

Dispersion modelling – particles, puffs, kernels and box averaging

by
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Note this is an early draft concentrating of the puff aspect (i.e. the aspect that is being developed for the first time in NAME-PPM). The box averaging and kernel approaches are well tried approaches (box averaging in the current NAME model), but are not yet discussed here. In due course this paper will be extended to describe these approaches and how they are applied in NAME-PPM.

1 Introduction

The dispersion in NAME-PPM uses a stochastic Lagrangian particle model. However in such models the dispersing material is located at a finite number of discrete points and some averaging is required to obtain a smooth concentration field. This paper describes the approach used.

The approach is quite complex with a number of options which need to be selected appropriately for the problem being considered. The three main possibilities are the use of (i) box averaging, (ii) kernel methods or (iii) puffs. Roughly speaking these are in order of increasing sophistication, but also increasing complexity. The main problem with box averaging is that the averaging widens the plume and reduces the magnitude of concentrations, and that, when the plume is narrow compared to the boxes, the effect of this can be large. The use of kernel methods still widens the plume and reduces the concentrations, but the scale of the smoothing used can be linked to the plume size, thereby preventing large errors from occurring. The puff approach is designed to avoid the systematic widening of the plume and reduction in concentrations. In the puff scheme the smoothing is introduced by replacing each particle by a puff centred on the particle location, and the tendency of this to widen the plume and reduce concentrations is compensated for by reducing the spread of the particles. The box averaging and kernel approaches are well established techniques [ref] whereas the puff scheme is essentially a new approach.

With the exception of some comments below on the approach of Rotach and de Haan, we are concerned throughout this paper with mean concentrations only, and for simplicity we drop the ‘mean’ and refer simply to ‘concentrations’.

2 One-dimensional case, instantaneous sources

To simplify matters we start by considering dispersion in one direction only, taken to be the z direction, and restrict consideration to instantaneous sources. We note that the source is not necessarily a point source and distributed sources are treated as follows. For the box averaging and kernel methods the initial particle locations are distributed appropriately across the source (e.g. randomly or more systematically spaced), while for the puff method we assume the source is a rectangular box or a Gaussian shape (with reflections as appropriate) and start with a single puff located at the centre of the source (more complicated shapes could be treated as multiple sources).

2.1 Box averaging

2.2 Kernel methods

2.3 Puffs

A problem with the two previous approach is that the concentration field is smoothed leading to underprediction of concentration magnitudes and overprediction of the area affected. To avoid this bias, we replace the particles by concentration distributions of finite size centred on the particles (i.e. puffs) as in the kernel method, but we reduce the dispersion of the particles (i.e. the puff centres) to compensate, as in the puff scheme of Rotach and de Haan 1999. However, unlike Rotach and de Haan who base their puff sizes on the relative dispersion of instantaneous releases, we choose the puff sizes with the sole purpose of obtaining a smooth concentration field. Our puffs play not a physical role but a mathematical or numerical role in helping to obtain a good approximation to the true solution of the stochastic Lagrangian particle model (the true solution being only obtainable in general in the limit of a simulation with infinitely many particles). This means we cannot use the puffs to estimate concentration fluctuations as Rotach and de Haan do, but equally we avoid the problem of representing the concentration distribution in areas of high concentration fluctuations where the Rotach and de Haan approach requires large numbers of puffs. We also split/recombine puffs as required to ensure enough puffs to adequately represent the concentration field as in SCIPUFF (although the approach does not follow the SCIPUFF approach in detail – see below). Our scheme is designed so that for homogeneous Gaussian turbulence it is unbiased and indeed exact in the limit of a large number of particles (relative to the underlying particle model). For inhomogeneous or non-Gaussian turbulence there will be systematic differences, but the approach is designed to keep these acceptably small.

To explain the scheme we need some definitions:

σ_p : The size of each puff (before any reflections are applied) is indicated by σ_p .

N : N indicates the number of times the puff has been split.

G : G is a flag indicating whether the puff is Gaussian (it is convenient to allow non-Gaussian top-hat shaped puffs near sources with top-hat shaped distributions). $G = \top$ indicates that it is Gaussian while $G = \perp$ indicates that it is top-hat shaped. Note in this context the shape of the puff refers to the shape before any reflections are applied.

R : R is a flag indicating whether the puff's displacement can have a random component. $R = \top$ indicates that it can have a random component, while $R = \perp$ indicates that it can't. Once R is set to \top it will usually quickly acquire a random component. However it may not have a random component at the point that R is set to \top , so R is best thought of as indicating that a puff has 'randomness enabled'. Randomness cannot be enabled unless the puff is Gaussian.

σ_h : For each puff we define σ_h as the spread which the entire release would have if the turbulence had been homogeneous but varying in time in the same way that the turbulence properties at the particle location actually vary. We call this the quasi-homogeneous spread (hence the notation).

σ_a : We define σ_a as the total spread of the entire cloud of puffs.

σ_h and σ_a will often differ in size. For example in a boundary layer σ_a will be constrained by the boundary layer depth, unlike σ_h which will grow more like the plume in a Gaussian plume model before reflections are applied at the ground and boundary layer top. Also, if we consider a plume released above and fumigating into a growing boundary layer, then σ_h will be quite small for a puff that hasn't yet entered the boundary layer while σ_a could be much larger and of order the boundary layer depth.

Δ : We denote the spatial resolution required for the concentration field (effectively the desired upper limit for puff size) by Δ . Δ could in general vary in space and time. There are a number of possible choices for Δ . The most basic is the choice $\Delta = \infty$. With this choice puffs will never be split and we have in effect a Gaussian puff model. This choice would be possible for passive releases within the boundary layer (if reflections at the ground *and* boundary layer top are applied) but is far from ideal (i) for buoyant sources which may only partially penetrate the boundary layer top, or (ii) if the geometry of the domain is not at straightforward (e.g. building or terrain effects or earth curvature at very long range).

A more sophisticated choice is to choose Δ to reflect the scale of aspects of the geometry (e.g. building or hill size, or curvature of the earth) or the scale of any inhomogeneity in the flow which we want to resolve (e.g. boundary layer depth, horizontal scale of variation of the meteorology). This option would give a model which has a similar level of treatment of the flow and dispersion to SCIPUFF, but with a stochastic treatment of the puffs which arise from the splitting process rather than the deterministic treatment used in SCIPUFF. Isolated inhomogeneities have little effect once the dispersing cloud is much bigger than the inhomogeneity, e.g. the effect of a building is not important if the cloud is much bigger than the building and the variation of turbulence properties with height very near the ground is unimportant if the cloud is mixed throughout a substantial depth of the atmosphere. We can avoid generating unnecessarily small puffs in such cases by making Δ also dependent on the cloud size σ_a .

Finally one could also restrict Δ by some fraction of σ_h , thus restricting Δ even when the turbulence is homogeneous or the dispersing cloud is much smaller than the scale of the inhomogeneity. This would enable effects due to the non-Gaussianity of the turbulence to be treated such as those due to skewness of the velocity distribution in convective boundary layers.

z_s : The source centre (before any reflections are applied) is indicated by z_s .

σ_s : The source size (before any reflections are applied) is indicated by σ_s .

Note that σ_h , σ_a and σ_p include any contribution to the spread arising from the source size.

To ensure that the concentration field is adequately resolved we aim to adjust σ_p so that $\sigma_p \leq \Delta$. We also need to ensure that there are enough puffs to describe the concentration field – equivalently for a given number of puffs we need to ensure that the puffs are not too small. To achieve this we aim to ensure that $\sigma_p \geq (A_1/2^{N/2}) \min(\sigma_h, \sigma_a)$ whenever $R = \top$. The parameter A_1 characterizes how much statistical noise is acceptable, and is the first of several tunable parameters which can be adjusted in our approach. Values of these parameters are discussed below. As discussed above, σ_h and σ_a could be very different in size and so it is necessary to use both quantities in limiting σ_p to avoid the need for an unnecessarily large number of puffs.

To achieve this we adopt an approach along the lines of the following (note that some of the steps will have no effect the first time they are carried out).

1. **Initialize puffs:** Initialize a single puff at the source.
2. **Compute σ_a**
3. **Recombine puffs:** If $\sigma_p \geq (A_2 A_1 / 2^{(N-1)/2}) \min(\sigma_h, \sigma_a)$ with $R = \top$ for a pair of puffs with a common parent, then one of the puffs is chosen at random and this puff is deleted with the contaminant being moved to the other in puff in the pair. Here A_2 is a number slightly larger than unity to prevent puffs which have just been split immediately recombining. Note this allows recombining of puffs only in rather restricted circumstances – in particular both puffs must have a common parent. This might seem a problem which might lead to the existence of too many puffs. However it should be noted that the splitting criteria is not expected to produce so many puffs as in a model such as SCIPUFF. In SCIPUFF, puffs always grow in size (puff growth is the only dispersion mechanism in SCIPUFF) and then split when they become too big, whereas, in the current approach, puffs split only when there are not enough puffs to represent the concentration field.
4. **Approximate by Gaussian:** If $G = \perp$ and σ_p is greater than A_3 times the spread of the puff resulting from the source, then we can ignore the details of the source shape and set the puff shape to a Gaussian with $G = \top$. A_3 is a tunable parameter which controls the error allowed in this step.
5. **Reduce σ_p :** If $R = \top$, $\sigma_p > \Delta$ and $\sigma_p > (A_1/2^{N/2}) \min(\sigma_h, \sigma_a)$, then reduce σ_p until either $\sigma_p = \Delta$ or $\sigma_p = (A_1/2^{N/2}) \min(\sigma_h, \sigma_a)$, with the reduction in σ_p replaced by a random displacement of the puff centre.

6. **Split puffs:** If $\sigma_p > \Delta$ or $\sigma_p < (A_1/2^{N/2}) \min(\sigma_h, \sigma_a)$ with $R = \top$, then split the puff into two. Generally the two new puffs will be identical to the old puff but with half the amount of contaminant and with R set to \top (if it wasn't already) so that the new puffs can subsequently move in random (and different) ways. However, if we have a top-hat shaped puff with $G = \perp$ arising from a top-hat shaped source (which implies the puff must also be deterministic with $R = \perp$), it is convenient to, in effect, split the source into two sources of half the size of the original source and to keep the new puffs resulting from the two parts of the source deterministic. By not introducing randomness before it is needed, we avoid the need for extra puffs to reduce the statistical noise. The split puffs are treated as new puffs and need to be treated in the same way as the others starting from step 4.
7. **Time-step puffs:** Any puff reaching this stage will have $\sigma_p \leq \Delta$ and either $R = \perp$ or $\sigma_p \geq (A_1/2^{N/2}) \min(\sigma_h, \sigma_a)$. We then evolve the puff over one time step Δt , with the aim of putting as much of the dispersion as possible into puff growth rather than random displacement of the puff centre while not causing σ_p to exceed Δ . Note this aim is not always exactly achievable because Δ may itself change as the puff evolves and, if the underlying stochastic Lagrangian model has time correlated velocities, it is not possible to instantaneously change the fraction of the spread going into puff spread and random displacements (see details below).

Steps 2 to 7 are repeated as required. Note that if σ_p is too large we allow it to decrease instantaneously with the spread being replaced by random displacement of the puff centre (step 5). However if σ_p is smaller than desired we allow it to grow only gradually over time (step 7). This is because it is not possible to convert spread represented as random displacements of puffs to spread represented by σ_p – one cannot reduce the spread due to random displacements because one doesn't know the point about which this spread occurs (indeed such a concept doesn't really make sense at all in an inhomogeneous flow).

The above provides an overview of the approach but there are a number of details left to clarify. However before doing this it is useful to review the form of the evolution equations in the underlying stochastic Lagrangian model. These equations take one of two forms depending on whether the model is Markovian in terms of the particle position z or in terms of the particle position and velocity (z, w) . For a z -model we have

$$dz = \langle w \rangle(z, t) + (2K(z, t))^{1/2} d\xi$$

while for a (z, w) model we have

$$dw' = a(z, w', t) dt + \left(\frac{2\langle w'^2 \rangle(z, t)}{\tau(z, t)} \right)^{1/2} d\xi$$

$$dz = (\langle w \rangle(z, t) + w') dt.$$

Here $\langle w \rangle$ is the fixed point mean velocity, $\langle w'^2 \rangle$ is the fixed point velocity variance, K is the eddy-diffusivity, τ is the Lagrangian time scale used in the stochastic model, a is a function which is determined on the basis of the 'well-mixed' condition (see e.g. Thomson 1987), w' is the departure of the particle velocity from the mean, and $d\xi$ is the increment of a Wiener process. Note that we have allowed $\langle w \rangle$ to depend on z . This is of course possible only if the air density varies. In the homogeneous Gaussian turbulence

approximation discussed above where the flow properties are assumed to vary in time in the same way as they vary along the particle trajectory, these models simplify to

$$dz = \langle w \rangle(t) dt + (2K(t))^{1/2} d\xi$$

and

$$dw' = -\frac{w'}{\tau(t)} dt + \left(\frac{2\langle w'^2 \rangle(t)}{\tau(t)} \right)^{1/2} d\xi$$

$$dz = (\langle w \rangle(t) + w') dt.$$

These equations yield equations for the evolution of various moments of the particle positions and/or velocities. For the z -model we obtain

$$\frac{d\overline{z'^2}}{dt} = 2K$$

and for the (z, w) -model we have

$$\frac{d\overline{z'^2}}{dt} = 2\overline{z'w'}$$

$$\frac{d\overline{z'w'}}{dt} = \overline{w'^2} - \frac{\overline{z'w'}}{\tau}$$

$$\frac{d\overline{w'^2}}{dt} = -\frac{2\overline{w'^2}}{\tau} + \frac{2\langle w'^2 \rangle}{\tau}.$$

Here z' and w' indicate departures from the mean over the particles. In deriving the last equation, note that $(d\xi)^2$ is of order dt and so can't be neglected in comparison to dt . As a result, formal application of the product rule for differentiation fails, and Itô's formula should be used instead. [add time dep terms and dW/dz terms]

It is now possible to describe the complete scheme based on the above ideas. First we list the variables characterizing the puff's state (from the perspective of describing the motion):

- z_p : centre of puff
- w'_p : turbulent velocity of the centre of the puff
- $\overline{z'^2}_h (\equiv \sigma_h^2)$, $\overline{z'w'}_h$, $\overline{w'^2}_h$: moments of the spread of the contaminant in the entire cloud about its centre in the quasi-homogeneous approximation introduced above (w' here is the velocity relative to that of the cloud centre)
- $\overline{z'^2}_p (\equiv \sigma_p^2)$, $\overline{z'w'}_p$, $\overline{w'^2}_p$: moments of the spread of the contaminant in a single puff about its centre (w' here is the velocity relative to that of the puff centre)
- N, G, R : as defined above
- σ_T : puff spread due to top-hat source shape
- Information on which puffs the puff is related to as a result of puff splitting.

We will now explain in detail how each of the steps 1 to 7 described above are implemented.

Step 1, Initialize puffs: Initialize a single puff at the source as follows:

$$\begin{aligned}
z_p &= z_s, & w'_p &= 0 \\
\overline{z'^2}_h &= \sigma_s^2, & \overline{z'w'}_h &= \overline{w'^2}_h = 0 \\
\overline{z'^2}_p &= \sigma_s^2, & \overline{z'w'}_p &= \overline{w'^2}_p = 0 \\
N &= 0, & R &= \perp \\
G &= \begin{cases} \perp & \text{if top-hat shaped source} \\ \top & \text{otherwise} \end{cases} \\
\sigma_T &= \begin{cases} \sigma_s & \text{if top-hat shaped source} \\ 0 & \text{otherwise} \end{cases}
\end{aligned}$$

Step 2, Compute σ_a : Compute σ_a from

$$\sigma_a^2 = \sum \frac{\overline{z'^2}_p + z_p^2}{2^{N/2}} - \left(\sum \frac{z_p}{2^{N/2}} \right)^2.$$

Step 3, Recombine puffs: If $\sigma_p \geq (A_2 A_1 / 2^{(N-1)/2}) \min(\sigma_h, \sigma_a)$ with $R = \top$ for a pair of puffs with a common parent, then one of the puffs is chosen at random and this puff is deleted with the contaminant being moved to the other in puff in the pair. Note step 3 is applied to all of the puffs before proceeding. However the subsequent steps 4 to 7 are all applied to one puff before being repeated for each of the others.

Step 4, Approximate by Gaussian: If $G = \perp$ and $\sigma_p > A_3 \sigma_T$, then set $G = \top$ and $\sigma_T = 0$.

Step 5, Reduce σ_p : If $R = \top$, $\sigma_p > \Delta$ and $\sigma_p > (A_1 / 2^{N/2}) \min(\sigma_h, \sigma_a)$, then proceed as follows:

Choose λ so that $\lambda \sigma_p = \max[\Delta, (A_1 / 2^{N/2}) \min(\sigma_h, \sigma_a)]$

Add random numbers to z_p and w'_p with variances $(1 - \lambda^2) \overline{z'^2}_p$ and $(1 - \lambda^2) \overline{w'^2}_p$ and covariance $(1 - \lambda^2) \overline{z'w'}_p$

Multiply $\overline{z'^2}_p$, $\overline{z'w'}_p$ and $\overline{w'^2}_p$ by λ^2

Note that if this step is implemented exactly, it may result in σ_p being exactly equal to Δ . If this is the case, it is important that rounding errors in the numerical implementation preserve this behaviour, in order to prevent unnecessary puff splitting in step 6.

Step 6, Split puffs: If $\sigma_p > \Delta$ or $\sigma_p < (A_1 / 2^{N/2}) \min(\sigma_h, \sigma_a)$ with $R = \top$, then split the puff into two. If $G = \top$ then we do this as follows:

Replace puff with two new puffs which are identical to the old puff but with half the amount of contaminant and with R set to \top and N replaced by $N + 1$.

If however $G = \perp$ then the puff is replaced by two new puffs with the following characteristics (where ‘=’ here is interpreted as a Fortran-like assignment):

$$\begin{aligned} z_p &= z_p \pm (\sqrt{12}/4)\sigma_T, \quad w'_p = 0 \\ \overline{z'^2}_h, \overline{z'w'}_h \text{ and } \overline{w'^2}_h &\text{ unchanged} \\ \overline{z'^2}_p &= \overline{z'^2}_p - (3/4)\sigma_T^2, \quad \overline{z'w'}_p \text{ and } \overline{w'^2}_p \text{ unchanged} \\ N &= N + 1, \quad R = \perp \quad G = \perp \\ \sigma_T &= \sigma_T/2. \end{aligned}$$

Note $\sqrt{12}\sigma_T$ is the width of a top-hat source with rms spread σ_T . The new puffs are treated as separate puffs and need to be stepped forward in the same way as the others, starting from step 4. The original ‘parent’ puff is abandoned and not processed any further.

Step 7, Time-step puffs: Any puff reaching this stage will have $\sigma_p \leq \Delta$ and either $R = \perp$ or $\sigma_p \geq (A_1/2^{N/2}) \min(\sigma_h, \sigma_a)$. We step the puff forward in time using the following algorithm where β is the fraction of the randomness used in the stochastic Lagrangian model. When the underlying Lagrangian model is Markovian in z we use

$$dz_p = \langle w \rangle(z, t) + (2\beta K(z, t))^{1/2} d\xi$$

$$\frac{d\overline{z'^2}_h}{dt} = 2K$$

$$\frac{d\overline{z'^2}_p}{dt} = 2(1 - \beta)K,$$

while when the model is Markovian in (z, w) we use

$$dw'_p = a(z_p, w'_p, t) dt + \left(\beta \frac{2\langle w'^2 \rangle(z_p, t)}{\tau(z_p, t)} \right)^{1/2} d\xi$$

$$dz_p = (\langle w \rangle(z_p, t) + w'_p) dt$$

$$\begin{aligned} \frac{d\overline{z'^2}_h}{dt} &= 2\overline{z'w'}_h, \quad \frac{d\overline{z'w'}_h}{dt} = \overline{w'^2}_h - \frac{\overline{z'w'}_h}{\tau}, \quad \frac{d\overline{w'^2}_h}{dt} = -\frac{2\overline{w'^2}_h}{\tau} + \frac{2\langle w'^2 \rangle}{\tau} \\ \frac{d\overline{z'^2}_p}{dt} &= 2\overline{z'w'}_p, \quad \frac{d\overline{z'w'}_p}{dt} = \overline{w'^2}_p - \frac{\overline{z'w'}_p}{\tau}, \quad \frac{d\overline{w'^2}_p}{dt} = -\frac{2\overline{w'^2}_p}{\tau} + \frac{2(1 - \beta)\langle w'^2 \rangle}{\tau}. \end{aligned}$$

The choice of β now needs to be discussed. There are a number of possibilities depending on R , on whether we have a z or (z, w) random walk model, and on whether Δ is determined by some limiting external scale (e.g. boundary layer depth) or is limited by some fraction, f , of σ_h . For $R = \perp$ we choose $\beta = 0$. For $R = \top$ with a z model we choose β as small as possible subject to $\overline{z'^2}_p$ at the end of the time-step being no bigger than an estimate of Δ at the end of the time-step. We estimate the latter quantity as

being the same as Δ at the start of the step if Δ is limited by an external scale and as $f\sigma_h|_{\text{end of timestep}}$ if Δ is limited by $f\sigma_h$. Finally when $R = \top$ with a (z, w) model we choose

$$\beta = \begin{cases} 0 & \text{if } \sigma_p \leq A_4\Delta \\ 1 & \text{if } \sigma_p > A_4\Delta \text{ and } \Delta \text{ is limited by an external scale} \\ 1 - f^2 & \text{if } \sigma_p > A_4\Delta \text{ and } \Delta \text{ is limited by } f\sigma_h. \end{cases}$$

Here A_4 is a tunable constant slightly less than unity. The idea is to keep σ_p in the range $[A_4\Delta, \Delta]$.

Conceptually steps 4 to 7 are repeated for each of the puffs and then the whole of steps 2 to 7 are repeated for subsequent time steps. However in practice there are two reasons why this prescription is not followed exactly. The first reason is that the time step used may depend on the position of the puff, and so different puffs may need to repeat certain steps a different number of times. The second reason is that obtaining the met data needed in the neighbourhood of a puff can be a computationally expensive step and the data volume may be too large for it to be desirable to store the data separately for each puff; it therefore makes sense to carry out several steps with a particular puff while the met data is at hand. As a result steps 2 and 3 are not carried out in every time step and steps 4 to 7 are repeated several times for one puff before proceeding to the next puff. When steps 2 and 3 are performed it is essential that the puffs are all synchronized in time. In repeating steps 4 to 7 for one puff, the fact that step 3 has not been invoked does not matter (at worst it can mean that more puffs are being tracked than is necessary) but the absence of step 2 is a potential problem. We get round this by extrapolating σ_a in time from the last two calculated values, and, if only one value has so far been calculated, we approximate σ_a by σ_h .

The remaining issue to discuss is the issue of the concentration distribution associated with a puff. We first consider the concentration distribution in the absence of boundaries. For $G = \top$, the distribution is Gaussian, whereas for $G = \perp$, the distribution is given by convoluting a Gaussian distribution (representing the spread of material emitted from a single point) with a top hat distribution (representing the source) to give

$$\frac{Q}{2\sqrt{12}\sigma_T} \left(\operatorname{erf} \left(\frac{z_p - z + \sqrt{12}\sigma_T/2}{(\sigma_p^2 - \sigma_T^2)^{1/2}} \right) - \operatorname{erf} \left(\frac{z_p - z - \sqrt{12}\sigma_T/2}{(\sigma_p^2 - \sigma_T^2)^{1/2}} \right) \right)$$

where Q is the total mass released. In the one-dimensional situation considered here, boundary geometry is simple, and boundaries are represented simply by reflecting the concentration distribution at the boundaries. Of course when reflections occur, step 2 above needs amending to account for the actual spread of a puff (after reflection) instead of the nominal spread. Note that if the source distribution is wide or close to a boundary, the effective source distribution involves reflection terms as well. For efficiency reasons it is best if every puff does not contribute to the concentration at all output points, and so we truncate the distribution for $|z - z_p| > A_5\sigma_p$.

3 Multi-dimensional case, instantaneous sources

The box averaging and kernel approaches trivial to extend. For the puff approach, the extension to two-dimensional puffs in the horizontal is also a trivial extension. A full

3-d puff model is more complex, especially in connection with reflections (see SCIPUFF solution) and puffs being stretched out by wind shear. However it is possible we may not develop a full 3-d scheme and instead use puffs which have a finite extent in either the vertical or the horizontal (but not both) so that the puffs look more like particles in the other direction. This would give us most of the advantages of a puff approach, without all the complication of the full 3-d scheme (this is analogous to the approach adopted by Hurley, 1994). In any case, even if we do develop a full 3-d scheme, we will include an option to treat the horizontal and vertical directions separately. We postpone a final decision on this till we can try out the options with real met fields.

4 Continuous sources

It is useful to consider the cases of fixed and changing meteorology separately. This is because the fixed met case is much simpler and is likely to be one of the main ways in which the model is used for short range environmental impact assessments. For fixed met, puffs and particles will be released at one time only. The effect of continuous or finite duration releases can then be treated by integration over measurements times (using the stationarity of the flow). For changing met this is not possible. Instead releases (for the puff approach) will be made at intervals and interpolations made between release times or averages made over long enough periods to avoid discrete release errors.

5 Choice of A_1 , A_2 , A_3 , A_4 , A_5 and Δ

Tests in simple situations (horizontally homogeneous boundary layers) show good results for $A_1 = 10$, $A_2 = 1.2$, $A_3 = 1$, $A_4 = 0.8$ and $A_5 = 4$. Choosing Δ to be one-fifth of the boundary layer depth seems adequate in many cases, although for sources in a low turbulence region above the boundary layer (with fumigation of the material into the boundary layer) it is also useful to limit Δ by $A_6\sigma_p$, with $A_6 = 0.5$ providing good results. $A_6 = 0.5$ implies a quarter of the variance of the cloud spread is carried by the finite size of the puffs, with the rest being represented by the puff displacements. For real meteorological fields we will also need to limit Δ by the scale of the horizontal inhomogeneity. The best values for all these quantities (which represent the trade off between accuracy and computational cost) may well need revising however in the light of experience with the full NAME-PPM model applied to real flow fields.

6 Complications

There are some further complications to consider, namely the interaction of the puff scheme with plume rise, fall speed, meandering, other extra velocity components (e.g. round buildings?), deep convection, discontinuities (e.g. at the boundary layer top),

complicated reflection geometries (e.g. round buildings) etc. These interactions with other aspects of NAME-PPM will need resolving as the other aspects are developed.

References

de Haan P. and Rotach M.W., 1998a, 'The treatment of relative dispersion within a combined puff-particle model', *Air Pollution Modeling and Its Application XII*, Plenum Press.

de Haan P. and Rotach M.W., 1998b, 'A novel approach to atmospheric dispersion modelling: the puff-particle model', *Q. J. R. Meteorol. Soc.*, **124**, 2771-2792.

Hurley P., 1994, 'PARTPUFF – a Lagrangian particle-puff approach for plume dispersion modeling applications', *J. Appl. Met.*, **33**, 285-294.