective dose rate is the sum of beta, gamma and inhalation rates.

Soon after the accident of the Fukushima Daiichi nuclear power plant we have presented ABR simulations with good agreement to preliminary measurements (Scheuermann et al., 2011). However, a closer look reveals some potential for improvement: It is not possible to perform simulations with multiple sources. In the frame of a benchmark, see van Arx et al., (2014), deviations between various German dispersion codes were detected, in particular when atmospheric conditions are vary in time and space. The turbulence description is not adapted to the variation of local conditions. Therefore, more detailed analysis and model development for varying atmospheric conditions should be performed. Testing and validation may be done with reference to the Atmospheric Transport and Diffusion Data Archive http://www.jsirwin.com/.

TURBULENCE MODEL

Particle transport in the ABR is treated as a combination of separate effects: convection with the time-averaged (mean) wind field and turbulent diffusion. The mean velocity is provided by the WINDO module as described above. To model the turbulent diffusion a random displacement is imposed with uniform probability within a given interval. The magnitude of the displacement can alternatively be taken from the dispersion experiments 'Karlsruhe-Jülich' (Thomas et al., 1976) or from the 'Prairie Grass Project' (Pasquill, F., 1978; Gifford, F. A., 1961). Each experimental data set estimates it depending on Pasquill's stability classes and an additional parameter, either the height h of the source or the distance from the source. The stability class is derived from the Monin-Obukhov length L and the roughness factor z_0 of the surface. The magnitudes of displacements in transverse and in vertical directions, σ_y and σ_z, calculated from the respective experimental data set, differ in the method of evaluation: Pasquill and Gifford fitted two parameters using a power law function with source distance-dependent parameters. In contrast, in the Karlsruhe-Jülich experiments the power law parameters depend on the source height.

In both cases the physical nature of the Gaussian plume, see e.g. Pal Arya, S. (1999), as described by

$$\bar{c}(x,y,z) = \frac{Q}{2\pi\sigma_y\sigma_z\bar{u}_x} \cdot exp\left(-\frac{y^2}{2\sigma_y^2} - \frac{(z-h)^2}{2\sigma_z^2} \right) \tag{1}$$

is reproduced for constant atmospheric conditions, in particular the mean downwind velocity $\bar{u}_x$. In eq. (1) the mean concentration $\bar{c}$ depends on the source strength Q. This turbulence model treats the horizontal directions as equivalent.

An alternative turbulence approach, which is valid for both constant and changing atmospheric conditions, has been introduced by Smith, F. B. (1968). He proposed a 'random-walk' method to determine the fluctuation velocity u_i' of the next time step Δt in the three coordinate directions as

$$u_i'(t+\Delta t) = R_i(\Delta t) \cdot u_i'(t) + k_i \cdot \left(1 - R^2{}_i(\Delta t)\right)^{0.5} \cdot \eta(t) \quad ; \quad i = x, y, z \qquad . \tag{2}$$

The first part of the eq. (2), the 'correlated' part, represents the fluctuation history. The second is purely statistical and is called the 'uncorrelated' part. The influence proportion of each term is expressed by the auto-correlation function $R_i(\Delta t)$. $\eta(t)$ is a Gaussian-distributed dimensionless random number with zero mean and variance 1.

For the uncorrelated part the anisotropic turbulent kinetic energy k_i of the direction i is taken into account. The auto-correlation function can be parameterized as $R_i(\Delta t) = exp(-\Delta t / T_{L,i})$ (Taylor, G. I., 1921). It triggers the influences by the ratio of integration time step size Δt and the Lagrange time scale $T_{L,i}$. In a turbulent flow the Lagrange time scale is a measure for the eddy life time. So in this case turbulence in each direction i will be described as a two parameter problem: The first parameter is k_i and the second is the Lagrange time $T_{L,i}$. For both parameters approaches will be discussed further.

In literature there are different model approaches to consider k_i. One is the description by similarity theories, a second is the boundary-layer parameterisation and a third is the turbulence description as it is implemented in the atmospheric dispersion modeling system AERMOD. All approaches are discussed in this paper.

Three similarity theories are considered:

A first, the 'Monin-Obukhov similarity theory', provides a prediction for the normalized standard deviations k_i / u_* as a function of L and z_0. But this approach ignores the thickness of the planetary boundary layer. So it is only validated for an unstable and convective atmosphere. For neutral or stable atmospheric conditions turbulence becomes very low.

A second is the 'local free-convection similarity theory'. It uses only velocity and temperature to model turbulence in the convective surface layer. For the calculation of velocity and temperature a parameterization for turbulence is set up and the friction velocity u_* is ignored (Panofsky, H. A., 1977).

A third is the 'mixed-layer similarity theory', Deardorff, J. W., (1970). Here, surface-layer variables describe a stationary and horizontally homogeneous planetary boundary layer. There is also a calculation of velocity and temperature as in the free-convection similarity theory. These parameters provide a description of cells for the up- and down drafts even close to the surface.

Boundary-layer parameterisation describes turbulence in a different way (van Ulden, A. P. and A. A. M. Holtslag, 1985). The parameterisation provides estimations for surface stress and heat flux. Thus, the Richardson number can be calculated to define stability of the atmosphere. The turbulence is then calculated by u_*, the mixing height h_{mix} and the particle height z.

The atmospheric dispersion modelling system AERMOD, see de Visscher, A., (2013), divides turbulence into two influencing parts: The first part is turbulence based on shear stresses and the other part is based on thermal heating. This model concept is related to the idea of the atmospheric layers. In the Prandtl layer shear stresses and thermal heating influence the turbulence production. Above the mixing height, in the Ekman layer, turbulence is caused by thermal heating only. The geostrophic wind determines the particle transport. The AERMOD turbulence model calculates both components by h_{mix} and convective velocity w_* .

The description of the Lagrange time $T_{L,i}$ is proposed by Hanna, S. R. (1981) as a function of k_i , h_{mix} , L and the mean velocity $\bar{u}$. Computation of $T_{L,i}$ is related to h_{mix} and is different for stable, neutral and unstable atmospheric conditions. However, there are also descriptions to evaluate $T_{L,i}$, where the travel time is taken into account. Another proposal by Tennekes, H., (1979) is the calculation of the Lagrange time by the energy dissipation rate and the Lagrangian structure function constant.

Another option is to determine the model parameters k_i and $T_{L,i}$ from the forecast weather data of the DWD. The simulation of the COSMO model, see. Doms et al., (2005), uses a 3D prognostic closure. The parameterization consists of a sub-grid-scale model with a grid resolution of about 2.8 km. The sub-grid turbulent kinetic energy is calculated in an algebraic way. Momentum and heat influences are taken into account by horizontal and vertical coefficients. These assumptions lead to the turbulent energy formulation.

MODEL COMPARISON

In order to compare the present model and the random-walk model, advantages and disadvantages are discussed in the following paragraphs:

The present model of the ABR is a fast running turbulence model with a stable numerical process. It simulates a 200 km x 200 km x 1000 m model area in less than five minutes. The resolution of the area is 1000 m x 1000 m in the horizontal layer and 25 terrain-following layers in the vertical direction. In order to run a simulation only a few input parameters are necessary. A simulation needs the stability class of the atmosphere, varying wind speed and wind direction, the source height, the topographic conditions and the nuclide vector for input parameters. The WINDO module is able to calculate the mean wind for changing topographical conditions of the model area. All the input values for a simulation are easy to provide.

However, the ABR turbulence model is only a stochastically method, where the influences of past turbulence are not taken into account. Moreover, there are several numerical and model-based influences in the calculation of turbulence. The turbulence parameters are calculated by the six Pasquill stability classes; thus the model is discontinuous. Furthermore, the turbulence parameters depend on the source height for the Karlsruhe-Jülich parameters and on the source distance for the Pasquill-Gifford parameters. Both experiments provide a power law, which is derived for a Gaussian plume expansion of 10 km. These parameters are also used for greater travel distances. Finally, constant turbulence parameters are used even if conditions change with time and space. Thus, an improvement in this model could be a description for changing conditions. In spite of these approaches, accurate results can be achieved.

The random walk method uses a model, which consists of two terms, for the turbulence estimation. This model takes previous turbulence events into account. There is a probability that a particle transported by eddies is able to follow the trajectory of the eddy or to follow another trajectory. It also provides continuous description of turbulence depending on potential temperature by using the Monin-Obukhov length and the roughness of the surface for the turbulence calculation. Thus, topographical facts are modeled and turbulence with varying conditions is provided. It also correlates the time scale for an eddy with the integration time. Thus relates the history and the stochastically part of the turbulence calculation. In this model there is no dependence on the source height or the source distance. The turbulence calculation is independent from its traveled trajectory. Further, the turbulence is descripted as a two parameter problem of anisotropic turbulence k_i and Lagrange time T_L .

However, input data for the random-walk model have to be provided on a fine model grid. In particular Monin-Obukhov and roughness lengths have to be calculated for a highly resolved topography on a 250 m – 1000 m grid. This is numerically expensive and costs calculation time. It is also necessary to provide height h_{mix} and the friction velocity u_* for the turbulence calculation in the random walk process. There are various models for the description of anisotropic turbulence k_i and Lagrange time T_L . Validation simulations have to be done to evaluate the models.

CONCLUSION

Improvements to the present turbulence model should be implemented in order to take account of varying atmospheric conditions such as the stability of the atmosphere and the Lagrangian time-scale of the turbulence structures. However, care should be taken to guarantee, that the numerical effort remains within the time-restrictions of the civil-protection regulations.

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