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Validation of a Lagrangian model plume rise scheme using the Kincaid data set

H.N. Webster*, D.J. Thomson

Climate Research Division, Met Office, Bracknell, Berks RG12 2SZ, UK

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Abstract

Correct prediction of the initial rise of a plume due to momentum and buoyancy effects is an important factor in dispersion modelling. A new plume rise scheme, based upon conservation equations of mass, momentum and heat, for the Lagrangian model, NAME, is described. The conservation equations are consistent with the well-known analytical plume rise formulae for both momentum- and buoyancy-dominated plumes. The performance of the new scheme is assessed against data from the Kincaid field experiment. Results show that the new scheme adds value to the model and significantly outperforms the previous plume rise scheme. Using data from assessments of atmospheric dispersion models using the Kincaid data set, it is shown that NAME is comparable to other models over short ranges.

Keywords: Dispersion modelling; Buoyancy; Conservation equations; Model evaluation; Turbulence

1. Introduction

Emissions from power station stacks and many other anthropogenic sources have substantial vertical velocities and are often hot compared with the surrounding ambient air. These momentum and buoyancy effects cause the emitted plume to rise, increasing the effective source height to between 2 and 10 times the actual release height for typical elevated sources (Arya, 1999). In turn, this plume rise can reduce maximum ground level concentrations by a factor of 3 to 100 (Briggs, 1984). It follows that the modelling of plume rise within atmospheric dispersion models is important, particularly at distances near to source and at times when the boundary layer is shallow enough for plume rise to enable the effluent to penetrate through the boundary layer top into the stable layer aloft. Plume rise can, therefore, have a long-range effect through processes such as fumigation.

The inclusion of plume rise within Lagrangian particle models has been considered by a number of authors (Luhar and Britter, 1992; Van Dop, 1992; Anfossi et al., 1993; Hurley and Physick, 1993; Hurley, 1999; Heinz and Van Dop, 1999). The problem is non-trivial since the rise of each particle is influenced by the buoyancy of the plume as a whole (which depends on relative or two-particle dispersion), whereas the basic idea underlying Lagrangian models is that the particle motions are independent (at least in the so-called 'single-particle' models). The buoyancy of the plume depends on the entrainment of ambient air into the plume and this generally needs to be parametrised in some way.

In the simplest models the problem is avoided by using a separate plume rise model to calculate the final rise height. The effects of plume rise are then accounted for by releasing particles from the final rise height and allowing them to be advected and dispersed passively by ambient winds and turbulence. More detailed schemes describe the transition of the particles from the stack to the final rise height, with plume buoyancy/momentum and ambient winds/turbulence acting together. These schemes fall into two main classes. In the first class, a

*Corresponding author.
E-mail address: helen.webster@metoffice.com (H.N. Webster).

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separate model for plume rise and entrainment is adopted and the velocities generated added to the motion of the particles (Luhar and Britter, 1992; Anfossi et al., 1993; Hurley and Physick, 1993; Hurley, 1999). The plume rise model might be a plume rise formula (such as those due to Briggs), or it might be an integral model solving a set of ordinary differential equations for the evolution of the bulk properties of the plume with time or downwind distance. Sometimes the plume rise model is used to obtain a single plume rise trajectory with the result added to each particle's motion, while in other approaches the plume rise model is applied separately for each particle using flow properties at the particle location. In addition, the plume spread is generally enhanced to account for plume rise induced turbulence, either by including a random adjustment to the plume rise or by enhancing the model's ambient turbulence. For models in this first class, the problem of representing the plume buoyancy and relative dispersion in a single-particle model is solved by treating such matters in the separate plume rise model. The second class consists of models where each particle carries its own temperature (or potential temperature) which evolves according to a stochastic equation. The buoyancy force on the particle is calculated from the particle temperature and is included directly in the equation for the evolution of the velocity (Van Dop, 1992; Heinz and Van Dop, 1999). This type of approach gives a more unified approach and has advantages from the perspective of turbulence closure theory (Heinz and Van Dop, 1999). Also the approach enables the rise of each particle to respond to local flow properties. However, in such models the treatment of turbulent entrainment into the plume and the relative dispersion aspects are less direct and not yet well understood with, for example, adjustments to the constants being required to generate the correct power law rise in a neutrally stratified atmosphere.

NAME is a Lagrangian model in which large numbers of particles are released into the model atmosphere (Maryon et al., 1999). Each particle represents a certain mass of the pollutant which is depleted over time, if appropriate, by wet and dry deposition processes, radioactive decay or chemical transformation. The particles are advected by three-dimensional ambient winds obtained from the Met Office's numerical weather prediction model, the Unified Model. Dispersion due to atmospheric turbulence is simulated by random walk techniques. The random walk scheme uses velocity variance and Lagrangian time scale profiles determined from empirical fits to observational data to simulate the turbulent motion (Maryon et al., 1999). Gaussian velocity distributions are assumed and the components of the turbulent motions are assumed uncorrelated. The plume rise scheme, modelling the rise of the plume due to momentum and buoyancy effects, is used until the plume becomes passive (i.e. neutrally buoyant) and subsequently follows the ambient air motion.

The original plume rise scheme within NAME used the well-known Briggs formulae for both stable and neutral/convective conditions (see Briggs, 1984; Seinfeld, 1986; Weil, 1988, for details). These formulae have been tested and fitted to observational, wind tunnel and water tank data (Briggs, 1984; Weil, 1988). There are, however, a number of disadvantages with the original NAME plume rise scheme. Firstly, the Briggs formulae are only valid in specific meteorological conditions (e.g. uniformly stratified environments with steady horizontal winds of constant speed and direction). Secondly, the scheme assumes that a particle released into unstable (or stable) conditions remains in unstable (or stable) conditions for the whole of the plume rise. This is clearly incorrect in certain situations, for example, a particle released into an unstable boundary layer may subsequently, whilst under the effects of plume rise, penetrate the boundary layer top into the elevated stable layer above. Thirdly, the original NAME scheme assumes, for the purpose of terminating the rise, that all ambient air entrained into the plume has a single potential temperature, taken to be the potential temperature at stack height. Whilst it is true that most of the entrainment occurs in the initial stages, in reality entrainment of ambient air occurs throughout the plume rise process.

Here we investigate a new plume rise scheme for NAME. The scheme solves an integral model based on the governing conservation equations of mass, momentum and heat (or enthalpy) as used in the atmospheric dispersion modelling system (ADMS) (Robins et al., 1999). The ADMS equations are based upon the work of Ooms (1972) and Ooms and Mahieu (1981) with some modifications and are introduced here into a Lagrangian framework. The integral model is solved following each particle separately, using local mean flow properties at the particle location. As a result the rise of each particle responds to local conditions. The solutions of the integral model for quantities such as plume radius do not really refer to the actual plume radius since they are different for each particle. The plume radius can, however, be interpreted as the initial radius multiplied by a measure of the average dilution in the neighbourhood of the particle. In short, each 'particle' could be regarded as a 'plume' driven by local ambient conditions in the sense that each particle carries (estimates of) a number of bulk plume properties. Mixing of ambient air into the plume is modelled using the concept of an entrainment velocity (Ooms, 1972).

The proposed new scheme has a number of advantages over the original NAME scheme. It caters for a wider range of meteorological conditions and allows entrainment of ambient air to occur throughout the plume rise process. Furthermore, the effect on the plume of the detailed wind and temperature profiles obtained from the Unified Model, including the temperature inversion at the top of the boundary layer, will be modelled in a more realistic way. The new scheme and its incorporation into the NAME framework is described in more detail in Section 2.

Validation is an integral part of model development. The new plume rise scheme is validated against data from the Kincaid experiment. The Kincaid data set has been used extensively in model validation exercises and we conclude this study by comparing NAME with other leading atmospheric dispersion models.

2. The plume rise scheme

The coupled system of conservation equations upon which the new plume rise scheme is based is now described.

Assuming that the effluent consists mainly of hot air, we can ignore differences in the specific heat and molecular weight between the species and the ambient air. The basic conservation equations are given by the coupled system

$$\frac{\mathrm{d}}{\mathrm{d}\zeta}\begin{pmatrix} F_\mathrm{m} \\ F_{Mx} \\ F_{My} \\ F_{Mz} \\ F_h \end{pmatrix} = \begin{pmatrix} E_\mathrm{m} \\ -F_\mathrm{m}(\mathrm{d}u_\mathrm{a}/\mathrm{d}\zeta) - D_x \\ -F_\mathrm{m}(\mathrm{d}v_\mathrm{a}/\mathrm{d}\zeta) - D_y \\ -F_\mathrm{m}(\mathrm{d}w_\mathrm{a}/\mathrm{d}\zeta) + B - D_z \\ -F_\mathrm{m}c_p(\mathrm{d}\theta_\mathrm{a}/\mathrm{d}\zeta) \end{pmatrix}, \tag{1}$$

where ζ is the distance along the plume axis, $\mathbf{D} = (D_x, D_y, D_z)$ is the drag force, B is the buoyancy force, E_m is the mass entrainment rate and $\mathbf{u}_\mathrm{a} = (u_\mathrm{a}, v_\mathrm{a}, w_\mathrm{a})$ is the mean velocity of the ambient flow. The mass, momentum and heat fluxes are denoted by F_m, $\mathbf{F}_M = (F_{Mx}, F_{My}, F_{Mz})$ and F_h, respectively, and are given by

$$F_\mathrm{m} = \pi b^2 \rho_\mathrm{p} u_\zeta,$$

$$\mathbf{F}_M = (\mathbf{u}_\mathrm{p} - \mathbf{u}_\mathrm{a})F_\mathrm{m},$$

$$F_h = c_p(\theta_\mathrm{p} - \theta_\mathrm{a})F_\mathrm{m},$$

where $b = b(t)$ is the plume radius, c_p is the specific heat capacity of the ambient air at constant pressure and $u_\zeta = |\mathbf{u}_\mathrm{p}|$, where $\mathbf{u}_\mathrm{p} = (u_\mathrm{p}, v_\mathrm{p}, w_\mathrm{p})$ is the velocity of the plume. Subscripts p, a and s denote plume, ambient and source variables, respectively. Density, ρ, satisfies the equation of state, $p = \rho RT$, and potential temperature, θ, is related to the actual temperature, T, through

$$\theta = T\left(\frac{p}{p_0}\right)^{-R/c_p},$$

where p is the pressure, p_0 is a reference pressure and R is the specific gas constant. The buoyancy force, B, is given by the formula

$$B = \pi b^2 g(\rho_\mathrm{a} - \rho_\mathrm{p}),$$

where g is the gravitational acceleration constant. The mass entrainment rate is calculated using

$$E_\mathrm{m} = 2\pi b \rho_\mathrm{a} u_\mathrm{e},$$

where u_e is the entrainment velocity. The entrainment velocity consists of two parts (Ooms, 1972),

$$u_\mathrm{e} = u_\mathrm{e}^{(\mathrm{rise})} + u_\mathrm{e}^{(\mathrm{turb})}.$$

The first component, $u_\mathrm{e}^{(\mathrm{rise})}$, is due to the relative motion of the plume and ambient air and is given by

$$u_\mathrm{e}^{(\mathrm{rise})} = \alpha_1|\Delta\mathbf{u}_\zeta| + \alpha_2|\Delta\mathbf{u}_N|,$$

where α_1 and α_2 are constants and $\Delta\mathbf{u}_\zeta$ and $\Delta\mathbf{u}_N$ are the components of the relative velocity along and perpendicular to the plume's axis. The second component, $u_\mathrm{e}^{(\mathrm{turb})}$, is due to the ambient turbulence and is given by

$$u_\mathrm{e}^{(\mathrm{turb})} = \alpha_3 \min\left\{(\varepsilon b)^{1/3}, \sigma_w\left(1 + \frac{t}{2T_\mathrm{L}}\right)^{-1/2}\right\},$$

where α_3 is a constant, ε is the turbulence dissipation rate, σ_w is the root mean square (r.m.s.) vertical velocity fluctuation and T_L is the Lagrangian time scale. The drag force, $\mathbf{D}$, is given by the formula

$$\mathbf{D} = \pi b \rho_\mathrm{a} \Delta\mathbf{u}_N |\Delta\mathbf{u}_N| c_\mathrm{D},$$

where c_D is a constant referred to as the drag coefficient. The plume trajectory, $\mathbf{x}_\mathrm{p} = (x_\mathrm{p}, y_\mathrm{p}, z_\mathrm{p})$, is calculated from

$$\frac{\mathrm{d}\mathbf{x}_\mathrm{p}}{\mathrm{d}t} = \mathbf{u}_\mathrm{p}.$$

In a number of specific meteorological scenarios (e.g. uniformly stratified environments with steady horizontal winds of constant speed and direction as detailed in Table 1) the coupled system of conservation equations (1) can be solved analytically if drag is neglected for both momentum- and buoyancy-dominated plumes to give the plume rise formulae of Briggs, Weil, etc. This shows that the conservation equations are consistent with previously published formulae and highlights that the new scheme should be suitable for a wider range of meteorological conditions. For vertical plumes (no ambient mean wind), drag has no effect. In the case of a bent over plume (strong ambient wind), drag reduces plume rise. For a buoyancy-dominated plume the effects are relatively small (Webster and Thomson, 2001). Suggested values for the entrainment parameters for vertical and bent over plumes, α_1 and α_2, can be obtained by comparing the analytical solutions of the coupled system (1) with the plume rise formulae of Briggs and Weil. Details of the inferred entrainment parameter values under certain meteorological conditions, for both momentum- and buoyancy-dominated plumes, are given in Table 1.

In stable conditions with no ambient mean wind, the conservation equations form a rather complicated

Table 1
Inferred entrainment parameter values for momentum- and buoyancy-dominated plumes

Meteorological conditions	Momentum-dominated plume	Buoyancy-dominated plume
Strong ambient wind (a bent over plume) Zero stratification	$\alpha_2 = 0.35$ (Briggs, see Arya, 1999) $\alpha_2 = 0.6$ (Weil, 1988)	$\alpha_2 = 0.61$ (Briggs, see Hanna et al., 1982) $\alpha_2 = 0.6$ (Weil, 1988)
No ambient mean wind (a vertical plume) Zero stratification	$\alpha_1 = 0.11$ (Weil, 1988)	$\alpha_1 = 0.125$ (Briggs, 1984) $\alpha_1 = 0.11$ (Weil, 1988)
Strong ambient wind (a bent over plume) Stable stratification	$\alpha_2 = 0.6$ (Weil, 1988)	$\alpha_2 = 0.6$ (Weil, 1988)

system which cannot be solved analytically. By dimensional analysis arguments an expression for the final rise height is obtained. A comparison with final rise formulae by Briggs, etc. does not, however, yield a value for the entrainment parameter as in other cases.

Atmospheric dispersion models which use a conservation approach to modelling plume rise, commonly assume constant values for the entrainment constants, α_1 and α_2. Within ADMS, α_1 and α_2 are set to be 0.057 and 0.50, respectively (Robins et al., 1999). The Air Pollution Model, TAPM (Hurley, 1999), uses $\alpha_1 = 0.1$ and $\alpha_2 = 0.6$.

The coupled system of conservation equations (1) are introduced into NAME using a simple forward time step numerical scheme. The values of the entrainment parameters, $\alpha_1 = 0.11$ and $\alpha_2 = 0.5$, are chosen from the range of values given by Briggs, Weil, ADMS and TAPM; namely $\alpha_1 = 0.1$ (TAPM) – 0.125 (Briggs) and $\alpha_2 = 0.35$ (Briggs) – 0.6 (TAPM). Note that the ADMS value of $\alpha_1 = 0.057$ is disregarded since it is out of keeping with other suggested values and numerical simulations in calm, stable conditions using $\alpha_1 = 0.057$ give poor agreement with the final rise formulae of Briggs and Weil (Webster and Thomson, 2001). The ADMS values of the parameter for entrainment due to atmospheric turbulence, $\alpha_3 = 0.655$, and the drag coefficient, $c_D = 0.21$, are adopted in the absence of any other suitable published values. The calculated fluxes of mass, momentum and heat together with ambient meteorological variables at the particle position are used to calculate the mean particle velocity, $\mathbf{u}_p$. The particle is then advected using

$$\mathbf{x}(t + \Delta t) = \mathbf{x}(t) + (\bar{\mathbf{u}} + \mathbf{u}')\Delta t,$$

where $\bar{\mathbf{u}}$ is the mean velocity and $\mathbf{u}'$ is the turbulent velocity component obtained from the random walk scheme. Whilst under the plume rise scheme, $\bar{\mathbf{u}} = \mathbf{u}_p$. For efficiency, when the effects of plume rise become minimal, the plume rise scheme is turned off and $\bar{\mathbf{u}} = \mathbf{u}_a$, thereafter. This termination is enforced after 1 h or when $|F_{Mz}/F_m| = |w_p - w_a| < 0.1$ m s^{-1}, whichever is sooner.

As well as altering the mean height of the plume, plume rise generates turbulence which will increase the plume size. This plume rise induced turbulence is greatest in the initial stages and is included within our scheme by adding a random component at each time step with prescribed mean and variance. Following the approach of the ADMS model (Robins et al., 1999), we adopt a second mass conservation equation

$$\frac{dF_{m0}}{d\zeta} = E_{m0}, \tag{2}$$

which includes entrainment of ambient air due to the plume rise process only (i.e. entrainment of ambient air due to ambient turbulence is neglected). ($F_{m0} = \pi b_0^2 \rho_p u_\zeta$ is the mass flux, b_0 is a measure of the plume radius and $E_{m0} = 2\pi b_0 \rho_a u_e^{(\text{rise})}$ is the mass entrainment rate.) Initially, $F_{m0} = \pi r_s^2 \rho_s w_s$ and $b_0 = r_s$ where r_s is the radius of the stack. The plume radius, b_0, at time t is calculated from

$$b_0(t) = \sqrt{\frac{F_{m0}(t)}{\pi \rho_p u_\zeta}}. \tag{3}$$

It is difficult to offer a convincing justification of the details of this approach because the plume width cannot be split unambiguously into a part due to plume rise induced turbulence and a part due to ambient turbulence. This is because the two effects interact and are not linearly additive. For example, in Eq. (3), ρ_p and u_ζ are plume variables calculated using the coupled system (1) which also includes entrainment due to ambient turbulence. It could be argued that these quantities should be recalculated. Equally, one could argue that E_{m0} in (2) should be based on b not b_0. However, for simplicity we have followed the ADMS scheme.

A circular plume of radius b_0 with top hat profiles of various plume properties has a probability density function given by $1/(\pi b_0^2)$. The r.m.s. spread in either cross-plume direction, σ_0, of such a profile is given by

$\sigma_0 = b_0/2$. By definition

$$\sigma_0^2 = \overline{\left(\sum_i r_i\right)^2},$$

where r_i are the random turbulent displacements due to plume rise induced turbulence in successive time steps. The random components in the model are assumed uncorrelated for simplicity and hence

$$\sigma_0^2 = \sum_i \overline{r_i^2} = \frac{b_0^2}{4}.$$

In the numerical scheme, plume rise induced turbulence is modelled by adding a random displacement, $\mathbf{r} = (r_x, r_y, r_z)$ to each trajectory at each time step. The components of the random displacement have zero mean and variance $\overline{r_i^2} = (b_0^2(t + \Delta t) - b_0^2(t))/4$.

3. The Kincaid experiment

The Kincaid field experiment was an extensive experimental campaign carried out during 1980 and 1981 as part of the Electric Power Research Institute plume model validation and development project (Bowne and Londergan, 1983; Hanna and Paine, 1989). The Kincaid power plant is located in Illinois, USA (39.59°N, 89.49°W) in an area of flat farmland with some lakes. The roughness length, z_0, is approximately 10 cm. Surrounding terrain is homogeneous and at an elevation of 180 m above mean sea level (a.m.s.l.).

During the campaign, a buoyant plume containing SF_6 was released from a stack of height 187 m and diameter 9 m. Two hundred monitors were placed at ground level along arcs at distances ranging from 500 m to 50 km from the stack. Hourly averaged concentrations were measured and from this data, for each hour and along each arc at a fixed distance from the source, the maximum hourly averaged concentration was calculated and recorded. In total, the Kincaid data base contains 1284 records over 171 h. Each record consists of the recorded maximum hourly averaged concentration at a particular time and distance from source. A quality indicator, QUAL, has been assigned to each record by Sigma Research Corporation (SRC) to indicate the reliability of the value in representing the true arc-wise maxima. A quality indicator of 0 implies that the plume probably missed the monitors and hence the value should clearly be disregarded. An indicator of 1 suggests that the observed value is probably not the maximum. Where a maximum is observed but it is believed that the true maximum may well be different, a quality indicator of 2 is assigned. (This category also includes cases where the observed maximum is zero but evidence shows that a plume is present aloft.) Quality 3 indicates that a well-defined maximum believed to be representative of the true maximum is detected. It is recommended (Olesen, 1994) that only data with quality indicator 2 or 3 is used for analysis.

Meteorological data was observed throughout the campaign on a 100 m tower at the power-plant site. Radiosonde data is available from a single on-site sounding obtained several times a day. Meteorological conditions ranged from neutral to convective with an overrepresentation of daytime convective hours. Observed wind speeds varied between a calm 1.5 m s^{-1} to a breezy 13.7 m s^{-1} over the period.

Observed concentrations and meteorological data from the Kincaid experiment are distributed as part of the Model Validation Kit (Olesen, 1994) developed at a series of workshops on 'Harmonisation of Atmospheric Dispersion Modelling for Regulatory Purposes'.

4. Model set-up

The NAME model is designed to run using output from the Met Office's numerical weather prediction model, the Unified Model, as ambient meteorological input. Unfortunately, Unified Model output for the experimental period is unavailable and consequently some pre-processing is required to extend the hourly single site data provided with the Model Validation Kit into three-dimensional fields acceptable by NAME. Pre-processing of input meteorological data is far from trivial with a variety of options available to modellers all of which can in some way be justified. For example, observed values of a parameter could be used or the value could be predicted from other meteorological parameters. Details of the pre-processing undertaken are now discussed.

All meteorological variables were assumed to be horizontally homogeneous. A grid of 0.5° resolution was used only in order to put the data in the correct format for NAME and not to represent any horizontal inhomogeneities. In the vertical, 38 levels were inserted in the model domain at 10, 30, 50 and 100 m, then at every 100 m until 3000 m and at 3750, 5000, 7500, 10 000 and 15 000 m.

Observations of wind speed and wind direction are available at 10, 30, 50 and 100 m. From this, the horizontal velocity components, u and v, were obtained. At higher levels, u and v were fixed at 100 m values. The vertical velocity component, w, was assumed to be zero.

Observed values of temperature are available at 10, 50 and 100 m. The surface temperature, T_s, was assumed to be equal to the temperature at 10 m. The temperature at 30 m was obtained by interpolating between 10 and 50 m. At levels above 100 m, temperature was assumed to decrease at the dry adiabatic lapse rate, $\Gamma_d = 0.0098$ K m^{-1} (i.e. constant potential temperature) within the boundary layer and at the lower rate of

$0.006\ \mathrm{K\ m^{-1}}$ above the boundary layer. A temperature jump, ΔT, at the top of the boundary layer was included, where ΔT is calculated using (Thomson, 2000)

$$\Delta T = \begin{cases} \dfrac{\gamma_\theta z_i c_F}{1+2c_F} & \text{if } H_0 > 0, \\ 0 & \text{otherwise,} \end{cases}$$

where γ_θ is the rate of increase of potential temperature with height above the ground (taken to be $0.0038\ \mathrm{K\ m^{-1}}$), z_i is the depth of the boundary layer, H_0 is the surface sensible heat flux and c_F is a constant. The constant c_F takes the value 0.2 recommended by Driedonks (1982).

The Monin–Obukhov length, L, and the friction velocity, u_*, derived by SRC using pre-processor methods detailed in Hanna and Paine (1989) were adopted. An observed value for surface pressure was used and mean sea level pressure was calculated by adding 20 mb to the surface pressure to compensate for the terrain being at an elevation of 180 m a.m.s.l.

The Model Validation Kit contains two values for boundary layer depth: an observed value determined manually by interpretation of radiosonde data and a predicted value derived using the methods described by Hanna and Paine (1989). The observed mixing heights represent an upper estimate. Following recommendations issued with the Model Validation Kit (Olesen, 1995), observed values of boundary layer depth were used in our model assessment study. Initial validations of other atmospheric dispersion models against the Kincaid data set (including that of ADMS) used observed values of boundary layer depth. It has become more common in recent model validation exercises using the Kincaid data set to use the boundary layer depth calculated by the model's own meteorological pre-processor.

A model output grid with a resolution of 0.5 km and centred roughly on the Kincaid power plant was used. Near to the source, particularly along the arc at 0.5 km from the stack, this output grid is clearly too large. A finer output grid with a resolution of 0.05 km was therefore constructed to be used for very near-source measurements up to 5 km away. However, the results from this finer grid are encumbered with an excessive number of zeros in the modelled concentrations. There is evidence that these zero values are caused, at least partly, by statistical noise but the computational expense prevents us from using more particles. Consequently, we have not considered these fine resolution results further here and all results presented below are obtained with the 0.5 km grid.

NAME runs were performed using both the new plume rise scheme and the old plume rise scheme (Maryon et al., 1999). The maximum predicted hourly averaged ground level concentration for each arc was compared with the observed arc-wise maxima. In other model validation exercises against the Kincaid data set, observations and model predictions have been normalised by the emission rate, Q. During the Kincaid experiment, the emission rate varied from hour to hour by a significant amount. Most models provide a steady-state solution in which the plume is instantly present some distance downwind. NAME, however, is a time-dependent model with a continuously evolving plume. The NAME particles contributing to the hourly averaged model concentration predictions would have been released at different times and are likely to have different emission rates associated with them (especially at the furthest arc (50 km)). Hence, it is not clear, when normalising concentrations by the emission rate, what the correct value of Q to use is. Furthermore, it does not appear that our results are unduly affected by outliers (over the measurement period, Q varied only over a relatively modest range from 8.2 to $22.6\ \mathrm{g\ s^{-1}}$). For this reason, we choose not to normalise concentrations and compare observations against model predictions directly.

5. Model assessment

The Kincaid data set is used to assess the ability of a model to predict maximum observed concentrations along arcs of fixed distance from a source in mainly convective conditions. A large scatter between observed and model predictions is expected due to the turbulent nature of the atmosphere. Hence, even a perfect model would not be able to reproduce the observations exactly. In addition, Olesen (1995) comments that since the observed maximums might have been larger if the monitoring network had been denser, a 'perfect' model should exhibit some degree of overprediction. Alternatively, concentration fluctuations could result in the observed maximums being greater than the ensemble mean predicted by the model and hence one could argue that some degree of underprediction should be expected.

The mean and standard deviation (σ) of both observations and model predictions are calculated. Performance measures obtained as part of the model assessment procedure are the bias, normalised mean square error (NMSE), correlation (r), fractional bias (FB), fractional bias in the standard deviation (FS) and proportion of values within a factor of 2 (FA2) of the observed maximum concentrations (Hanna et al., 1991). The ratio of the predicted concentrations to the observed concentrations, `C MOD/C OBS`, is known as a residual. In a good model, the residuals should not demonstrate any dependence on variables such as downwind distance, stability and wind speed.

6. Results

The plume rise scheme has been assessed using observational data of quality 2 and 3. The performance statistics for observations of quality 3 are shown in Table 2. Table 2 clearly shows that the new plume rise scheme outperforms the old scheme. The new scheme slightly underpredicts (positive bias) but gives good agreement with the observed mean and standard deviation. The old scheme overpredicts significantly (negative bias) and exhibits too much variation (σ). The new scheme also shows significantly better performance in the bias, NMSE, FB and FS statistics. The fraction of modelled values within a factor of two of observations reaches a respectable 67% for the new scheme. Correlation is the only statistic for which the new scheme is outperformed, with a value of just 0.3.

Extreme values are of particular interest in assessing exceedences of air quality standards for regulatory purposes. The average of the ten highest concentrations, the maximum concentration and the robust highest concentration (RHC) with $R = 11$ (Cox and Tikvart, 1990) are given in Table 3 for data of quality 3. The new plume rise scheme outperforms the old plume rise scheme in predicting extreme values. The highest concentrations are significantly overpredicted by the old scheme, whereas the new scheme, performs well.

Fig. 1 shows the corresponding scatter plots of observations against model predictions for data of quality 3. Quantile–quantile plots for the same data are given in Fig. 2. Within a quantile–quantile plot, the largest observed concentration is plotted against the largest model prediction regardless of whether they occurred at the same time, distance from source, etc. Figs. 1 and 2 reinforce many of the conclusions drawn from the statistical analysis, namely that the old scheme overpredicts whereas the new scheme, performs better. The behaviour of the residuals, `C MOD/C OBS`, of quality 3

Table 2
Performance statistics obtained using data of quality 3

	Mean (μg m^{-3})	σ (μg m^{-3})	Bias (μg m^{-3})	NMSE	r	FB	FS	FA2
Observations	0.692	0.513	0.0	0.0	1.0	0.0	0.0	1.0
New plume rise	0.578	0.575	0.114	1.07	0.306	0.180	−0.113	0.667
Old plume rise	1.19	1.05	−0.501	1.51	0.341	−0.531	−0.687	0.616

Table 3
Extreme value statistics for data of quality 3 (in μg m^{-3})

Extreme statistics	Observations	New plume rise	Old plume rise
Maximum concentration	3.928	3.929	6.389
Top-ten average	2.477	2.919	4.949
RHC ($R = 11$)	3.727	4.328	6.823

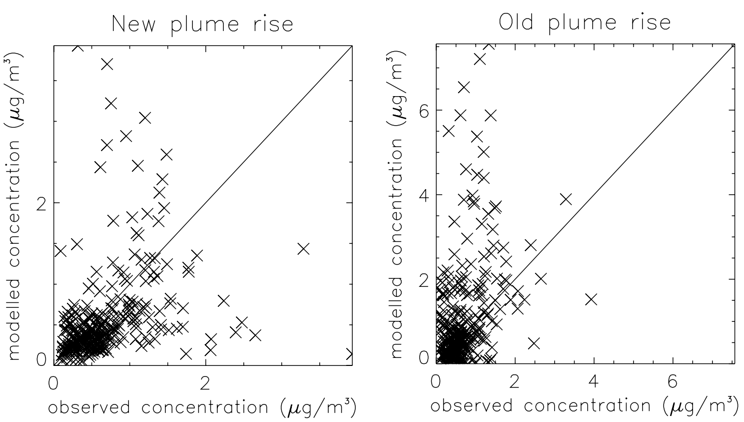

Fig. 1. Scatter plots using data of quality 3.

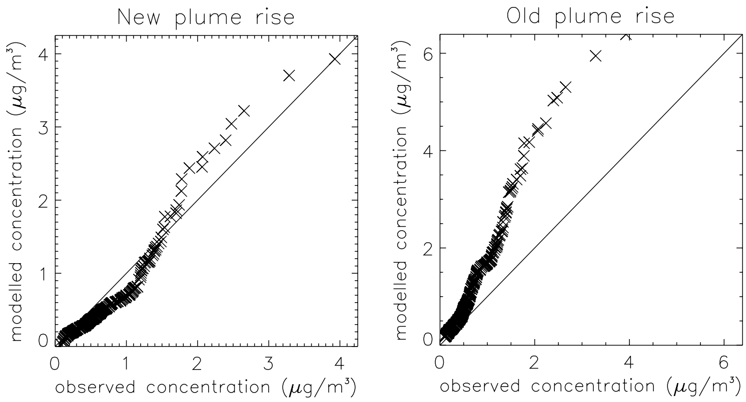

Fig. 2. Quantile–quantile plots using data of quality 3.

is displayed in Figs. 3 and 4. Data has been grouped according to a number of physical and meteorological variables namely distance from source, wind strength, stability (as characterised by z_i/L, where z_i is the boundary layer depth and L is the Monin–Obukhov length), boundary layer depth and time of day. The cumulative distribution function of the residuals within each group is denoted by the 5th, 25th, 50th, 75th and 95th percentiles. These five significant points are plotted in a box format (see Figs. 3 and 4). For a good model, the residual boxes should be small and should not deviate too much from unity. The dashed horizontal lines in Figs. 3 and 4 define the boundaries of the area within which modelled values lie within a factor of two of observations. The old plume rise scheme (Fig. 4) overpredicts at distances of 2 km or less and to a lesser extent at distances between 2 and 5 km. The old scheme also shows a tendency to overpredict at large distances. The new scheme (Fig. 3) performs well at all ranges including near source with a large proportion of the residuals lying within the factor of two lines.

The residuals show no apparent dependence on wind speed (represented by u_*) for any of the NAME runs (see Figs. 3 and 4).

The old scheme (Fig. 4) tends to overpredict in neutral conditions. Fig. 3 shows that the new scheme performs better in neutral conditions with less suggestion that the residuals have some dependence on stability.

Both runs appear to have problems with shallow mixing heights of 400 m or less and with large mixing heights of more than 2500 m. The observed mixing depth used in the model is an upper estimate and so some degree of underprediction of concentrations is perhaps to be expected. On the other hand, in situations with shallow boundary layers an overestimate of the boundary layer depth could result in an overprediction of surface concentrations. In such cases a plume which, in reality, is present above the boundary layer top could be modelled as though it is within the boundary layer and mixed down to the ground. The new scheme underpredicts for both shallow and deep mixing depths whereas the old scheme suffers from the inverse problem with large overprediction at small and large mixing heights. The new scheme residuals do not show any dependence on the hour of day. The old scheme, however, overpredicts during the morning when the boundary layer is most likely to be shallow.

Details of the comparison of model predictions against observations of quality 2 and 3 combined are presented in Webster (2001). To summarise, NAME overpredicts slightly against observations of quality 2 and 3 and the performance statistics are marginally worse (larger NMSE, smaller proportion of values within a factor of two of observations, etc.) than those obtained for observations of quality 3 only. There is also some evidence of overprediction near source, at low wind speeds and during early morning.

7. Comparing the performance of NAME with other atmospheric dispersion models

In order to put the performance of NAME in context, it is appropriate to compare its performance with other atmospheric dispersion models. In doing this, we adopt the protocol recommended with the Model Validation Kit (Olesen, 1994).

The performance of NAME is compared in Table 4 against the following atmospheric dispersion models: HPDM (Earth Tech., USA), ADMS (CERC, UK), OML (NERI, Denmark), AERMOD (USA) and ISCST (EPA, USA). Since NAME is a Lagrangian model, it is computationally expensive to run. The run time is therefore several magnitudes more than other models of a simpler nature. The data for HPDM and OML are obtained from the model validation exercise at Mol (Olesen, 1995). The statistics for ADMS 3, AERMOD

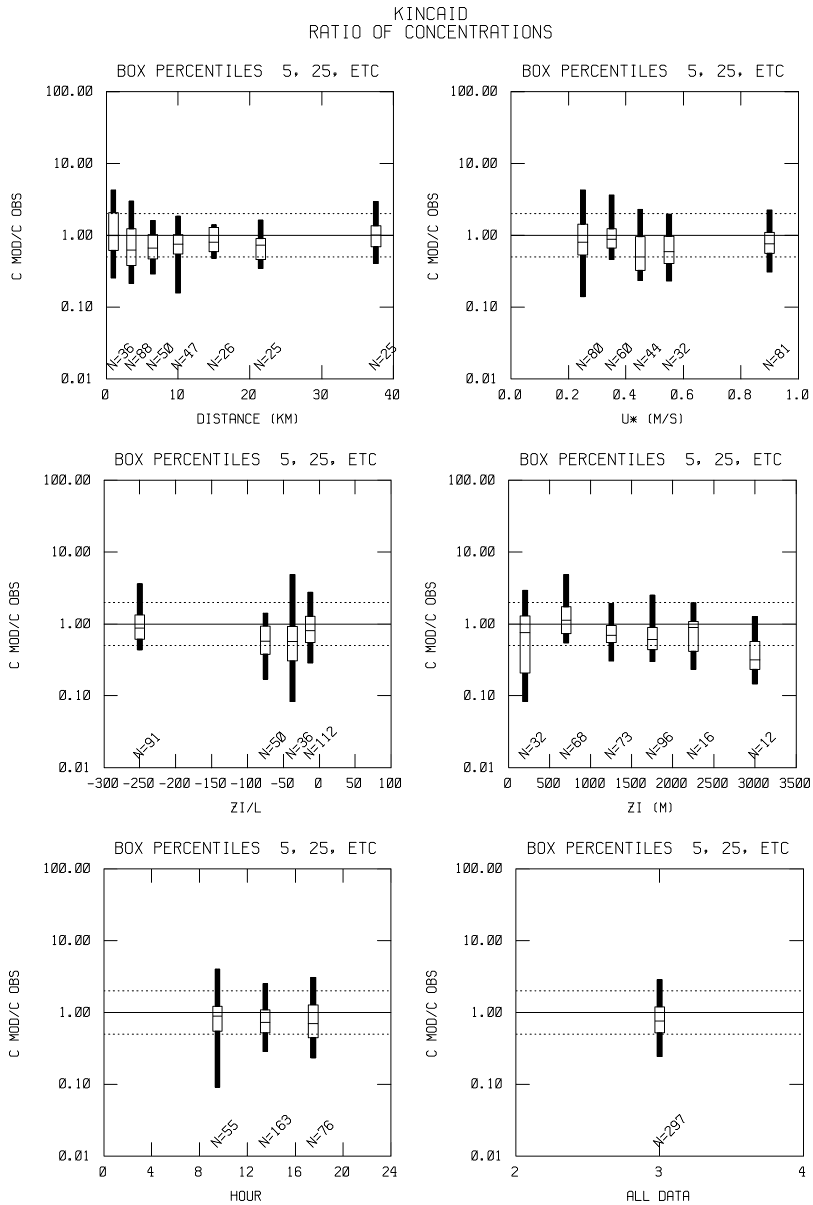

Fig. 3. Residual box plots for new plume rise using quality 3 data.

and ISCST are reproduced from the ADMS validation summary (CERC, 1999).

It is difficult to interpret the statistical data given in Table 4. A variety of pre-processing methods for the meteorological data have been used and the Kincaid data set has been used for some models during model development. Consequently, the validation exercise does not constitute an independent test of the models. In addition, there are difficulties in comparing steady-state models with time-dependent models. However, the following general conclusions can be drawn.

AERMOD and ISCST show significant under estimates. NAME also shows a degree of general underprediction. Early versions of ADMS showed substantial over estimates but ADMS 3 performs well.

NAME is comparable to other models. The fraction within a factor of two of observations from NAME is highly respectable. Correlation, however, is disappointingly low. Statistical measures of mean, standard deviation, bias, NMSE, FB and FS are similar to other atmospheric dispersion models.

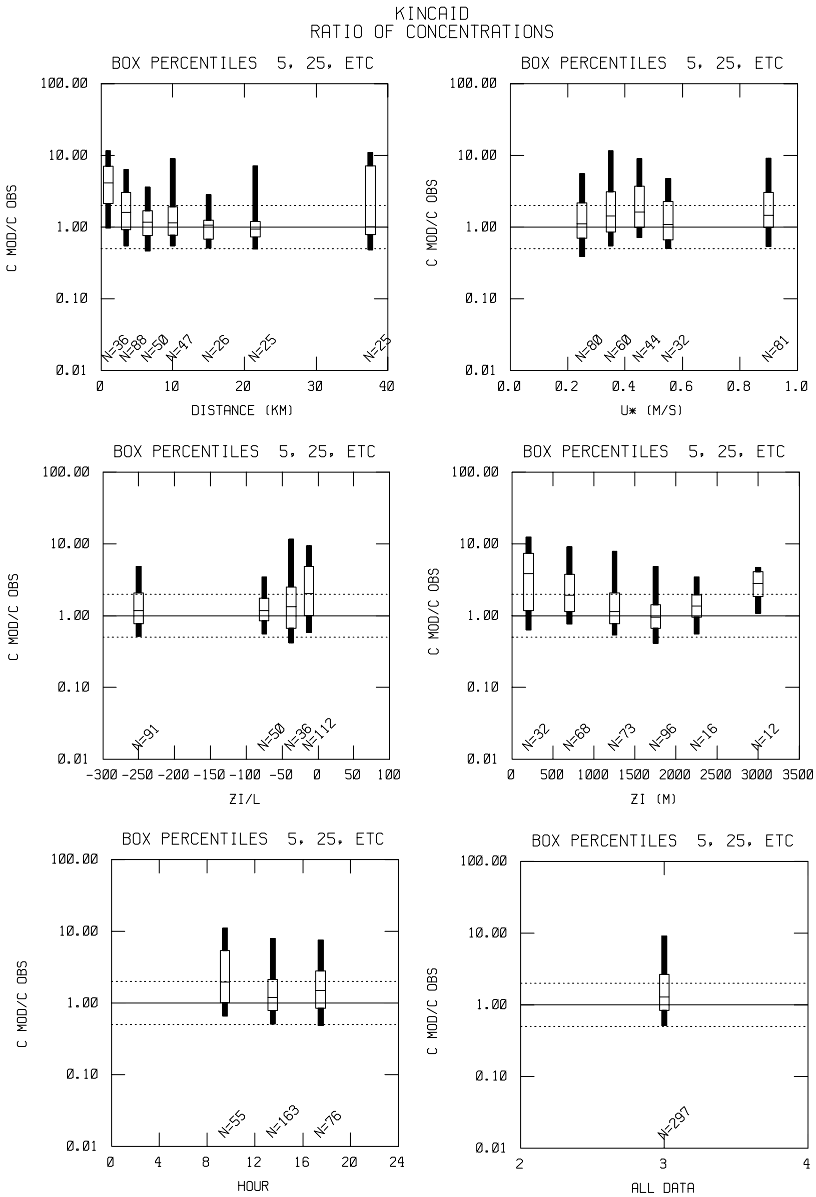

Fig. 4. Residual box plots for old plume rise using quality 3 data.

Table 4
Performance statistics from atmospheric dispersion model assessments using Kincaid data of quality 3. (Concentrations are normalised by the emission rate, Q, in keeping with the protocol recommended with the model validation kit)

Model	Mean	σ	Bias	NMSE	r	FB	FS	FA2
Observations	54.34	40.25	0.00	0.00	1.000	0.000	0.000	1.000
HPDM	44.84	38.55	9.50	0.75	0.441	0.192	0.043	0.565
OML	47.45	45.48	6.89	1.24	0.146	0.135	−0.122	0.547
ADMS 3	51.7	34.7	2.7	0.6	0.45	0.05	0.15	0.67
AERMOD	21.8	21.8	32.6	2.1	0.40	0.86	0.59	0.29
ISCST3	30.0	60.0	24.3	2.8	0.26	0.58	−0.39	0.28
NAME	40.6	40.4	13.8	1.15	0.279	0.290	−0.005	0.615

It is likely that the performance of NAME could be improved by tuning model parameters and/or alternative pre-processing methods of the meteorological data. However, no tuning has been undertaken in this study because tuning to a single data set is felt to be inappropriate. This is particularly true in this case since the Kincaid experiment was conducted in the US and the data set is biased towards unstable conditions. NAME, however, is used for mainly UK purposes over a range of stability conditions.

8. Conclusions

The conservation equations of mass, momentum and heat used by ADMS to calculate plume rise have been introduced successfully into a Lagrangian particle model framework. The new scheme has many advantages over the original scheme which calculated plume rise using formulae by Briggs. Since the Briggs-type formulae are particular solutions of the more general conservation equations, the new scheme is able to cater for a wider range of meteorological conditions. It also enables the entrainment of ambient air to be modelled throughout the plume rise process and consequently the effect on the plume of the inversion at the top of the boundary layer will be more realistically modelled.

Despite insufficient available meteorological data, NAME has been successfully assessed against the Kincaid data set. This validation work has shown that the new plume rise scheme is superior to the old scheme. The new scheme handles well a variety of meteorological conditions although the Kincaid data set does not enable the testing of the new scheme against very stable conditions. Unlike the original scheme, the new scheme residuals show very little, if any, systematic dependence on stability and downwind distance. For observational data of quality 3, the performance of the new plume rise scheme is good.

Data from other model validation exercises using the Kincaid data set has been used to compare the performance of NAME with other atmospheric dispersion models. We conclude here that, with the new plume rise scheme, NAME, which historically has been a medium to long-range model, is on a par with other models at short ranges.

It would be of interest to assess how much the results presented here are impacted by the pre-processing of the meteorological data. Therefore, it is intended, in the future, to investigate the use of European Centre for Medium range Weather Forecasting meteorological data with the Kincaid experiment data set. In view of the difficulty in estimating boundary layer depth from radiosondes alone, it would also be of interest to assess the performance of NAME against the Kincaid data set using boundary layer depths calculated using the model's own meteorological pre-processor or those determined by other pre-processors. It should also be noted that validation of the plume rise scheme in stable conditions has not yet been done. This would complete the validation work if suitable data sets could be identified. In addition, it would be appropriate to assess the sensitivity of model predictions on the values chosen for the entrainment and drag coefficients.

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