INTRODUCTION OF A PUFF-PARTICLE APPROACH FOR NEAR-SOURCE DISPERSION INTO THE CALPUFF MODEL

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Abstract—CALPUFF is a Lagrangian puff dispersion model for pollutant transport simulations for inhomogeneous and non-stationary conditions using a one-hour time step. Using so-called „absolute disersion" parameterizations, the model predicts one-hour-averaged concentrations. In order to be able to predict not only „average" but also „possible" concentrations, i. e. the higher moments of the concentration probability density function, the „absolute dispersion" has to be separated in its puff-growth part and the additional contribution from the meandering of the plume during the averaging time. For this, the concept of the Puff-Particle Model (PPM) is introduced as a new near-source dispersion model within dispersion models such as CALPUFF. The PPM combines the advantages of both, puff and particle dispersion models by moving the center of mass of each puff along a trajectory which mimics the quickly changing turbulent flow field (artificial meandering). This trajectory is derived from the low-frequency part of trajectories as simulated by a Lagrangian stochastic particle model. It allows for a new puff-plume meandering scheme. The combination of CALPUFF and PPM improves the prediction of the highest possibly occurring near-source concentration, as well as the distance down-wind from the source where it occurs, while retaining the advantages of the CALPUFF model.

Key words: concentration pdf, puff models, plume meandering, relative dispersion.

INTRODUCTION

Within the field of dispersion modeling, puff models show a variety of advantages compared to Gaussian plume models. They can take into account the spatial variability of meteorological and dispersion conditions, causality effects, wet and dry deposition, low wind speed dispersion, etc. Lagrangian stochastic particle models, on the other hand, are the state-of-science of dispersion modeling, especially for the simulation of inhomogeneous (convective) turbulence. However, their demand of computing time generally limits their application to the simulation of short episodes rather than a full year. Furthermore, physical processes like dry and wet deposition, buoyant plume rise, and chemical transformations within a cluster, are much easier to implement within the framework of a puff model.

There are two types of puff models. The most common type can be called „plume segment" puff models. Within the framework of these models, a puff (consisting of a center of mass, the actual velocity of the puff, and a 3D distribution of the total mass around the center) stands for the ensemble average of

the concentration distribution belonging to a „piece“ (in time) of the pollutant release. These puffs do not correspond to a single cluster in nature, but are an ensemble average over many individual clusters. Dispersion parameterizations predicting such ensemble mean statistics are called „absolute dispersion“.

The second type is the group of „cluster dispersion“ puff models. These models identify the puff with an individual, physically realistic cluster of particles. They use the concept of relative dispersion (i. e. 2-particle statistics; Borgas and Sawford 1994): turbulent eddies smaller than the actual puff size will contribute to its growth (increasing the ensemble 2-particle separation), while larger eddies move the puff as a whole (without changing the separation of the particles). Hence, absolute dispersion is the combined effect of relative diffusion and of the meandering of the puff respective to a fixed point, caused by turbulent eddies larger than the puff.

The missing link between relative and absolute dispersion is the dispersing effect of meandering over time-scales shorter than the averaging time for which the absolute dispersion parameterization used applies (normally equaling the spectral gap, i. e. roughly one hour). For small (newly released) puffs, absolute dispersion is dominated by meandering rather than by puff-growth. Therefore, in contrast to „cluster dispersion“ models, „plume segment“ puff models are not suited to give correct concentration predictions for a single (instantaneous) release, especially in the near field.

In practice it is difficult to provide the flow field at a sufficiently high temporal rate. This means that the effect of meandering has to be simulated. For this, in the Puff-Particle Model (PPM) (de Haan and Rotach 1999), a „cluster dispersion“ puff model using relative diffusion, the meandering of the puffs’ centers of mass is generated artificially. These meandering trajectories simulate the effect of all those eddies not resolved by the flow field but still larger than the puff. Models like the PPM are especially suited for the simulation of accidental hazardous releases. For preliminary risk assessments, the actual flow field is not known. But the artificial meandering scheme of the PPM allows the simulation of an ensemble of possible realizations, identifying worst-case scenarios. Thus, the PPM can determine the probability of a certain concentration level: a concentration probability density function (C-pdf).

The disadvantage of „cluster dispersion“ models is their need to simulate a large ensemble of individual releases to obtain the ensemble average. The additional information they generate is not needed all the time. In the present paper, the „cluster dispersion“ Puff-Particle Model (PPM) is introduced as a sub-model into the „plume segment“ CALPUFF model. In the next three sections, the basic philosophy and major features of CALPUFF and PPM are summarized. Then, we present the design of the interface between these two models, and describe how the concentration pdf are obtained. Finally. the form of such concentration pdf’s for different down-wind distances and averaging times is discussed.

THE CALPUFF DISPERSION MODEL

CALPUFF is a Lagrangian puff dispersion model (Scire *et al.* 1995, 1997). Among its main fields of application are pollutant transport simulations for inhomogeneous and non-stationary conditions. The model is a member of the „plume segment“ puff model family, using "absolute dispersion", i. e. the time-averaged dispersion of an ensemble of pollutant releases. Together with the flow fields of its meteorological model, CALMET, CALPUFF is applicable to complex terrain and coastal situations.

The CALPUFF model is a non-steady-state puff dispersion model. The user-defined grid size allows for high-resolution simulation of episodes as well as for runs for one year or more with a one-hour time step for environmental impact assessments, and studies of air quality and pollutant transport on regional scales. By its puff-based formulation, it can account for a variety of effects such as spatial variability of meteorological and dispersion conditions, causality effects, dry deposition, plume fumigation,

low wind speed dispersion, pollutant transformation, wet removal, and complex terrain effects. It has various algorithms for parameterizing dispersion processes, including the use of turbulence-based dispersion coefficients derived from similarity theory or observations. Evaluation studies of CALPUFF have been done for long range transport distances (U.S. EPA 1995), intermediate distances (Irwin 1998) and short to intermediate distances (Strimaitis *et al*. 1998).

THE PUFF-PARTICLE MODEL

The fact that instantaneous releases require puff models using relative dispersion, but that at the same time, the update frequency of the flow field information in almost all applications is too low to resolve all those turbulent eddies not covered anymore by the relative dispersion concept, gave rise to the development of the Puff-Particle Model (PPM). It represents the group of so-called „cluster dispersion“ puff models. The PPM in its current version is a research model for tracer pollutants, focusing on near-source dispersion, and neglecting deposition and chemical processes. It features a full stochastic Lagrangian particle dispersion model, which fulfills the well-mixed criterion (Thomson 1987). For convective conditions, the vertical component of the pdf is the same as in Luhar and Britter (1989). To provide a perfectly smooth transition between stable/neutral Gaussian turbulence to convective skewed turbulence, the transition function of Rotach *et al.* (1996) has been adopted. Further details on the PPM can be found in de Haan and Rotach (1999).

Every puff within the PPM follows a turbulent puff trajectory derived from a stochastic particle trajectory. The kinematic turbulent energy belonging to those eddies which are smaller than the puff's size-already covered within the concept of relative dispersion-is removed from the particle trajectories. For this, a Kalman low-frequency filter is used, where the cut-off frequency depends on the size of the puff (de Haan and Rotach 1998). Hence, every puff carries along its own position as well as the position and turbulent velocity components of the stochastic particle it 'belongs to'. The effect of meandering (caused by turbulent eddies larger than the puff but not resolved by the flow field) is simulated by the puff center trajectories, yielding a complete description of dispersion. It has been shown on the basis of tracer data, that the correct treatment and interpretation of the two contributions to the dispersion process is crucial for reproducing experimental results to a good correspondence (de Haan and Rotach 1998).

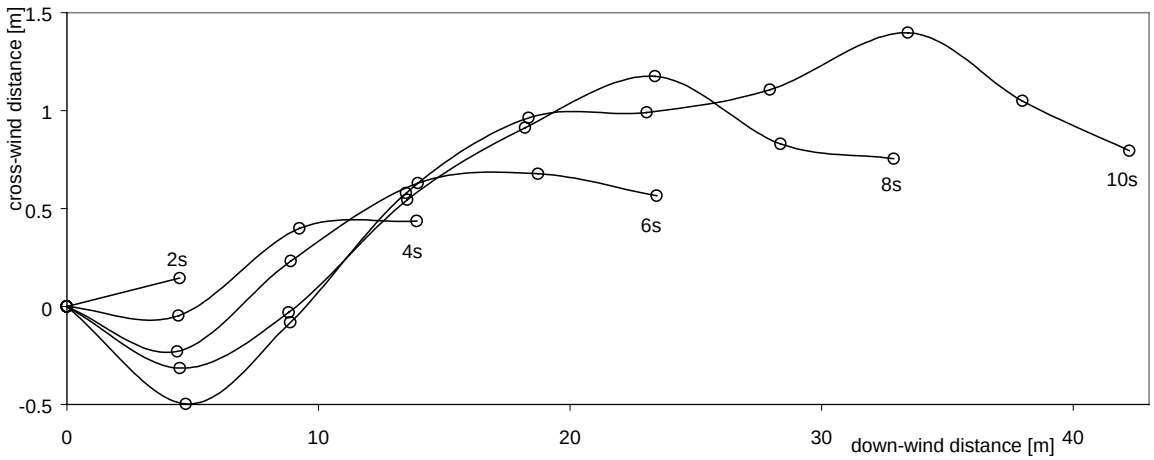

Figure 1. Illustration of the meandering puff-plume scheme. The released puff-plume is depicted 2, 4, 6, 8 and 10 seconds after its release. Puffs belonging to the same puff-plume are connected by a thin line. Circles indicate the position of the center of each puff (not the puff size). View from above.

THE PUFF-PLUME MEANDERING SCHEME

Within the PPM, the puffs use stochastic paths to artificially produce the correct meandering behavior. To obtain correct C-pdf's for any user-specified averaging time, however, that is not sufficient. „Neighbor" puffs should show „similar" meandering: the spatial and temporal correlation of turbulence has to be taken into account. If this is neglected, the most extreme concentration events will be underestimated, and the C-pdf will not be correct.

The PPM employs a plume meandering scheme based on the puff meandering scheme. Plumes are described as threads of puffs which are correlated in their turbulent movements to their next neighbors in the puff-plume. The PPM puff-plume meandering scheme is illustrated in Figure 1 and consists of two steps. *Step 1:* At the beginning of the time-step, each puff has its initial 3D stochastic velocities. After moving the puff-plume with the mean flow and by the stochastic velocities, the newest puff is released. Its stochastic velocities are correlated with those of the second-newest puff (its „mother" puff) by copying the mother's turbulent velocities and computing a puff trajectory over a time which corresponds to the spatial separation from this second-last puff to the source. *Step 2:* The size of the puffs is enlarged using relative dispersion, and new stochastic velocity components are computed (again, by computing a puff trajectory starting with the turbulent velocities from the „mother" puff). The first (most distant from the source) puff of the puff-plume follows a normal (non-correlated) PPM puff-center trajectory.

This meandering scheme can be illustrated by thinking of a spectrum of turbulent eddies „rolling back" towards the source along the puff-plume with the average mean wind speed (introducing the spatial correlation). Such a spectrum of eddies is „released towards the origin" from the front of the plume every time step, based on the puff path of the front puff (temporal correlation) (see Figure 2).

The Lagrangian particle model within the PPM yields a Lagrangian spectrum, when the turbulent velocity of a particle is followed over time. It has the correct „–1" slope of the inertial subrange, in contrast with the „–2/3" slope required for Eulerian spectra. The current approach will thus give a „–1" instead of a „–2/3"-inertial subrange slope when considering the turbulence at a fixed point in space. However, since these spectra are filtered and only their low-frequency part is used, this shortcoming has only a minor influence. The main difference between Eulerian and Lagrangian spectra is the location of the maximum of the spectrum, $f_{max,E}$ and $f_{max,L}$, respectively. This is corrected by shifting the Lagrangian spectrum towards higher frequencies by a factor $\beta = f_{max,E} / f_{max,L}$. So the turbulent velocities of a puff with a separation x to its „mother" are computed as a puff trajectory over a time $\beta \cdot x/U$ rather than x/U.

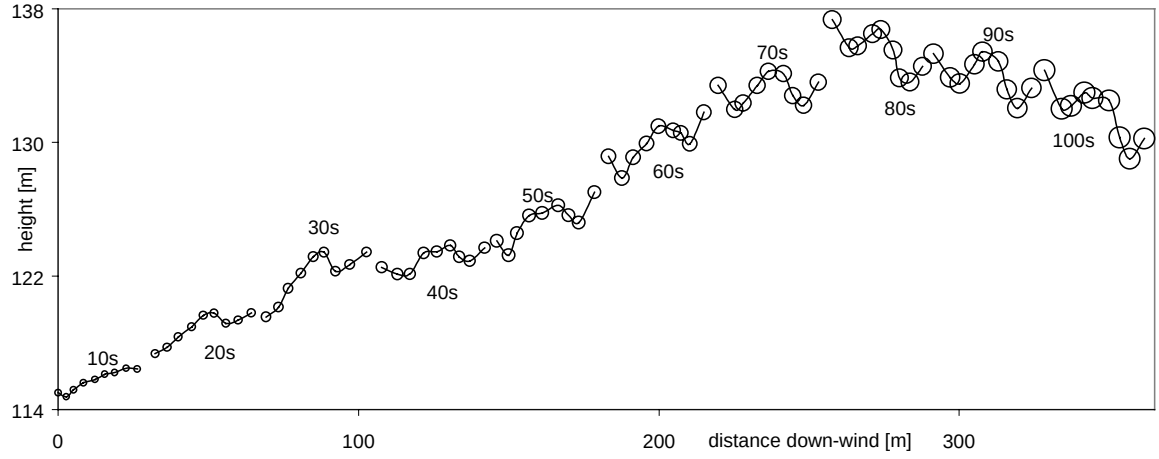

Figure 2. Possible evolution of a plume (consisting of 9 puffs released with a one second interval) over time, when using PPM's meandering puff-plume scheme. The position of the plume's puffs is shown every ten seconds. Example for convective conditions, release height 115 m. View from the side.

INTRODUCTION OF THE PUFF-PARTICLE MODULE INTO CALPUFF

The CALPUFF model has been developed for a broad range of applications, from micro-scale to meso-scale, from short-term to long-term, with treatments of wet and dry deposition, chemistry, coastal interactions, complex terrain, visibility impacts, etc. The PPM will be one additional option in this list, providing additional information on the near-source concentration moments. Due to the flexibility of the CALPUFF model on the side of the user, its code has reached a high grade of complexity. Therefore, one of the main objectives for the implementation of the Puff-Particle module into CALPUFF was to introduce as few interactions between the CALPUFF code and the PPM option as possible, in keeping with the module coding concept. Thus, the underlying thought of the concept adopted was that CALPUFF's puff treatment will not change; it is only within the Puff-Particle module that the simulation of artificial meandering of relatively dispersed puffs is computed.

Figure 3 illustrates the basic set-up of the PPM within CALPUFF:

- To every newly released puff, a so-called 'mirror ensemble' is attached. Such a mirror ensemble consists of a user-defined number, *N*, of puff-particles.
- In order to take into account the information from all grid cells through which the puff will pass in one hour, CALPUFF divides the one hour model time step into a varying number of sampling steps for each puff. For the duration of the sampling step of the parent puff within CALPUFF's main routine, the mirror-ensemble is advected with an internal user-defined PPM-timestep between, say, 1 and 10 seconds. For every internal PPM-timestep, new particle trajectories are computed, from which puff trajectories are derived. Additionally, the puff-particles are advected by the mean flow.
- At the end of the sampling step, from the mirror ensemble's first and second moments of the mass distribution, the position and size of the parent puff are calculated and handed back to CALPUFF's main routine. CALPUFF may then compute any physical process possibly changing the (parent) puff's mass or chemical composition, but not its size or location. The mirror ensemble remains in existence for use in the next sampling step.

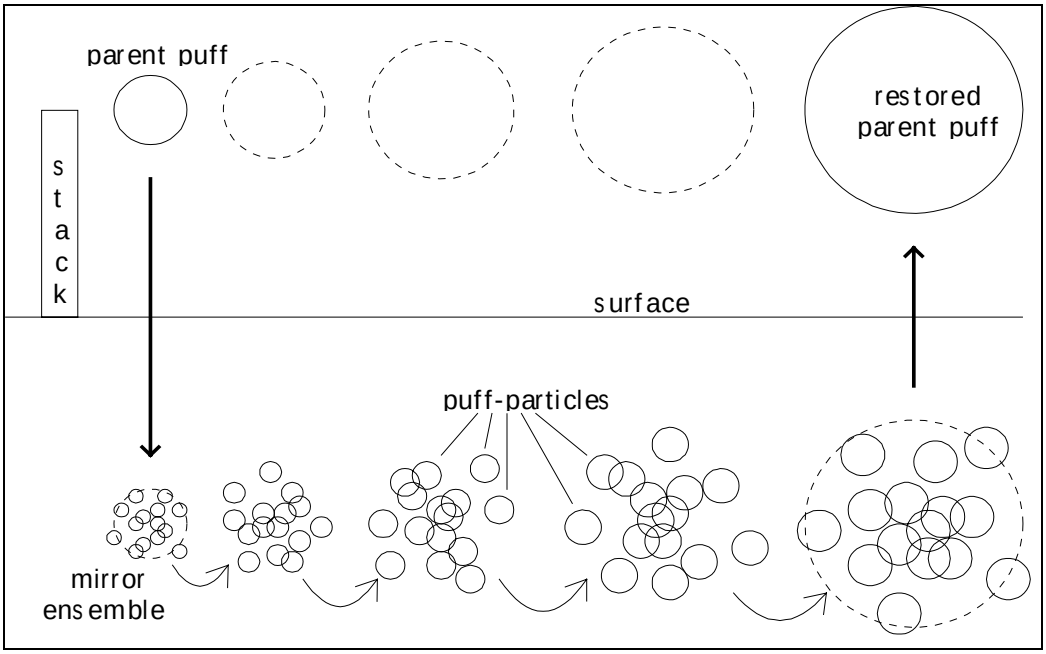

Figure 3. Illustration of the imbeddement of the PPM into the CALPUFF model. The procedure for one sampling time step is depicted. After „restoring" the new location and size of the parent puff, the mirror-ensemble remains stored for use at the beginning of the next sampling step of the same puff, until the puff reaches a mature stage where the mirror-ensemble will be deleted.

- After a certain time, the size of the relatively dispersed particle-puffs in the mirror ensemble will be

such that the largest part of the energy spectrum of turbulent eddies will be 'within' the puff-particle. This means that the relative and absolute dispersion for that ensemble become similar. The artificial meandering will show only little variation of the particle-puff's paths. Then, the 'parent puff' location and size is recomputed, the mirror ensemble deleted and the parent puff restored, which from then on is treated with the common absolute dispersion within the CALPUFF model.

The initial position of the particle-puffs at the time of creation of a mirror ensemble is taken randomly from a three-dimensional Gaussian distribution with mean at the center of the parent puff, and the standard deviations of the parent puff being the second moments of the Gaussian distribution. Analogously, the initial turbulent velocity components of the puff-particles of the mirror ensemble are taken from a three-dimensional Gaussian distribution with zero mean and with the ambient turbulence $\left(u_i'^2, i = 1,2,3\right)$ as the second moments.

DETERMINATION OF A CONCENTRATION PDF

The puff-particle approach gives a realistic picture of the transport (caused by the mean wind, provided by the flow field updates), the amount of meandering (covered by the stochastic puff center trajectories) and the diffusion of the release (caused by eddies smaller than the puff, and taken into account by relative diffusion). For each parent puff, an ensemble of mirror puff-particles is released. Since the meandering part of their motion is reigned by random particle motion, their trajectories will not be identical. Each of them is a possible realization of what might have happened to the parent puff in reality.

To obtain the mean (ensemble averaged) concentration at any receptor, the average over all mirror puff-particles can be taken, where each realization is assumed to represent 1/*N* of the total mass of the parent puff. In theory, the ensemble average concentration thus obtained should be close to the concentration estimation obtained by using the parent puff only, together with absolute dispersion. Of course, in practice, minor differences will appear. To let these differences vanish, it would be necessary to use the same set of parameterized spectra of turbulent energy as a foundation of the absolute as well as the relative dispersion parameterization and at the same time derive the particle pdf within PPM's particle model from this set of spectra.

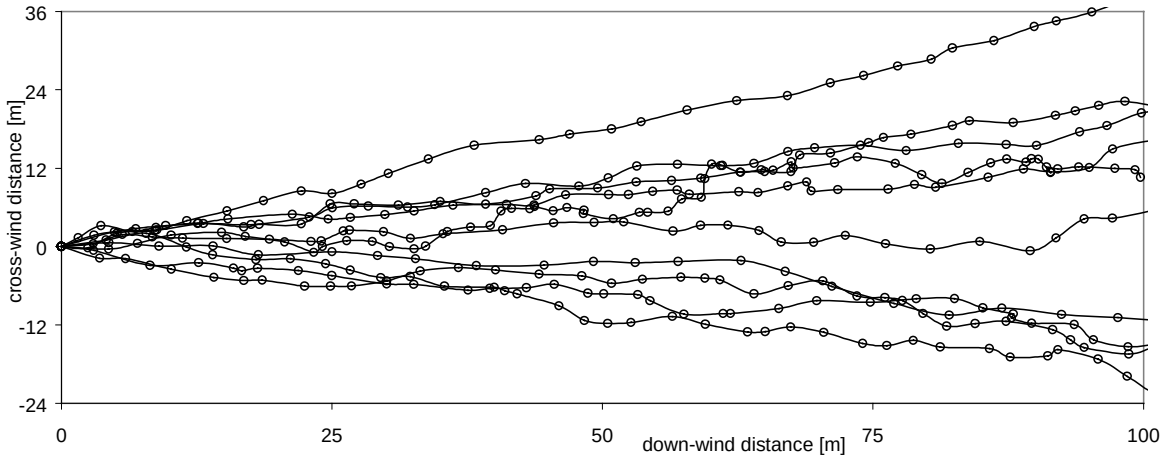

Figure 4. Method to construct a C-pdf. Many individual meandering puff-plumes are simulated. Each is treated as one possible realization that could actually have happened for the given meteorological data. The sorted concentration impacts (for a user-determined averaging time) at specified receptor locations from these many realizations constitute the C-pdf.

To obtain the pdf of concentration at such a receptor, every realization (i. e. mirror puff-particle)

carries the whole mass of the parent puff, and the concentration due to this particular realization is computed (Figure 4). This leads to *N* possible concentrations, from which the concentration pdf easily can be derived. Of course, to make the concentrations thus computed comparable to the standard CALPUFF results, these *N* possible concentrations have to be computed using all puffs in the modeling domain impacting the receptor, whether they possess a mirror-ensemble or not. In the intermediate to far field, the will lead to a narrowing of the concentration pdf, reflecting the fact that well dispersed pollutant clusters will indeed lead to a higher degree of determination of the corresponding concentration. Therefore, the PPM option within CALPUFF will produce valuable results mainly in the near field, where the differences in puff position due to meandering potentially are of the same order of magnitude as the size of the puff.

CHARACTERISTICS OF CONCENTRATION PDF'S

When looking at the changes in the form of the C-pdf for increasing down-wind distances (Figure 5), two effects are occurring simultaneously. First, a shift of the mean (and the maximum) to the left, i. e. to lower ensemble average concentrations. Second, a narrowing of the C-pdf: the slopes to the left and to the right of the maximum are getting steeper. This means that the ensemble average becomes „better defined", due to the fact that the relevant time scales of fluctuation at these distances are much larger than the averaging time.

The form of the C-pdf also is a function of the averaging time *T*. Whereas a short averaging time of 60 s leads to a wide-spread C-pdf (in Figure 5, for 1000 m down-wind, the probability that the actual concentration is at least five times higher than the ensemble average is 5%), the C-pdf narrows for larger averaging times (without changing its mean, i. e. ensemble concentration). Additionally, C-pdf's for stable conditions are wider than for convective conditions, because more dispersion leads to a more well-defined ensemble mean, hence a narrowing of the C-pdf.

The form of the C-pdf often is assumed to be log-normal. For most models predicting concentration fluctuation probabilities, this is an input rather than a result. The results from the present model, however, suggest that the C-pdf is log-skewed towards lower concentrations.

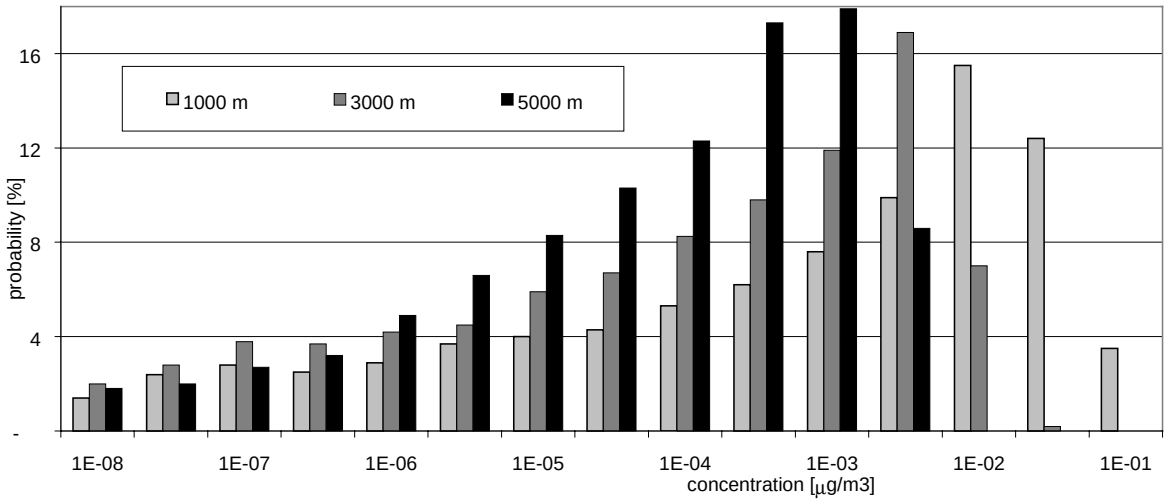

Figure 5. Example of C-pdf's for the plume centerline position at three distances down-wind from the source; averaging time 60 s. Example for the Copenhagen experiment (release height 115 m, conditions of forced convection).

SUMMARY AND CONCLUSIONS

The combination of two models, CALPUFF and PPM, using different approaches to describe the dispersion of pollutants, allows for the combination of the advantages of the CALPUFF model, with additional information on the higher moments of the concentration distribution at near-field receptors from the PPM module. This allows for an additional assessment of concentrations that actually could be observed at a given receptor, together with the corresponding probability. This additional feature is particular useful for the assessment of hazardous pollutants, where the question of the average exposure is less relevant than the highest exposure which could actually occur under the given meteorological conditions.

Acknowledgments—The present work was partly financed by the Swiss Agency of Education and Sciences (BBW) and the Swiss Agency of Environment, Forest and Landscape (BUWAL) through a project in the framework of COST 615 (citair), and by the Swiss National Science Foundation through Grant Nr. 21-46849.96.

REFERENCES

Borgas, M. S. and Sawford, B. L. (1994): A Family of Stochastic Models for Two-Particle Dispersion in Isotropic Homogeneous Stationary Turbulence. *J. Fluid. Mech*., **279**, 69–99

de Haan, P., and Rotach, M. W. (1998): The Treatment of Relative Dispersion within a combined Puff-Particle Model (PPM). In: Air Pollution Modeling and Its Application XII, S.-E. Gryning and N. Chaumerliac (eds.), Plenum Press, New York, 389–396

de Haan, P., and Rotach, M. W. (1999): A novel approach to atmospheric dispersion modelling: the Puff-Particle Model (PPM). Accepted for publication in *Quart. J. Roy. Meteorol. Soc*.

de Haan, P., and Scire, J. S. (1999): Prediction of higher moments of near-source concentration by simulating the meandering of pollutant puffs. Preprints 13th Conf. Boundary Layers and Turbulence, Jan. 10–15, 1999, Dallas. American Meteorol. Soc., Boston, USA

Irwin, J. S. (1998): A comparison of CALPUFF modeling results with 1977 Inel field data results. In: Air Pollution Modeling and Its Application XII, S. E. Gryning and N. Chaumerliac (eds.), Plenum Press, New York, 143–151

Luhar, A. K. and Britter, R. E. (1989): A Random Walk Model for Dispersion in Inhomogeneous Turbulence in a Convective Boundary Layer. *Atmospheric Env.*, **23**, 1911–1924

Rotach, M. W., Gryning, S.-E. and Tassone, C. (1996): A Two-Dimensional Stochastic Lagrangian Dispersion Model for Daytime Conditions. *Quart. J. Roy. Meteorol. Soc.*, **122**, 367–389

Scire, J. S., Strimaitis, D. G., Yamartino, R. J., and Zhang, X. (1995): A User's Guide for the CALPUFF Dispersion Model. Prepared for the USDA Forest Service, Cadillac MI, by Earth Tech, Inc., Concord, MA 01742, USA.

Strimaitis, D. G., Scire, J. S., and Chang, J. C. (1998): Evaluation of the CALPUFF Dispersion Model with two Power Plant Data Sets. Preprints 10th Joint Conf. Appl. Air Poll. Meteorology, 11–16 Jan. 1998, Phoenix, Arizona.

Scire, J. S., Strimaitis, D. G., Yamartino, R. J., and Insley, E. M. (1997): A User's Guide for the CALPUFF Dispersion Model (Version 5.0). Earth Tech, Inc., Concord, MA 01742, USA.

Thomson, D. J. (1987): Criteria for the Selection of Stochastic Models of Particle Trajectories in Turbulent Flows. *J. Fluid Mech.*, **180**, 529–556

U.S. Environmental Protection Agency (1995): Testing of meteorological and dispersion models for use in regional air quality modeling. U.S. EPA, Research Triangle Park, NC.

DISCUSSION

D. WILSON: When using a discrete numerical model to simulate concentrations pdf's it is necessary to release a very large number of puffs to capture the extreme values of high concentration that occur at a fixed (Eulerian frame) receptor. Do you have a procedure for estimating the required number of puffs (N) needed to correctly simulate a concentration peak such as the C_{99} that is exceeded 1% of the time?

P. de HAAN: The current simulations were performed with $N = 1000$. This is believed to give reliable results for C_{95}. Hence $N = 10\,000$ would do for C_{99}. But it depends on the assumed form of the C-pdf. Statistically correct confidence limits, however, would also be a function of the averaging time T.

M. KAASIK: An experiment with measurements very near to the source is the Lillestrøm experiment. Will you use this data set?

P. de HAAN: The Lillestrøm data set consists of only four independent experiments. These took place under very stable conditions, but during sunrise. The concentration statistics are influenced by one very high observation. I consider the Prairie Grass data to be more adequate for near-source assessments.

S. RAFAILIDIS: A comment relating to the need of validation of your model. By the end of 1998 the University of Hamburg and the German „Umweltbundesamt" will release a comprehensive wind tunnel data set. It contains information on the spectral characteristics of the incoming flow, and concentration time series down-wind of the release (www.mi.uni-hamburg.de).