Predicting concentration fluctuations with a puff-particle model

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Abstract: This paper demonstrates that the puff-particle model (PPM) allows for the prediction of concentration fluctuations (in addition to the estimation of the concentration itself). Several models have been developed based on Gifford's meandering plume concept to separate the dispersing effect of instantaneous plume (or puff) growth, and of meandering. They all have in common the assumption of a certain shape of the probability density function of concentration, and that the variance of concentration fluctuations is derived from the properties of turbulence. In contrast, the PPM aims at simulating a realistic 3-D meandering of the puffs, which allows for direct determination of the higher moments of concentration, whilst enabling the individual puffs to account for inhomogeneous conditions.

Keywords: concentration fluctuations, particle model, plume meandering, puff model, relative dispersion.

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1 Introduction

When modelling pollutant transport and dispersion using gridded meteorological flow fields on an hourly basis, significant parts of the turbulence spectra are not resolved in space and time. Parameterizations of puff or plume dispersion commonly account for this by estimating one-hour averaged dispersion. For risk assessments and odour impact analyses, the highest possible occurring concentration during a time considerably shorter than one hour is more decisive. For this, the probability density function of concentration for a given location and a specific averaging time is required.

In order to estimate concentration probability density functions, dispersion can be divided into two components: the instantaneous puff/plume growth (driven by turbulent eddies being smaller than the size of the puff), and the dispersion caused by meandering (large eddies displace the puff without enlarging it) of the puff during the time-averaging period. This contribution presents predicted higher moments of near-source concentrations for different averaging times, using the Lagrangian puff-particle model (PPM). The performance of the PPM in predicting one-hour averaged concentration values has been extensively validated using the Model Validation Kit, and compared with other dispersion models (de Haan and Rotach, 1998a). The use of the PPM to estimate concentration fluctuations was first discussed in de Haan *et al*. (1999) and de Haan and Scire (1999).

In the following sections, the basic philosophy and major features of the PPM are summarized. The puff-plume meandering scheme, which is proposed to simulate the meandering behaviour of a continuously emitting source within the PPM, is introduced. By interpreting any single meandering puff trajectory as a possible realization, a probability density function of concentration (hereafter denoted as *C*-pdf) can be computed. This is performed for a tracer experiment.

2 The need for the modelling of concentration fluctuations

Assessment of flammability or toxicity on the basis of ensemble-averaged concentrations can be seriously in error. These effects depend on short temporal and spatial scale fluctuations and thus the variance is essential for these predictions (Sykes, 1988). Short temporal scale effects call for short (concentration) sampling times. This violates a basic assumption of many common air pollution models, since such averaging times are considerably shorter than the spectral gap (approximately one hour). Most models assume that the sampling time is sufficiently long to include most of the turbulent energy spectrum (Hanna, 1982).

In practice it is difficult to provide the flow field at a sufficiently high temporal rate to resolve all meandering motions, especially for small puffs. This means that the effect of meandering has to be simulated. In the PPM (de Haan and Rotach, 1998a), a ‘cluster dispersion’ puff model using relative diffusion, the meandering of the centre of mass of the puff is generated artificially. These meandering trajectories simulate the effect of all the eddies which are not resolved by the flow field but are still larger than the puff.

The present contribution calculates concentration fluctuations with a plume meandering model. This can be applied to near-source cases, since the internal (within the puff) fluctuations are neglected. Internal fluctuations become important when the release becomes approximately well mixed in the vertical direction (Hanna, 1984; 1986). In buoyant plumes, internal fluctuations are driven by the relative motion (plume rise) and may be relevant at all fetches. The present contribution does not apply to buoyant releases.

Savunen and Rantakrans (1999) present an odour model based on the assumption of a log-normal *C*-pdf, based on Gifford (1959) and Hanna (1986). Its second moment is estimated as the standard deviation of the meandering motion or, when the plume becomes well-mixed, as the standard deviation of turbulent velocity. Sykes *et al*. (1984) present a second-order turbulence closure scheme which accurately describes the near-field meandering and is able to predict the concentration variance along with the ensemble-mean concentration.

Borgas (1998) and Wilson and Hilderman (1999) focus on the prediction of the highest occurring concentration caused by internal fluctuations. Borgas (1998) uses theoretical relative dispersion considerations to derive the higher moments of the *C*-pdf, whereas Wilson and Hilderman (1999) use a stochastic Markov process to emulate the time-series of internal concentration fluctuations, when the moments of the *C*-pdf are supplied by any plume meandering model.

Several models have been developed based on Gifford’s (1959) meandering plume concept to separate the dispersing effect of instantaneous plume (or puff) growth and of meandering (e.g. Hanna, 1984, 1986; Savunen and Rantakrans, 1997; Sykes, 1988). They all have in common the assumption of a certain shape of the probability density function of concentration, and that the variance of concentration fluctuations is derived from the properties of turbulence. SCIPUFF (Sykes, 1997) uses a second-order turbulence closure scheme predicting both the mean concentration and its variance. In contrast, the PPM aims at simulating a realistic 3-D meandering of the puffs, which allows for the direct determination of the higher moments of concentration, whilst enabling the individual puffs to account for inhomogeneous conditions.

3 The puff-particle model (PPM)

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 no longer covered by the relative dispersion concept, gave rise to the development of the puff-particle model (PPM). 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 fulfils 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 and 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 (1998a).

Every puff within the PPM follows a turbulent puff trajectory derived from a stochastic particle trajectory. The cinematic turbulent energy belonging to those eddies which are smaller than the size of the puff — already covered within the concept of relative dispersion — is removed from the particle trajectories. For this, a low-frequency Kalman filter is used, where the cut-off frequency depends on the size of the puff (de Haan and Rotach, 1998b). Hence, every puff carries 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 centre 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 with good accuracy (de Haan and Rotach 1998a). In order to avoid the double counting of dispersion, only the low-frequency part of the trajectory is used by applying the Kalman filter (de Haan and Rotach, 1998b).

4 The puff-plume meandering model

Gifford’s (1959) meandering plume dispersion model neglects dispersion in the direction of the mean wind, leading to a ‘spreading disk’ plume dispersion model. The mean concentration distribution as predicted by Gifford’s (1959) model is identical with predictions from ensemble-averaged plume models. Additionally, it predicts statistical properties like the variance of point concentrations. The ‘split’ between instantaneous plume growth and dispersion due to meandering is a function of downwind distance, i.e.

it is different for each disk of the fluctuating plume. These disks do not actually move; it is the statistical property of their movement that is predicted. From this it follows that the statistical properties of concentration as predicted by the Gifford (1959) approach apply to instantaneous (point) concentrations, i.e. with zero-averaging time.

However, for a non-zero, arbitrary concentration averaging time, the correlation of the meandering movements between two neighbouring disks, or puffs, has to be taken into account. Even though the statistical properties of concentration fluctuations for each point are correct, the statistical properties of concentration averages over time differ from non-correlated to correlated meandering. Sykes (1984) and Sykes and Gabruk (1997) present an extension to the Gifford (1959) model, introducing an auto-correlation function for concentration fluctuations. This allows for the computation of the influence of averaging time on the concentration variances.

Within the PPM, the puffs use stochastic paths to artificially produce the correct meandering behaviour. In this way, the ensemble mean concentration, together with its higher moments can be computed for a puff release, for any user-specified averaging, i.e. sampling, time. However, to obtain correct *C*-pdfs for continuous plume releases, these stochastic puff meandering trajectories are not sufficient. They are derived from Lagrangian particle trajectories which are stochastically independent. But ‘neighbour’ puffs, i.e. subsequently released 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 neighbours in the puff-plume. The PPM puff-plume meandering scheme is illustrated in Figure 1 and consists of three steps:

- *Step A.* At the beginning of the time-step, each puff has its initial 3-D stochastic velocity components.
- *Step B.* After moving the puff-plume with the mean flow and by the stochastic velocities, the newest puff is released. The stochastic velocities are correlated with those of the second-newest puff (the ‘mother’ puff). This is done by first copying the mother’s turbulent velocities, and then evolving, i.e. decorrelating, this velocity by computing a puff trajectory (starting with the mother’s turbulent velocity) over a time which corresponds to the spatial separation from the mother puff to the source. The resulting turbulent velocity (decorrelated over the distance between mother and child puff) is then assigned to the child puff.
- *Step C.* The size of the puff 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 (noncorrelated) PPM puff-centre trajectory.

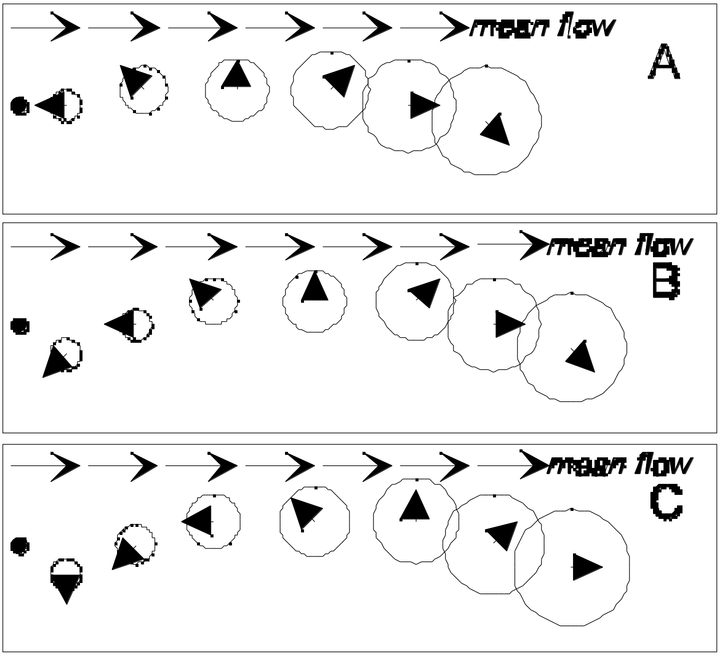

Figure 1 Scheme to produce artificially meandering puff-plumes. The source location is indicated by a solid black dot. The solid triangles depict the stochastic velocity of the puff centres (3-D in the model), without the mean wind flow component.

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

5 Use of the PPM to predict concentration fluctuations

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 (by the stochastic puff centre trajectories), and the diffusion of the release (caused by eddies smaller than the puff, and taken into account by relative diffusion). Since the meandering part of any puff is controlled by random particle motion, their trajectories will not be identical, even for identical meteorological conditions. Each of them is a possible realization of what might have happened to the puff in reality.

To obtain the mean (ensemble-averaged) concentration at any receptor, the average over an ensemble has to be computed, where each realization is assumed to represent $1/N$ of the total mass of the ‘real’ puff. The C-pdf, on the other hand, i.e. the concentration fluctuations, may be computed by treating every possible realization (as depicted in Figure 2) as having the total mass of the real puff. The N different concentration impact scenarios, each being a possible realization of what might have been the impact of the source on the receptor location chosen, can then be used to construct a C-pdf.

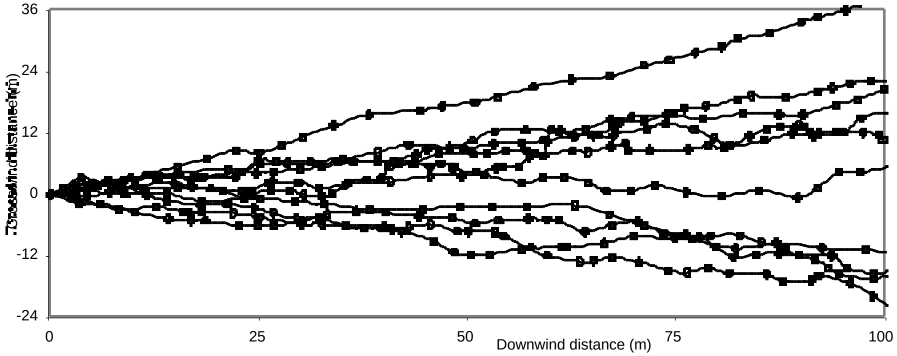

Figure 2 Method to construct a *C*-pdf. Many individual meandering puff-plumes are simulated. Each is treated as one possible realization that could have happened for the given meteorological data. The sorted concentration impacts (for a user-determined averaging time) at specified receptor locations from these many realizations constitute the *C*-pdf.

As a first example of the application of the PPM, Figure 3 depicts the cumulative *C*-pdf for the Copenhagen tracer experiment (Gryning and Lyck 1984) for $N = 1000$ for an averaging time of 60 seconds. The 60 second averages are considered representative for odour problems here. For the example of 1000 m downwind plume centreline concentrations, the chance that the 'true' concentration will not exceed the average is 74%. In 5% of all cases, the actual concentration will be higher than five times the ensemble average.

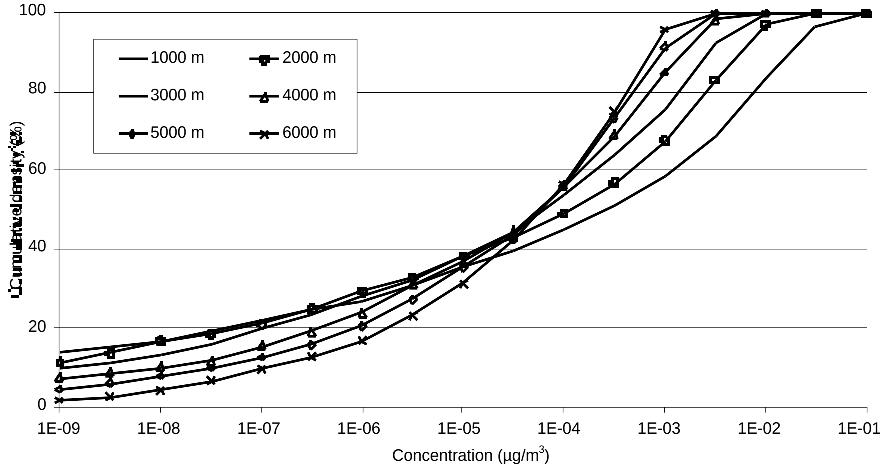

Figure 3 Cumulative concentration pdf for the plume centreline position at six distances downwind from the source. Averaging time 60 s. Release height 115 m, conditions of forced convection.

Observations show that the most pronounced plume concentration fluctuations are produced very near to the source (Fackrell and Robins 1982), and the form of the pdf changes from a near-source exponential to an intermediate-field normal distribution. Despite these forms, the ratio of peak to ensemble-averaged concentrations seems to remain constant. The relative amount of meandering (with respect to ensemble-averaged dispersion) depends on atmospheric stability. For example, for stable (night-time) conditions Hanna (1983) observed very high lateral plume meandering.

When looking at the changes in the form of the *C*-pdf for increasing downwind distances (Figure 3), two effects occur simultaneously. First, there is a shift of the mean (and the maximum) to the left, i.e. to lower ensemble-average concentrations. Second, there is a narrowing of the *C*-pdf where 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 timescales of fluctuation at these distances are much larger than the averaging time. The form of the *C*-pdf is often assumed to be log-normal. For most models predicting concentration fluctuation probabilities, this is an input rather than a result. However, the results from the present model, suggest that the *C*-pdf is log-skewed towards lower concentrations.

6 Summary and conclusions

Hazardous gases and odour complaints show a highly non-linear relationship between their impact and the average concentration. The total dose or the peak concentration is more relevant. To assess such releases, short averaging times are needed, as well as higher moments of concentration, i.e. a *C*-pdf. For this, the sub-averaging time and sub-grid meandering of the pollutant release has to be modelled separately from the dispersion itself. Using the PPM, this paper shows a method to simulate the meandering of puffs while dispersing the puffs with relative dispersion. For every emitted pollutant puff, an ensemble of puffs is simulated within the PPM. Every individual meandering puff path is interpreted as one possible realization of the dispersion, meandering and transport of the pollutant puff. The *C*-pdf is based on the estimated concentration impacts of the individual realizations from the ensemble.

The particle model incorporated within the PPM, upon which the puff meandering is based, assumes that the particle trajectories be stochastically independent. This allows for the computation of concentration variances for an instantaneous puff release. However, for any continuous release, the correlation between subsequently emitted puffs has to be taken into account. In order to mimic this spatial and temporal correlation correctly, a puff-plume meandering scheme has been introduced. The puff and plume-meandering approach is suited to calculate near-source *C*-pdf for any user-specified averaging time. For the estimation of far-field concentration fluctuations, the effect of internal fluctuations has to be taken into account as well. This way, the PPM is especially suited for the simulation of accidental hazardous releases. The artificial meandering scheme allows the identification of worst-case scenarios.

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