Lagrangian Models in Urban Area Air Pollution Research

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Abstract The effects of air pollution in urban areas on the environment increase the demand for investigation in this field of research. Besides human and animal health, vegetation as well as matter are affected. By reason of the complex conditions in urban areas in terms of meteorology and topography, appropriate tools for the simulation of the dispersion of air pollutants are needed. The Lagrange-model theory enables transportation models to be formulated which meet these demands. The basic idea of the theory is the determination of trajectories of particles (or volumes). This gives the models a high degree of flexibility in respect to complex terrain, scale, number of emission sources, etc. The particles may represent gases or aerosols released by any kind of emission source. This paper describes and discusses the characteristics of Lagrangian models and presents some examples for urban area and further applications.

1 INTRODUCTION

Air pollution has become a general problem not only but especially in urban areas. To judge and interpret the current situation and the evolution of air pollution dispersion a variety of diagnostic and prognostic models are in use. In the area of dispersion models Lagrangian particle models (also referred to as Monte Carlo simulation models) are of special interest. Due to their flexibility in scale and the fact that they can be applied in complex terrain, Lagrangian models are an interesting tool for the application in urban areas.

Lagrangian models are usually coupled with a wind field/meteorological model or form part of a model system. The general idea and some of the relevant features will be discussed in the following sections. Some models for urban area use will be presented briefly and an insight in further fields of application given.

2 LAGRANGIAN MODELS

Lagrangian models belong to the class of stochastic dispersion models. Their basic concept is the determination of the pathway of individual particles or air volumes usually in a three-dimensional model domain. For this reason these models are also referred to as Lagrangian particle dispersion models or as trajectory models.

In the case of atmospheric dispersion, the term particle denotes any air pollutant, including gases, or any (neutrally) buoyant substance in the air. In this paper the term particles also refers to air volumes.

For physical reasons the particles are assumed to have no mass and no spatial extension so that they can follow every flow. However, each particle is associated with certain characteristics which will be modified and registered each time the particle moves. In general particles are assumed to be relatively inert over the period of interest. If a uniform mass is assigned to the particles, the density of the particles is proportional to the concentration.

The trajectory of a particle is considered to be the result of the advective wind and fluctuation caused by turbulence.

Particles may be released from any number of locations. The type of the emission source, e.g. point or line source, has no influence.

The form of Lagrangian models employed will depend on the chosen scale and the types of turbulences to be simulated as well as the available data and the aim.

2.1 Theory and Modelling

The fundamental concept for the particle motion in Lagrangian models is the statistical theory of Taylor [1921] for diffusion effects. As his theory is based on the the nearly ideal conditions of homogeneous and stationary turbulence fields, it was extended by Obukhov [1959] and Smith [1968]. They suggested simulating the trajectory of a particle by a Markov sequence of first order. The motion of a particle in

of track material in the atmosphere for a number of representative particles by a Lagrangian simulation. The model considers the sedimentation of heavy aerosols, rain scavenging, and wet deposition, as well as the flow around (simplified) buildings. The horizontal equidistant resolution is 5 m to 10 km with a maximum size of the calculation grid of 400 by 400 km. Vertically a maximum of 50 intervals can be applied up to the atmospheric boundary layer (approx. 2000 m height). The program LASAT includes a meteorological preprocessor for the data input needed by the Lagrangian model part as discussed above.
The software package is generally available and is used both by local German authorities and in industry. For further information see Janicke [1987] or http://www.janicke.de.

The main components of the LADM (Lagrangian Atmospheric Dispersion Model) are a mesoscale wind field model which provides the wind and turbulence fields for the dispersion component - the Lagrangian particle model. The particles here usually represent neutrally buoyant, relatively inert gases, as assumed in the general description. In the model plume rise effects are considered. The horizontal grid resolution is chosen to be 250 × 250 m near the emission source(s) (approx. 5 km) and 1000 × 1000 m far from the source. The ground level concentrations are computed for a vertical box height of 25 m.
LADM has been used for simulation in several areas in Australia, e.g. in the Perth Airshed Photochemical Study. For more details see Physick et al. [1994].

RAPTAD (Random Puff Transport and Diffusion) by Yamada [1986] represents another three-dimensional Lagrangian model for transport and diffusion forecast of airborne materials over complex terrain. It is thought to be coupled with HOTMAC (Higher Order Turbulence Model for Atmospheric Circulation) for the meteorological input. The models have been used internationally at the US EPA and industrial research centers and major universities. Further information is available in Yamada [1986] and by http://chili.rt66.com/ysa/index.html.

In the air pollution simulation system DYMOS (Dynamic Models for Smog Analysis) the main components are a meteorological model, a model concerning transport and dispersion of air pollutants and an optional air chemistry model. The individual models are selected for the specific application planned. For the transport and dispersion simulation a Lagrangian trajectory model may be used. The system includes a database for data input and a graphic user interface. DYMOS forms the base of EU funded projects. It has been applied in conurbations such as Berlin and Munich. In addition to smog, the dispersion of further air pollutants or radioactive substances are simulated. For more details refer to Gerharz [1997].

2.3 Further Fields of Application

Lagrangian models are, as pointed out above, not limited to mesoscale application or air pollution simulation, which are focused on here.
An example for the implementation of a macroscale Lagrangian model is the model for long-term prediction of ozone concentrations in Europe developed by IIASA, Laxenburg, Austria in cooperation with EMEP's Meteorological Synthesizing Centre-West (MSC-W) at the Norwegian Meteorological Institute, Oslo, and GMD FIRST (Heyes et al. [1996]). In this model the objects of interest are air boxes or air volumes for which the pathways will be determined over a time period of 96 hours. The resolution of the model is based on the latitude-longitude-grid with a grid spacing of approximately 150 km. The vertical coordinate is given by the atmospheric boundary layer.
In environmental risk management the application of Lagrangian models for real time transport simulation is of special interest. It is due to the fact that the structure of the models is easy to parallelize and that dispersion also in heavily structured terrain can be described. An example for an air pollution emergency system is LAGSIM (Mieth [1999]).
Another field of utilization which is relatively independent of scale is the field of nuclear dispersion. In this case the Lagrangian model includes the computation of the decay rate of the nuclear substance.

3 DISCUSSION

Compared with other model types, Lagrangian models often fill in their gaps. Numerical diffusion as in Eulerian model does not occur. In contrast to Gaussian models, Lagrangian trajectory models are appropriate for the description of dispersion in complex meteorological situations or complex structured orography. Lagrangian models offer the possibility to consider changes in meteorological conditions (and emission situations) in the computation as soon as the data is available.
An advantage of the Lagrangian approach is the flexible in use in respect to the spatial resolution: from a few centimetres to some kilometres. The scale of the model domain strongly influences the structure of the model and the setting of the model parameters. A specific application in a microscale domain is the simulation of flows around buildings in horizontal dispersion. In a macroscale model motion is assumed to be dominated by the advective wind and therefore turbulent effects are neglected. In addition the objects of interest chosen are air volumes and

not particles. The choice of the spatial resolution in Lagrangian models is limited by the scale of the data input, such as the wind and turbulence field, in order to meet accuracy.
The time step for the motion calculation also has to be chosen appropriate to the scale and the meteorological conditions (Physick et al. [1994]).
Adequate input data is crucial in regard to the determination of dispersion parameters like the standard deviations and the Lagrangian time scale. As pointed out in 2.2, in emergency management application the information about the emission rate is usually missing. In the example of LAGSIM data is provided by a release model based on Monte Carlo simulation (see Mieth [1999]). In most of the Lagrangian models a module for the computation of plume rise for stack release is implemented. The shape of emission source (e.g. line or point source) does not influence the model structure.
The particle methodology is not well suited for the treatment of chemically reactive species. As long as the reactions can be described by a linear rate, chemistry can be included. But in the case of complex nonlinear chemical reactions, a Eulerian approach should be used. Moreover, the computation of complex chemical reaction schemes often leads to coupled systems of stiff ordinary differential equations. The solution of this type of system is very time consuming.
Another computation time factor may be the number of released particles at each emission source as it strongly determines the amount of calculations needed. The time required for the simulation process may become extensive where a large number of sources are involved or high accuracy is required. However its structure makes the Lagrangian dispersion model well suited for numerical parallelization. A parallel implementation offers the possibility to use a large number of particles and guarantees a reasonable execution time. For further information see Mieth [1999].

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