Abstract

In this thesis a number of contributions on short-range dispersion modeling in the atmospheric boundary layer are collected. They include the development, validation and application of a model type called Puff-Particle Model (PPM), the investigation of a density kernel method to determine smooth concentration estimated for pure particle dispersion models, and the investigation of urban type surface structure on dispersion characteristics.

The PPM is a blend between a Lagrangian Gaussian puff model and a stochastic Lagrangian particle model. The pollutant puffs are advected by the mean wind; the dispersing effect of turbulent eddies smaller than the actual size of the puff is described by a relative dispersion parameterization. Additionally, the puffs exhibit artificial meandering on time scales shorter than the time interval between two consecutive updates of the mean wind field.

Commonly, puff models use either an absolute dispersion parameterization, which accounts for the dispersing effect of meandering as well. Such puff models provide predictions of the ensemble mean concentration. Alternatively, puff models may derive an estimate of the amount of meandering from the statistical properties of the ambient turbulence. This enables the specification of instantaneous ensemble mean concentration, together with its variance. In both cases, an instantaneous release is simulated by one puff. In contrast, in the PPM the puffs experience a stochastic but realistic meandering. To obtain ensemble statistics, an ensemble of puffs in the model has to be simulated for each released pollutant puff. Each simulated puff path is one possible realization of the release's dispersion. The main advantage is that all puffs are advected by the local wind at their current position. Concentration variances can be computed not only for instantaneous concentrations, but, due to the temporal correlation between subsequent positions of the meandering puffs, also for any other sampling time.

The puff meandering allows the PPM to compute the higher moments of concentration, along with the mean concentration, for any puff release. This provides a convenient way for risk assessment of hazardous releases, or for the computation of the frequency of exceedance of a given odor threshold. The particle model embodied within the PPM assumes that the evolution in time of particle velocity and position be a Markov process. This neglects the

spatial and temporal correlation between two neighboring particles. To extend the field of application of the PPM from puff to plume releases, a special puff-plume meandering scheme has been introduced. It constitutes a dependence of the individual puffs on their predecessors in the plume.

To ensure that the puff's meandering trajectory represents the correct amount of kinetic energy, the PPM computes a full three-dimensional particle trajectory, as supplied by a stochastic Lagrangian particle model. Such particle trajectories represent the entire spectrum of turbulent energy. A low-pass filter is thus applied which removes all eddies smaller than the actual puff size. The resulting time series of stochastic velocities is used as puff center trajectory. This avoids that an increasing part (as puff sizes grow) of the dispersion is double-counted both by the puff center trajectories and by the relative dispersion scheme.

The PPM can be used to compute ensemble-averaged concentrations by sampling over many individual puff trajectory realizations. For three tracer experiments, the PPM predictions are compared to those of other dispersion models. It is shown that, due to the built-in full-scale particle model, the PPM has approximately the same model prediction performance as pure stochastic particle models (which perform best). In the ensemble-average mode, the PPM is approximately one order of magnitude faster than pure particle models. This is due to the use of puffs, which lead to a smoother representation of the concentration density field. Particle models need to simulate more particles to allow for the same smoothness. A method is proposed for particle models to predict smoother concentration fields as well (and thus to speed them up accordingly), by assigning a density distribution to every particle. When concentrations are to be estimated, the size of these density distributions (called kernels) is chosen by optimizing between a smooth spatial concentration density and its oversmoothing.

Apart from the Puff-Particle Model, this thesis also focuses on the use of applied Gaussian plume models over urban environments. For single, high stack source configurations, Gaussian plume models give acceptable results. This is due to the fact that the condition of surface homogeneity is (more or less) fulfilled. Nowadays severe air pollution problems arise in the ever-growing cities. Built-up areas feature a different turbulence structure. It is shown for a specific example which adaptations in the use and computing code of an applied Gaussian plume model have to be undertaken in order to apply it to urban environments.