A NEW PUFF MODELLING TECHNIQUE FOR SHORT RANGE DISPERSION APPLICATIONS

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INTRODUCTION

Lagrangian particle models have proved very successful as an approach to treating a wide variety of dispersion problems. However they suffer from a problem of statistical noise. This arises from the way the concentrations are calculated by counting particles in boxes. This problem can in principle be overcome by following a very large number of particles, but this makes the models very expensive to run as the noise decreases only slowly, like the inverse of the square root of the number of particles.

Various approaches have been proposed to overcome this problem, the most common being the use of kernel methods (*de Haan, P.,* 1999) or hybrid models involving aspects of particle and puff approaches (e.g. *de Haan, P. and M. W. Rotach*, 1998; *Hurley, P.*, 1994). Here we present a new approach of the hybrid type which has the aim of reproducing the results of a Lagrangian particle model with reasonable accuracy, but with reduced noise and computational cost. The approach has similarities with that of de Haan and Rotach in that it uses multiple puffs, with some of the dispersion being represented by the growth of the puffs and some by random motion of the puffs as in a stochastic particle model. However, because our aim here does not include predicting statistics of the turbulent concentration fluctuations, the partitioning between these two ways of representing the dispersion is not done physically with the puff growth representing the "relative dispersion" and the random motion of the puffs representing the "meandering". Instead the partitioning is tuneable. At one extreme we have a model with a very large number of very small puffs which offers the accuracy of a pure particle model, while at the other extreme we have a few large puffs which gives a faster model with accuracy comparable to an ensemble mean puff or plume model. In this way the model is tuneable to give the desired balance between speed and accuracy. Note that, because the random part of the puff motion is reduced to compensate at least approximately for the puff growth, the approach avoids systematically overestimating the dispersion as occurs in kernel approaches.

THE PUFF MODEL

In the short range applications considered here, where the flow can be regarded as approximately horizontally homogeneous, the horizontal dispersion can be accurately represented by treating all of the horizontal growth through increases in puff size (*Hurley, P.*, 1994). We follow this approach and so only need to discuss the vertical dispersion in detail.

We assume that the underlying Lagrangian particle model which we wish to approximate with our puff model takes the form

$$dw = a(z, w, t)\,dt + (2\sigma_w^2 / \tau)^{1/2}\,d\xi\,, \qquad dz = w\,dt \qquad (1)$$

where z and w are the particle height and vertical velocity, σ_w^2 and τ are the velocity variance and time scale (at height z), and $d\xi / dt$ is white noise (see e.g. *Thomson, D. J.*, 1987, *Rodean, H. C.*, 1996). We note however that a similar approach is possible if the underlying model is diffusive with no velocity memory. We now write $z = z_0 + z'$, $w = w_0 + w'$ for the particles within a puff where z_0, w_0 refers to the puff centre. Conceptually we envisage that a certain fraction, β, of the white noise term in (1) (and of the initial velocity variance when the particle

is released) is used to drive the puff centre with the rest used to drive the expansion of the puff. This leads to

$$dw_0 = \langle a(z_0 + z', w_0 + w', t)\rangle\, dt + (2\beta\sigma_w^2/\tau)^{1/2}\, d\xi \qquad (2)$$

$$dw' = [a(z_0 + z', w_0 + w', t) - \langle a(z_0 + z', w_0 + w', t)\rangle]\, dt + (2(1-\beta)\sigma_w^2/\tau)^{1/2}\, d\xi' \qquad (3)$$

with $dz_0 = w_0\, dt$ and $dz' = w'\, dt$, where $\langle\rangle$ indicates an average over the particles in the puff. To use these equations we need to approximate $\langle a(z_0 + z', w_0 + w', t)\rangle$ in (2) and $a(z_0 + z', w_0 + w', t) - \langle a(z_0 + z', w_0 + w', t)\rangle$ in (3). The first of these we approximate by $a(z_0, w_0, t; \beta)$, where β indicates the term is evaluated with the velocity variance reduced by a factor β, plus an error term. In calculating the error term, we approximate a by its usual form in Gaussian turbulence, namely

$$a(z, w, t) = -\frac{w}{\tau} + \frac{w^2 + \sigma_w^2}{2\,\sigma_w^2}\frac{d\sigma_w^2}{dz},$$

and average over z', w' (approximating e.g. $1/\tau(z_0+z')$ by $1/\tau(z_0) - (z'/\tau^2)d\tau/dz$ and neglecting terms involving two derivatives in z) to get

$$\langle a(z_0 + z', w_0 + w', t)\rangle - a(z_0, w_0, t; \beta) = \frac{\langle w'^2\rangle + (1-\beta)\sigma_w^2}{2\,\sigma_w^2}\frac{d\sigma_w^2}{dz} + \frac{\langle w'\, z'\rangle}{\tau^2}\frac{d\tau}{dz}. \qquad (4)$$

For the second quantity to be approximated, we take the homogeneous (Gaussian) turbulence form of a (but with the turbulence statistics having the same time dependence as seen by the puff), leading to

$$a(z_0 + z', w_0 + w', t) - \langle a(z_0 + z', w_0 + w', t)\rangle = -\frac{w'}{\tau} + \frac{w'}{2\sigma_w^2}\frac{d\sigma_w^2}{dt}.$$

We now have a closed system of equations. Equation (3), being (with the approximations) linear in z' and w', gives rise to a Gaussian distribution of the positions and velocities within the puff whose second order central moments can be found by solving a coupled set of ordinary differential equations, while equation (2) describes the evolution of the puff centre. We note that the puff growth equations are very similar to those found in the SCIPUFF model (*Sykes, R. I. et al.*, 1998). β will be adjusted to give the desired mix between the dispersion which is represented by puff growth and that by puff motion and we turn to this matter next.

A constant value of β is used in the early stages of the puff growth. This value can be chosen as zero, so that all the early dispersion is treated via puff growth. However values greater than zero are required if we wish to include the effect of vertical velocity skewness (this cannot be represented through puff growth because our puffs are all Gaussian). At later times, puff size is limited by the scale Δ over which the flow is to be regarded as approximately homogeneous. Generally Δ is chosen as some fraction of the boundary layer depth. When the puff size reaches Δ, we set $\beta = 1$. This will stop the puff growing, but not at once because it takes some time for $\langle z'w'\rangle$, which determines the rate of puff growth, to decay. It also takes some time for $\langle z_0 w_0\rangle$ to increase and hence for the rate of dispersion due to the random puff motion to increase. While we could simply allow the puff size to increase a little beyond Δ, we choose instead to allow the puff to shed any excess size and we replace it with random increments in the puff position.

If $\beta = 0$ in the early stages of the dispersion, then, at least for an instantaneous source, we release a single puff at the source. However as soon as randomness in the puff position is introduced (i.e. when $\beta > 0$) it is necessary to have multiple puffs in order to obtain adequate statistics of the random component of the motion. This is done by splitting the puff a number

of times until there are an adequate number of puffs. The splitting process is different from that in e.g. SCIPUFF (*Sykes, R. I. et al.*, 1998) or HYSPLIT (*Draxler, R. R. and G. D. Hess*, 1997, 1998) in that the child puffs are identical in size and location to the parent puff but the mass of pollutant they carry is reduced. The value of the extra puffs is that they will have different evolutions after creation and so will provide a better sampling of the random component of the puff motion. Each split is always into two child puffs, but the child puffs may immediately split again if this is required. The number of splits is computed by requiring that the typical number of puffs contributing to any concentration estimate is sufficiently large. This is implemented by requiring that the number of splits n satisfies $2^n \sigma_p / \min(\sigma_h, \sigma_a) \geq A$. Here 2^n is the estimated number of puffs, A is the number of puffs we wish to contribute to a concentration estimate (choosing a large value will increase the cost of the simulation but reduce the noise), σ_p is the puff size, and $\min(\sigma_h, \sigma_a)$ is an estimate of the effective plume size which is 'seen' by the puff, so that $\sigma_p / \min(\sigma_h, \sigma_a)$ is the fraction of puffs that will contribute to a typical concentration estimate. σ_h is the spread which would occur for material experiencing homogeneous Gaussian turbulence with the velocity variances and time scales showing the same time dependence as the turbulence seen by the puff, while σ_a is the actual spread evaluated over all puffs. Generally σ_a will be less than σ_h. For example, within the boundary layer, σ_h will grow indefinitely while σ_a will be limited by the boundary layer depth. However, this is not always so. For a source above the boundary layer which then fumigates into the boundary layer, σ_h will be small for a puff that remains above the boundary layer while σ_a will reflect the increased spread of the puffs that have been mixed into the boundary layer.

For puffs near the ground, the puff concentration distribution is reflected following the approach used in Gaussian plume models. It is also important to advect the puffs with the velocity, not at their unreflected centre z_0, but at their true centre of mass z_r after reflection. This avoids the problem of puffs from a source at ground level not moving downwind. It is then simplest to take all flow properties at this height. However, because it is the evolution of z_0 which responds to the turbulence properities, we replace z derivatives by the derivatives 'seen' by the unreflected puff centre. For example, in (4)

$$\frac{d\sigma_w^2}{dz} \quad \text{becomes} \quad \frac{d\sigma_w^2(z_r)}{dz_0} = \frac{d\sigma_w^2(z_r)}{dz_r}\frac{dz_r}{dz_0}$$

with the understanding that dz_r/dz_0 is evaluated at constant (unreflected) puff size σ_p. This has some beneficial properties in terms of the well-mixed distribution of pollution (see below) as well as in reducing the upward drift in z_0 caused by the vertical derivatives of σ_w^2 and τ – this is desirable because z_r will increase even if z_0 is constant as the puff expands.

We would like the model to have the property that an initially well-mixed state remains well mixed. However the approximations necessary in puff models mean that this is unlikely to be achievable in all circumstances. In particular the well-mixed state can be achieved with various choices for the puff sizes and for the distribution of puff centres. These will not all lead to identical evolutions. However the model does have some good properties in this regard. If all the dispersion is represented by puff growth, then the first term on the right hand side of (4), when combined with the drift terms in $a(z_0, w_0, t; \beta)$, yields the usual drift acceleration used in well-mixed particle models. The second term in (4) is zero at the start but builds up to yield a total drift acceleration of $(1/\tau)\ dK/dz$ where K is the diffusivity $\sigma_w^2\tau$, leading to a drift velocity dK/dz in the diffusive limit as used in well-mixed diffusive models. Without the second term in (4), the faster growth of puffs in the high τ regions could lead to these regions being depleted preferentially. [Note that these drift effects are treated slightly

differently in the SCIPUFF approach, with, in effect, the whole drift acceleration $(1/\tau)\ dK/dz$ being used from the start.] Once all the puffs have ceased to grow, the distribution of puff centres will approach a well-mixed distribution based on the underlying particle model and, together with the way reflections are treated, will lead to a uniform concentration profile.

For a continuously emitting source there is a potential difficulty in that the puffs are small near the source, which would seem to require frequent puff releases to give a continuous plume. However the meteorology changes on a much slower time scale and so it is inefficient to have frequent releases which all behave in a very similar manner. To solve this problem the puffs are given a spread in time. They then contribute to concentrations at times either side of their nominal time. To ensure the results vary smoothly, the time-spread is taken to be triangular in shape (apart from the first and last puffs from a source) with an overlap in time between successive puff releases.

Extension of the model to take account of shear in the mean flow and to apply to non horizontally homogeneous flows is likely to be possible, using ideas similar to those used in SCIPUFF.

COMPARISON WITH THE KINCAID EXPERIMENT

The model described above has been implemented in the NAME model (*Jones, A. et al.*, 2007). Here we present a comparison of the model with the results of the Kincaid experiment (*Bowne, N. E. and R. J. Londergan*, 1983). This experiment involved dispersion from a tall power station stack with a generally convective boundary layer. We use the data in the form presented in the Harmonisation Initiative Model Validation Kit (*Olesen, H. R.*, 1995) and restrict attention to the "quality 3" experimental data. Modelled and measured arc-wise maxima of the hourly averaged ground level concentrations are compared along arcs at distances ranging from 500 m to 50 km from the stack.

The simulations use NAME III version 4.3. The input meteorology is hourly values of wind speed and direction at 100m, near surface temperature and cloud cover as measured at the power plant site. Surface sensible heat flux and boundary layer depth are estimated using methods similar to those in ADMS (*CERC*, 2005). For this application using single site observations of meteorology rather than 3-d meteorology from an NWP model, the mean flow and turbulence profiles are constructed using formulae based on surface fluxes, boundary layer depth and roughness length. The buoyant plume rise is represented by the model described by *Webster, H. N. and D. J. Thomson* (2002) using hourly information on the emission velocity and temperature (together with the stack diameter).

Table 1. Statistics of the model performance for the Kincaid experiment

FB	NMSE	COR	FA2	FS
-0.025	0.62	0.47	0.737	-0.086

Table 1 shows the results of the comparison in terms of fractional bias (FB), normalised mean square error (NMSE), correlation (COR), fraction of cases within a factor of 2 (FA2) and fractional bias in the standard deviation (FS) as defined by *Hanna, S. R. et al.* (1991). The results are comparable to the best performing models for this dataset (see e.g. *CERC,* 2001, *Olesen, H. R.*, 1995), giving confidence that the puff scheme is performing reasonably. We note that our statistics are evaluated slightly differently to those of CERC and Olesen in that we choose not to normalise the concentrations by the source strength. This is because the

source strength varies in time and there is a significant travel time from the source to the most distant receptors. However we do not believe this significantly affects the statistics.

In the future we aim to test the model against a wider range of datasets and develop the approach for longer ranges by removing the approximations which are valid only in horizontally homogeneous situations.

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