Chapter 3

The Treatment of Relative Dispersion Within a Combined Puff-Particle Model (PPM)*

Abstract—The Puff-Particle Model (PPM) combines the advantages of both, puff and particle dispersion models. In short, in this approach the centre of mass of each puff is moved along a 'particle trajectory', so trying to mimic the quickly changing turbulent flow field. However, particle models account for dispersion of turbulent eddies of all sizes (1-particle statistics, absolute dispersion) while puff models use relative dispersion to describe the puff growth. Therefore, on combining these two approaches as described above, the dispersing effect of small eddies (smaller than approximately the puff's size) is accounted for twice. A method is therefore presented to correctly simulate the relative dispersion of puffs within the framework of the PPM. It is based on removing the effect of the high-frequency part of the spectrum when using a 'particle trajectory' as the trajectory of the puff centre. It is 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.

Key words: dispersion modelling, puff models, particle models, relative dispersion.

3.1 CONCEPT OF THE PPM

One of the major advantages of puff models is their ability to simulate inhomogeneous and instationary conditions. In principle this allows for concentration predictions of a 'sudden release' of pollutants from a source. In such cases relative dispersion must be used to describe the growth of the puff. Relative dispersion only takes into account the dispersing effect of those turbulent eddies which are able to enlarge the size of the puff and do not move the puff as a whole without dispersing it. The use of absolute dispersion (like the widely used parametrizations of Pasquill and Turner), which accounts for the dispersing effect of turbulent

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eddies of any size, leads to underpredicted concentrations relatively close to the source due to too large a dispersion.

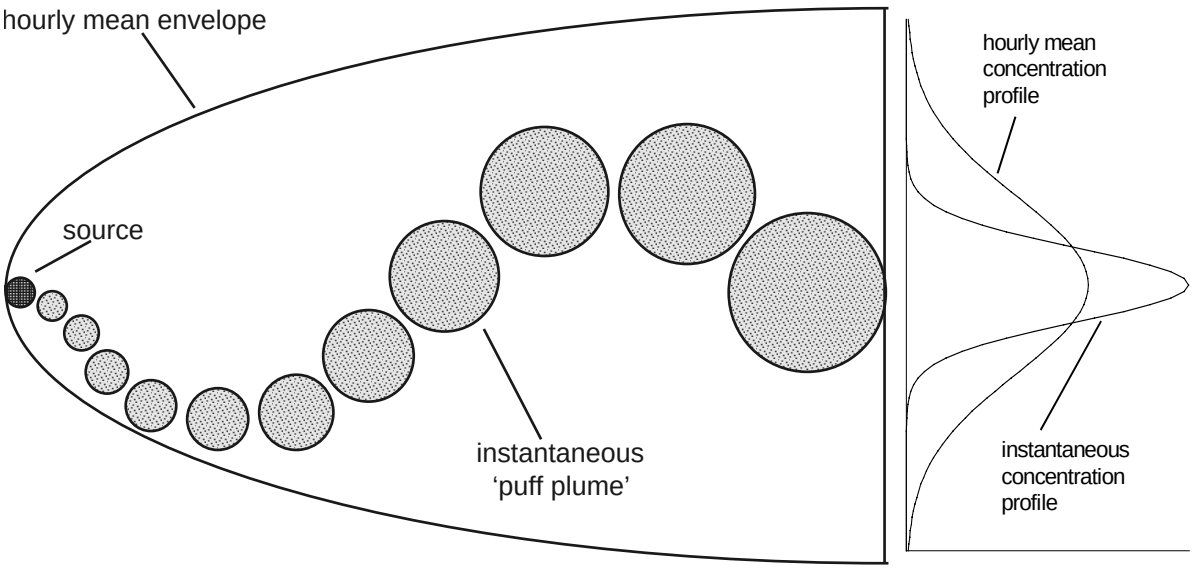

Figure 1 Conceptual sketch of the principle of the PPM. The meandering of the instantaneous 'puff plume' is modelled by moving the centre of mass of the puffs along a particle trajectory.

However, to correctly describe the dispersing effect due to the meandering of the released plume, a rather frequent updating of the flow field information is necessary. In principle, the updating of the flow field should resolve all turbulent eddies larger than the 'size' of the puff (characterized by its standard deviations). Since in practice such a frequent updating of the flow field and meteorological information is hardly possible, the puff-particle approach (de Haan and Rotach, 1995) aims at simulating the dispersing effect of plume meandering by introducing puff centre trajectories (see Fig. 1). These trajectories are determined by the low-frequency part of the turbulence spectrum, since relative dispersion only describes the effects of the high-frequency part. Clearly, as the puff's size grows, the relative dispersion covers an increasing part of the spectrum. Therefore, the trajectory of the puff's centre of mass has to simulate the effect of a decreasing amount of turbulent eddies, and thus has to become 'smoother' as puff sizes grow.

3.2 RELATIVE VS. ABSOLUTE DISPERSION

Relative dispersion corresponds to the expansion of a cluster of particles. The spread σ of an ensemble of marked passive particles from each other is

$$\sigma^2(t) = \left\langle \left(\int_0^t v(\xi) d\xi \right)^2 \right\rangle, \tag{1}$$

where $v = u - V_{cm}$, u is the absolute velocity of the particles and the velocity of the centre of mass of the cluster is denoted by V_{cm}. The overbar in Eq. (1) and hereafter denotes the average over all the particles within the puff, and the angular brackets refer to an ensemble average. In the concept of absolute dispersion, on the other hand, the spread σ is

$$\sigma^2(t) = \left\langle \left(\int_0^t u(\xi) d\xi \right)^2 \right\rangle. \tag{2}$$

For example, a turbulent eddy larger than the cluster of particles will displace the cluster as a whole. This will increase absolute dispersion, whereas the relative dispersion remains unchanged. From this it becomes clear that when using a particle model to simulate the meandering of a puff, as a surrogate for a frequently updated flow field, part of the spectrum is accounted for twice. This would cause the total dispersion to become overestimated more and more as the travel distance increases, leading to underestimated ground level concentrations far away from the source.

To separate the contribution of small eddies (contributing to an increase in puff size) for those of larger eddies (contributing to the meandering of the whole puff) the following procedure is introduced. From the actual puff sizes (i. e., the standard deviations) σ_x, σ_y, σ_z, a threshold frequency $n^*_{x,y,z} = \bar{u}(t) / (2\sigma_{x,y,z})$ is defined for each direction using Taylor's frozen turbulence hypothesis. The integral over the low frequency part of the turbulence spectrum is denoted as $\langle u_i^2 \rangle_{\text{eff}}$ $(i = u, v, w)$, where $\langle u_i^2 \rangle_{eff} = \int_{n_{\min}}^{n} S_i dn$. Then, the ratio $r_i = \langle u_i^2 \rangle_{\text{eff}} / \langle u_i^2 \rangle$ is determined (Fig. 2). The integration of the whole spectrum runs from $n_{\max} = \bar{u}/\eta$, where $\eta = (\upsilon^3/\varepsilon)^{1/4}$ is the Kolmogorov micro-scale, υ is the kinematic molecular viscosity and ε is the dissipation rate, to $n_{\min} = 1/T$, where T is the averaging time for the measurements of the turbulence statistics of the flow field.

In the present work velocity spectra models are taken from Højstrup (1981) for the unstable surface layer and Højstrup (1982) for the unstable planetary boundary layer. The model of Kaimal *et al.* (1972) is used for the neutrally stratified surface layer. For the stable surface layer, the model of Olesen *et al.* (1984) is adopted. For the upper part of the neutral and of the stable boundary layer, the same formulations as for the surface layer are used.

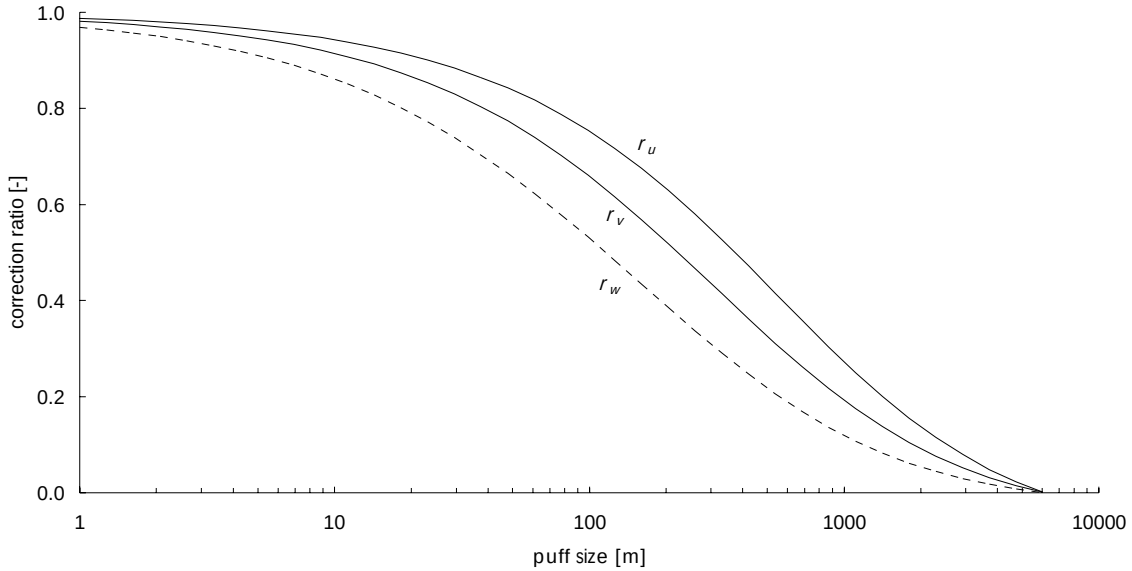

Figure 2 Plot of the correction ratios r_i *(i = u, v, w)* (*u*-component: solid line; *v*-component: dashed line; *w*-component: dotted line) as a function of puff size (conditions of forced convection; $u^* = 0.4\ \mathrm{ms}^{-1}$, $z/L = -2$, $z_i = 1000$ m, $\bar{u} = 3.4\,\mathrm{ms}^{-1}$, averaging time of flow field one hour).

3.3 REDUCTION OF THE TRAJECTORY VARIABILITY AS PUFF SIZES GROW

The combination of a puff model with a particle model representing the whole turbulence spectrum asks for the removal of the dispersing effect from the high-frequency part of the energy spectrum (i. e., the small turbulent eddies already covered by the puff model) from the particle trajectories. The procedure to remove this part of the turbulent fluctuations from the 'particle-part' of the PPM is straightforward: The time series of stochastic turbulent velocity components of each particle is smoothed. The trajectory of the centre of mass of a puff is then calculated based on these smoothed turbulent velocities. This leads to an increasingly smooth puff centre trajectory as the puff size grows.

The Kalman filter originates from the need to estimate the true value of an underlying stochastic process which can only be observed with an error, where it is assumed that the observational error is normally distributed with a standard deviation τ. Under such circumstances there is a need not to consider the measured time series of, for example, pressure, but to filter out the noise signal originating from the observational error, thus obtaining a smoothed time series as an improved, less fluctuating estimation of the quantity which originally had been measured. Often running mean values are used for such purposes, where the smoothed value is calculated as a weighted function of several values at both sides of the position for which a smoothed value has to be estimated. These running mean values

have two disadvantages with respect to the present need for smoothing the turbulent velocities calculated by a particle model: first, the future values of the turbulent velocity are not known at the moment where a smoothed value has to be estimated for use for the puff centre trajectory. This way, running mean estimations could only be based on past values of the turbulent velocities, leading to a biased estimation. Second, such a running mean makes it necessary to store an increasing number of 'past values' of the turbulent velocities of each particle, since the running mean is based on these past values.

The Kalman filter procedure, on the other hand, is computed recursively. This way, the filter estimation at the time step t is only based on the filter estimate at the time step $t-1$, the measured value at time step t and the parameters of the underlying stochastic process. Stochastic particle dispersion models generally are modelled as a so-called AR(1)-process, i. e. an auto-regressive process in which the position and velocity of a particle only depend on the velocity and position of the same particle one time-step ago.

If the underlying AR(1)-process is

$$X(t) = \alpha \cdot X(t-1) + E(t) \tag{3}$$

where X denotes the turbulent velocity vector (u', v', w'). The stochastic process from Eq. (3) has a part correlated with the turbulent velocities at the preceding time step and a uncorrelated stochastic distribution $E(t)$ which is normally distributed with zero mean and variance σ^2. The process given by Eq. (3) is our underlying, 'true' process. We assume it to be observed with a normally distributed observational error with variance τ^2. The Kalman filter estimate $\hat{X}$ for the next time step then is

$$\hat{X}_{t+1,t} = \alpha \cdot \hat{X}_{t,t} \tag{4}$$

where the filter probability density has a variance

$$R_{t+1,t} = \alpha^2 R_{t,t} + \sigma^2 \tag{5}$$

Here, the first subscript gives the time step for which the filter estimate is valid, and the second subscript indicates the time step of the last observation on which this filter estimate is based. Given the new observation at time step $t + 1$, $X(t + 1)$, the filter estimate is corrected to

$$\hat{X}_{t+1,t+1} = \hat{X}_{t+1,t} + \frac{R_{t+1,t}}{R_{t+1,t} + \tau^2}\left(X_{t+1} - \hat{X}_{t+1,t}\right) \tag{6}$$

with the new variance

$$R_{t+1,t+1} = \frac{R_{t+1,t} \cdot \tau^2}{R_{t+1,t} + \tau^2} \tag{7}$$

This recursive algorithm can be started as soon as initial values $\hat{X}_{0,0}$ and $R_{0,0}$ are chosen, the influence of which vanishes after just a few iterations.

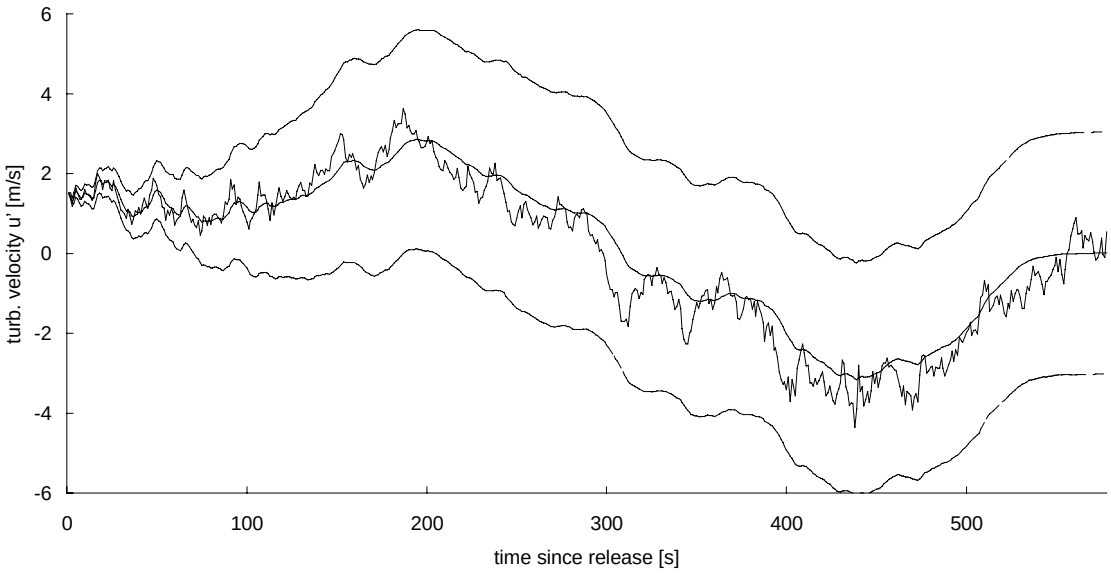

Figure 3 Smoothing of the turbulent velocity components calculated by the particle model (solid line) for use as puff centre velocities in the PPM (dashed line). The smoothing is increased as the correction ratios drop, i. e. the puff size grows. The dotted lines below and above of the smoothed turbulent velocity indicate the range $[u' - \tau, u' + \tau]$. Example for the *u*-component.

The concept used within the puff-particle approach is to consider the turbulent velocity components computed by the particle-part of the model to be 'observed values', where the 'observational error' is normally distributed with mean zero and standard deviation τ. By choosing τ proportional to the correction ratios r_i (and thus proportional to the growth of the size of the puff), increasingly smoothed time series of turbulent velocities are obtained. These smoothed velocity components are then used to calculate the trajectory of the puff's centre of mass. In the beginning, i. e. when the puff size is small and r_i approximately equals unity, τ is chosen to be zero. As puff sizes increase and the r_i decrease (Fig. 2), the high-frequency fluctuations of the turbulent velocity components are eliminated from the trajectory of the puff's centre (Fig. 3). This corresponds to the concept of relative diffusion where all fluctuations originating from turbulent eddies with sizes smaller than the size of the puff are

taken into account. As the puff size further increases, the r_i eventually drop to zero, and τ is chosen in such a way that the smoothed turbulent velocity time series remain constant.

Between the two limiting cases ($\tau_i = 0$ for $r_i = 1$ and τ_i large for $r_i = 0$),

$$\tau_i(r_i) = c\sigma \cdot \text{logit}\{d(0.5 - r_i)\} \tag{8}$$

is chosen in the PPM, where $\text{logit}(x) = \exp(x)/\{1 + \exp(x)\}$. In the present work, $c = 100$ and $d = 10$ are used. The ratios r_i are evaluated for each puff individually. As puff sizes grow, the values of the r_i decrease and eventually approach zero, leading to turbulent movements of the puff centres of very low frequency only. This allows the particle model within the PPM to be switched off as soon as r_i equals unity, and the puff centres are moved by the average flow field only. For far-field concentration predictions, this causes considerable computational savings.

Even when τ is large, the smoothed velocity fluctuation of a stochastic process will not give exactly zero. Therefore, to ensure that the smoothed turbulent velocities approach zero as $r_i \to 0$, the smoothed values are forced towards zero as soon as $r_i > 0.9$.

3.4 VALIDATION

For the prediction of concentrations averaged over approximately one hour, the puff-particle approach with smoothed puff centre trajectories should yield similar concentrations as a dispersion model based on absolute dispersion (e. g., a particle model). Therefore, the validation in this section aims at comparing the ground-level concentrations of four different models. The first model which is to be compared is a ‘pure’ particle model after Rotach *et al.* (1996) which fulfils the well-mixed criterion of Thomson (1987). The second and third model in this comparison are the PPM without and with additionally smoothed puff centre trajectories, respectively. The fourth model is a ‘pure’ puff model, in which the puffs are dispersed with relative dispersion. A second validation of the performance of the PPM with smoothed puff centre trajectories, against the data from three tracer experiments under different atmospheric conditions, can be found in de Haan and Rotach (1998).

The comparison of the predicted ground-level concentrations of these four models allows to validate the treatment of relative dispersion within the PPM. If the averaging time is one hour, the stochastic puff centre trajectories will account for almost the whole dispersing effect of plume meandering. Therefore the total dispersion will equal absolute dispersion, and this

leads to comparable ground-level concentrations predictions of both, the ‘pure’ particle model on the one side and the PPM with the smoothed puff centre trajectories on the other side. The PPM without the smoothing procedure, on the other hand, is expected to give too low concentration predictions, since a increasing part of the energy spectrum is taken into account twice, leading to an overestimation of the total dispersion. At the opposite, the ‘pure’ puff model does only cover part of the energy spectrum, leading to underestimated dispersion and hence to overpredicted ground-level concentrations.

To validate the predictions of the different models against measurements, the data from the Copenhagen tracer experiment are used. Data from 9 hours of measurements under conditions of forced convection are available. The non-buoyant tracer was released over a suburban surface at a height of 115 m. The receptors were placed on several arcs downwind of the source and hourly average measurements of the tracer concentrations were made at 2 m above ground. The mean wind speed was measured at different levels. The mixing height, the friction velocity and the Obukhov length were measured close to the release point, and measurements of the velocity statistics, $\langle u'^2 \rangle$ and $\langle w'^2 \rangle$, are available. More details about the experiment can be found in Gryning and Lyck (1984).

The simulation of the tracer experiment was performed by rebuilding the experimental set-up within the model and by predicting the concentrations at arcs of receptors at the same locations as in the tracer experiment. This allows the calculation of the cross-wind integrated concentration (CIC), the standard deviation on the arc in meters (SIGY) and of the maximum concentration occurring on an arc (ArcMax). Additionally, the ground-level concentrations in the plume centre line are predicted.

As an example, the resulting concentration profiles down-wind from the source for one of the hours of the tracer experiment are depicted in Fig. 4. The poor performance of the ‘pure’ puff model is completely due to the underestimated total dispersion, causing the maximum concentration to occur further down-wind and to remain on a high level as compared to the other three models as well as with the experimental data. The other three models all show very similar concentration patterns close to the source. This is due to the fact that in this early stage the relative dispersion of the puffs is only a minor contribution to the total dispersion, and also due to the fact that the ‘pure’ particle model is identical with the particle-part of the PPM used to calculate the stochastic puff centre trajectories. The removal of part of the

dispersing effect of these stochastic trajectories in the third model, the PPM with smoothed puff trajectories, leads to a larger predicted maximum concentration. It is similar to the maximum concentration as predicted by the 'pure' particle model. The PPM without smoothing procedure, on the other hand, predicts an about ten percent lower maximum concentration, due to the overestimation of total dispersion. Further down-wind, the concentration predictions of the particle model and of the smoothed PPM remain similar, whereas the PPM without smoothing simulates somewhat lower concentrations.

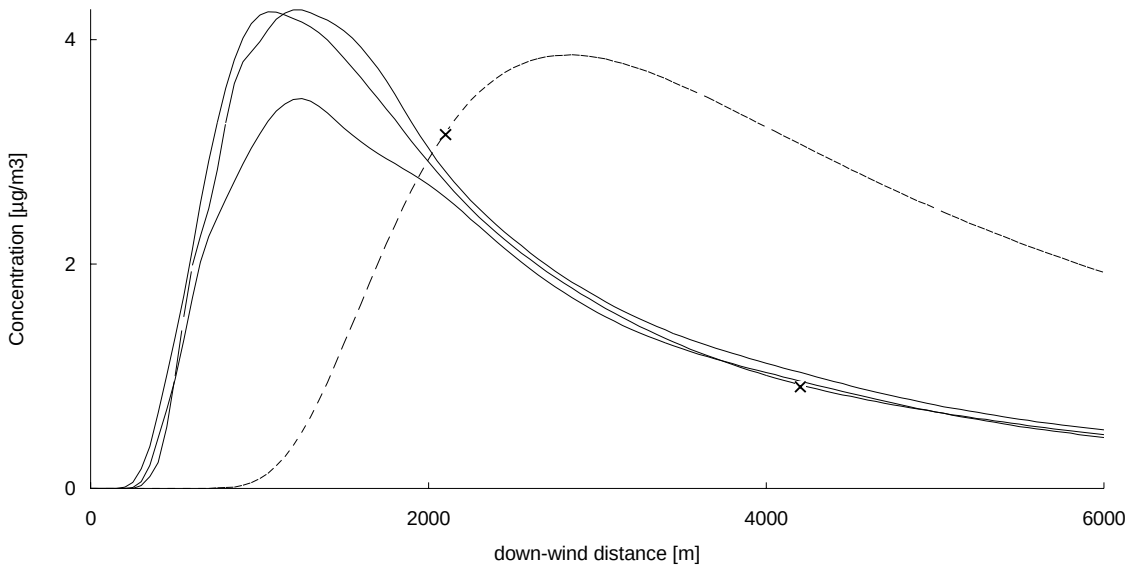

Figure 4 Example of the plume centre line concentration at 2 m above the ground for the particle model (dashed line), the puff-particle model without and with Kalman filter (lower and upper solid line, respectively) as well as for the puff model (right dashed line). Crosses depict the measurements (Copenhagen experiment from Sep. 26, 1978).

In Table 1 the following statistical measures are compared for the different simulations of the tracer experiments: the fractional bias $FB = \left(\overline{c}_{obs.} - \overline{c}_{pred.}\right) / \left\{0.5\left(\overline{c}_{obs.} + \overline{c}_{pred.}\right)\right\}$; the normalised mean square error $NMSE = \overline{\left(c_{obs.} - c_{pred.}\right)^2} / \left(\overline{c}_{obs.}\overline{c}_{pred.}\right)$; the correlation coefficient $COR = \overline{\left(c_{obs.} - \overline{c}_{obs.}\right)\left(c_{pred.} - \overline{c}_{pred.}\right)} / \left(\sigma_{obs.}\sigma_{pred.}\right)$; the percentage of simulations within a factor of two of the measurement, FAC2. $c_{obs.}$ is the observed, $c_{pred.}$ the simulated concentration.

As can be seen, the overall performance of the 'pure' particle model is better than the measures of the other three models. However, the smoothed PPM shows almost identical FB and NMSE. Additionally, the measures of the smoothed PPM are clearly improved as compared with the PPM without smoothing procedure. The puff model, finally, shows a

rather poor performance. Even the particle model, however, shows a general underprediction (a positive fractional bias). In Rotach and de Haan (1997) it is shown that taking into account the rough character of the suburban area where the tracer experiment took place leads to the vanishing of this systematic underprediction.

	ArcMax				**CIC**				**SIGY**			
	NMSE	COR	FAC2	FB	NMSE	COR	FAC2	FB	NMSE	COR	FAC2	FB
Observations	0.000	1.000	100%	0.000	0.000	1.000	100%	0.000	0.000	1.000	100%	0.000
Particle model	0.137	0.871	91%	0.029	0.189	0.700	87%	0.197	0.088	0.836	100%	0.006
PPM (Kalman f.)	0.186	0.858	87%	0.050	0.179	0.644	83%	0.123	0.091	0.879	100%	–0.08
PPM (no filter)	0.218	0.852	78%	0.047	0.180	0.654	83%	0.134	0.103	0.901	95%	–0.10
Puff model	1.687	0.255	30%	–0.47	1.057	0.029	39%	–0.12	0.388	0.947	60%	0.569

Table 1 Comparison of statistical measures (see text) for the different simulations.

It must be noted that the data from the Copenhagen experiment do not allow to validate one of the most important effects of the smoothing procedure within the PPM. The predicted maximum down-wind concentration closely resembles the predicted values from the ‘pure’ particle model, whereas the PPM without correction predicts lower maximum concentrations. Unfortunately, all arcs in the Copenhagen experiment were placed at relatively large distances from the source, so that the maximum concentration was not observed.

3.5 SUMMARY AND CONCLUSIONS

The puff-particle approach is suited to simulate the effect of plume meandering in absence of frequently updated meteorological and flow field information. However, the combination of a puff and a particle model leads to a double representation of the dispersing effect of part of the turbulence spectrum, dependent on the size of the individual puffs. In the present contribution, a method is proposed which corrects this overestimation of dispersion by filtering out the high-frequency part of the changes of turbulent velocity within the particle model. This filtering is realised using a Kalman filter. The extent of the smoothing depends on the proportion of the velocity spectrum of which the dispersing effect is taken into account by the puff part of the model. This way, the smoothing increases as puffs sizes grow. The validation against data from a tracer experiment and against the results of a pure particle model show than the corrected PPM (i. e., with smoothed puff centre trajectories) does not

over- nor underpredict the total dispersion and shows approximately the same results as does the particle model.

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