Mathematical modelling of aerosol transport and deposition: Analytic formulae for fast computation

Robert McKibbin

Follow this and additional works at: https://scholarsarchive.byu.edu/iemssconference

https://scholarsarchive.byu.edu/iemssconference/2008/all/230

This Event is brought to you for free and open access by the Civil and Environmental Engineering at BYU ScholarsArchive. It has been accepted for inclusion in International Congress on Environmental Modelling and Software by an authorized administrator of BYU ScholarsArchive. For more information, please contact scholarsarchive@byu.edu, ellen_amatangelo@byu.edu.
Mathematical modelling of aerosol transport and deposition: Analytic formulae for fast computation

Robert McKibbin

Institute of Information and Mathematical Sciences, Massey University at Albany,
Private Bag 102 904, North Shore Mail Centre, Auckland, New Zealand (r.mckibbin@massey.ac.nz)

Keywords: Modelling; Advection-dispersion; Particle transport; Deposition; Hazards.

Solid and liquid particles (aerosols) ejected into the atmosphere by volcanic or hydrothermal eruptions, dust and sand swept up by storms or from other pollution sources, and droplets from crop-spraying, are subsequently dispersed by atmospheric wind currents. The particles fall under gravity while being advected by the mean wind and dispersed by turbulence. Particle sizes are generally not uniform, and may also change during flight (perhaps by particle coalescence and/or fragmentation, or, in the case of fluids, by evaporation or condensation) with consequent change to the settling speed. The wind may also change with elevation (and with time) and particles may be trapped on crop or forest foliage as they near the ground.

A quantitative model that reflects these influences on particle dispersal is outlined. It is assumed that the wind does not change over the time of particle flight, and that there is no change of particle size due to evaporation or condensation. However, the other elevation-dependent features listed above are included. Changes of conditions with elevation are treated by using a piecewise-constant wind velocity, associated dominant turbulence length scale, settling speed and trapping rates. In any case, this is the way that data are provided for most of the numerical schemes currently available. When the vertical dispersion is assumed negligible (as is commonly supposed in such modelling), analytic solutions to the advection-dispersion equations that describe the motion of the particles may be found. Results calculated directly from the analytical formulae provide examples of the method.

1. INTRODUCTION

When particles are released in the atmosphere, perhaps from volcanic eruption columns, sand or dust storms, dust pollution sources, crop-spraying, aerial top-dressing or pollen from trees, they are generally blown by the wind while falling through the air as well as being dispersed by the wind's turbulence. Particles that fall through air that has been polluted by toxic gaseous discharges from industrial processes, may adsorb chemicals which are then present in the deposits of the particles on the ground. While the paths of individual particles may be of interest, it is usually the density of the eventual distribution of the fallout on the ground that is more important. In particular, being able to predict and estimate of the thickness of volcanic ashfall deposits or chemically-polluted dust is of most value to health and safety agencies which use such information for hazard maps.

Estimation of the characteristics of the wind during any event is essential in the modelling exercise. Meteorological measurement equipment is unlikely to give more than information about average wind-speed and direction at a sequence of elevations, so any model should be able to use that information, but no more than that. The model proposed in this paper is based on dividing the atmospheric wind-flow into a sequence of layers, within each of which the speed and direction are known layer-averaged values. It
generalises previous models where the particle settling speeds remain constant, and/or the dispersion is assumed isotropic (for example, see Bonadonna et al. [2002]; Lim, [2006]), and includes trapping by foliage.

Early models assumed uniform wind conditions and particle sizes (for a summary, see Lim [2006]). More recently, papers by Bonadonna et al. [2005] and Costa et al. [2006], amongst others, discuss settling speed calculations that take into account air density variation with elevation as well as the effect of non-sphericity of the particles. Particle sizes from discharges or releases are generally not uniform initially, and may change during flight, either by particle coalescence and/or fragmentation, or, in the case of liquid droplets, by evaporation or condensation, with consequent changes to the settling speed. The wind (speed, direction and dominant turbulence length scales) may also change with elevation (and with time, although not considered here). The inclusion of appropriate sink terms in the conservation equations allows for modelling the trapping of some particles on forest, orchard, crop or windbreak foliage (see, for example, McKibbin [2006a]; Harper et al. [2007]). This aspect is important in agriculture and horticulture, where spray drift onto nearby areas may be a health hazard. Predictions of deposits of tephra ejecta from volcanic (and hydrothermal eruptions: see McKibbin et al. [2005], McKibbin [2006b]) are useful for scenario-planning by civil defence organizations.

Results calculated directly from the derived analytical formulae are used to provide examples of the method. The new formulae allow extremely fast direct computation of deposit distributions. Because of this, fine discretizations of release zones, non-uniform wind profiles and ejected particle size distributions can be made with little computation cost. Space precludes much detail; only a summary of the method and some aspects of its implementation can be given here.

2. MATHEMATICAL MODEL FORMULATION

It is reasonably assumed that the air is of uniform density and that its motion is not affected by the small volume fraction of particles present. A Cartesian coordinate system is arranged so that the x-y plane is the ground and the z-axis is vertical upwards. The mean (locally time-averaged) mass concentration of particles per unit volume of the atmosphere is denoted \( C(x, y, z, t) \), and the principle of conservation of mass of the solid phase yields

\[
\frac{\partial C}{\partial t} = -\nabla \cdot \mathbf{q} + m_s - m_t
\]

(1)

where \( \mathbf{q} \) is the particle mass flux per unit cross-sectional area, \( m_s \) is a mass source term (mass rate per unit volume) and \( m_t \) is a mass removal term due to trapping, such as by foliage in a forest canopy or a crop. The specific mass flux has advection, dispersion and settling components, in the form:

\[
\mathbf{q} = \mathbf{Cu} - \mathbf{D} \otimes \nabla C - CSk
\]

(2)

where \( \mathbf{u} = (U, V, 0) \) is the mean (horizontal) wind velocity vector, with mean wind speed \( W = \sqrt{U^2 + V^2} \). The particles are small, and are assumed to have quickly reached their average terminal velocity \( \mathbf{u} - Sk = (U, V, -S) \) with respect to the mean motion of the air, where \( S \) is the particle gravitational settling speed in the downward direction (\( \mathbf{k} \) is a unit vector in the positive z-direction). The turbulence in the atmosphere is assumed to cause mechanical dispersion of the particles; \( \mathbf{D} \) is the dispersion tensor, which may be written in the form \( \mathbf{D} = W\mathbf{L} \) in terms of mean wind speed and a dispersion length tensor which involves characteristic dominant length scales of the atmospheric turbulence. This pragmatic model assumes a simple form where the dominant principal dispersion lengths are assumed horizontally constant, but not necessarily isotropic; this leads to Gaussian-type profiles with spreads that are directly calculable from the parameters and elapsed time (to which can be related explicitly the distance fallen and/or mean horizontal distance travelled).
For the case of a release of a mass \( Q \) of particles at point \((X_0, Y_0, H)\) above the ground at time \( t = 0 \), the mass source \( m_i \) may be written using Dirac delta functions in the form

\[
m_i = Q \delta(x - X_0) \delta(y - Y_0) \delta(z - H) \delta(t)
\]

Distributed releases may be composed by superposing suitable combinations of such sources (see further below). The trapping term, considered to be proportional to the particle concentration \( C \), is assumed to be of the form

\[
m_i = k(x, y, z)C
\]

where the trapping rate \( k(x, y, z) \), which is zero outside any trapping zone, is \{mass of particles trapped per unit volume of the trapping region, per unit time\}/\{mass of particles present per unit volume of the trapping region\}; in SI units, [\( k \)] = \( s^{-1} \). In general, \( k \) will depend on the foliage characteristics and the particle type and size, and possibly the wind speed (Mercer & Roberts [2005]).

It is assumed here that, in the case of fluid droplets, there is no particle mass change due to evaporation or condensation. If so, rather than include a mass loss term due to evaporation in (1), it may be better to use a particle number concentration \( N \) rather than a particle mass concentration \( C \). Earlier work on droplet trapping by agricultural shelterbelts is reviewed in, for example, Harper et al. [2006, 2007], and the inclusion of evaporation is comprehensively discussed in Harper [2008]. Solid or liquid particles may agglomerate at levels where such agglomeration occurs.

Substitution of expressions (2) – (4) into (1) and some rearrangement gives:

\[
\frac{\partial C}{\partial t} + \nabla \cdot \left( (\mathbf{u} - \mathbf{D}) \otimes \nabla C - C \mathbf{S} \mathbf{k} \right) = Q \delta(x - X_0) \delta(y - Y_0) \delta(z - H) \delta(t) - kC. \tag{5}
\]

For a horizontal wind, the dispersion tensor is taken to be of the form:

\[
\mathbf{D} = \begin{bmatrix} D_{xx} & D_{xy} & 0 \\ D_{yx} & D_{yy} & 0 \\ 0 & 0 & D_{zz} \end{bmatrix},
\]

which is a symmetric tensor of order 2. If the wind direction is at angle \( \theta \) to the x-axis (i.e. \( U / W = \cos \theta, V / W = \sin \theta \)), and the longitudinal (downwind) and transverse (crosswind) dispersion coefficients are \( D_x \) and \( D_y \) respectively (allowed to be different here, but assumed the same in previous studies), then the dispersion tensor has the form:

\[
\mathbf{D} = \begin{bmatrix} D_x \cos^2 \theta + D_y \sin^2 \theta & (D_x - D_y) \sin \theta \cos \theta & 0 \\ (D_x - D_y) \sin \theta \cos \theta & D_x \sin^2 \theta + D_y \cos^2 \theta & 0 \\ 0 & 0 & D_{zz} \end{bmatrix}.
\]

(Note that if the dispersion is isotropic, \( D_x = D_y \) and \( \mathbf{D} \) is a diagonal matrix.) If the settling speed, the mean wind speed and direction, as well as the turbulent dispersion, vary with elevation, then \( S = S(z) \), \( U = U(z) \), \( V = V(z) \) and \( \mathbf{D} = \mathbf{D}(z) \), and (5) can be written:

\[
\frac{\partial C}{\partial t} + U(z) \frac{\partial C}{\partial x} + V(z) \frac{\partial C}{\partial y} - S(z) \frac{\partial C}{\partial z} = \frac{dS}{dz} C
\]

\[
= D_{xx}(z) \frac{\partial^2 C}{\partial x^2} + 2D_{xy}(z) \frac{\partial^2 C}{\partial x \partial y} + D_{yy}(z) \frac{\partial^2 C}{\partial y^2} + D_{zz}(z) \frac{\partial^2 C}{\partial z^2} + \frac{dD_{zz}}{dz} \frac{\partial C}{\partial z} + Q \delta(x - X_0) \delta(y - Y_0) \delta(z - H) \delta(t) - k(x, y, z)C. \tag{6}
\]
In general, this equation has no analytical solutions, and usually a full-scale numerical approach is necessary for finding the concentration \( C \) and consequent deposits.

However, for the case where the vertical dispersion is small compared to other components, as is often proposed by other authors (for example, see Bonadonna et al. [2002]) for regions not very close to the ground, and the elevation-dependent profiles of wind characteristics and particle settling speeds are approximated by piece-wise (layer-wise) constant functions, then concentrations and deposits can be found as explicit analytic solutions. Fast direct computation is then possible without problems associated with accuracy and stability of spatial and temporal discretization schemes.

3 SOLUTIONS FOR THE PARTICLE CONCENTRATION

When the vertical dispersion \( D_{zz} \) is assumed negligible, and the wind and settling parameters are piecewise constant functions of elevation, it is possible to find analytic solutions for (6) with appropriate initial and boundary conditions. First, the solution for a single uniform layer is described, and then it is used to find the analytical solution for the general case.

3.1 Uniform atmosphere

A mass \( Q \) of particles with constant settling speed \( S \) is released at time \( t = 0 \) from a height \( H \) into a steady, uniform, horizontal wind of speed \( W \) (a constant), with constant dispersion coefficients and a uniform trapping parameter \( k \). A set of Cartesian coordinate axes \((x, y, z)\) is aligned so that the mean wind is in the positive \( x \)-direction, so \( u = (W, 0, 0) \), and the origin (take \( x_0 = y_0 = 0 \) for clarity) is directly below the point of release. Then (6), with associated initial and boundary conditions becomes:

\[
\frac{\partial C}{\partial t} + W \frac{\partial C}{\partial x} - S \frac{\partial C}{\partial z} = D_z \frac{\partial^2 C}{\partial x^2} + D_T \frac{\partial^2 C}{\partial y^2} + Q \delta(x) \delta(y) \delta(z - H) \delta(t) - kC
\]  

(7)

\(C(x, y, z, 0) = 0; \ C \to 0 \) as \( x, y \to \pm \infty, z \to +\infty\).

The concentration at time \( t \) after release can be found using a standard solution procedure involving Laplace and Fourier transforms, and is given by:

\[
C(x, y, z, t) = \frac{Q}{4\pi \sqrt{D_z D_T}} \exp \left[ -\frac{(x - Wt)^2}{4D_z t} - \frac{y^2}{4D_T t} \right] \exp(-kt) \delta(z - (H - St)).
\]  

(8)

The concentration in the atmosphere is zero except at the level \( z = H - St \); the particles fall steadily with speed \( S \), while spreading out in the \( x \)- and \( y \)-directions as time increases. The centre of mass moves at speed \( W \) in the \( x \)-direction and at speed \( S \) in the negative \( z \)-direction. The particles arrive at the ground at time \( t_1 = H/S \). The mass density \( f(x, y) \) of the deposit on the ground is given by integrating the downward mass flux there:

\[
f(x, y) = \frac{\tilde{z}}{0} SC(x, y, 0, t) dt = \frac{Q}{4\pi \sqrt{D_z D_T t_1}} \exp \left[ -\frac{(x - Wt_1)^2}{4D_z t_1} - \frac{y^2}{4D_T t_1} \right] \exp(-kt_1)
\]  

(9)

This deposition density \([f] = \text{kg m}^{-2} \) in SI units) has elliptical level surfaces (contours), centred on the point \((Wt_1, 0, 0)\). If \( k \neq 0 \), the distribution of the particles trapped in the foliage (in kg m\(^{-2}\)) may be calculated explicitly (see McKibbin [2006a]). The total amount trapped is \( Q_{Tz} = Q(1 - e^{-Wt_1/S}) \); this leaves an amount \( Q_D = Q - Q_{Tz} = Q e^{-Wt_1/S} \) distributed on the ground. Note that, interestingly, these total amounts do not depend on the wind speed or the dispersion parameters. Spatially-distributed trapped amounts are easily calculated – see McKibbin [2006a].
3.2 Layered atmosphere

In a system where the atmosphere is divided into $n$ superposed layers, the solution above describes the motion of the particles in the layer in which they are released. If this region is labelled Layer 1, occupying $Z_i < z \leq Z_n$ where $Z_n \geq H$, the particles all reach the bottom of the Layer 1 (= the top of Layer 2) at time $t = t_1 = (H - Z_n) / S_1$. The particles then form a horizontally-dispersed mass source at the top of Layer 2. Because the wind in Layer 2 may be moving in a different direction to that of Layer 1, the coordinate system is rotated for Layer 2 so that the wind is in the positive "x"-direction in that layer.

The procedure is as follows. The wind direction and hence the positive "x"-coordinate axis in the system in Layer $i$, $1 \leq i \leq n$, is rotated at an angle $\theta_i$ to the global coordinate system $(x,y,z)$, and is labelled $(X_i,Y_i,z)$. The coordinate systems are related by:

$$
\begin{align*}
X_i &= x \cos \theta_i + y \sin \theta_i \\
Y_i &= -x \sin \theta_i + y \cos \theta_i
\end{align*}
$$

The wind speed, settling speed, dispersion and trapping coefficients may vary with elevation, and so are subscripted accordingly. At time $t = t_1 = (H - Z_n) / S_1$, the particles arrive at the top of Layer 2 with an areal density distribution given by:

$$
f(X_1,Y_1) = \frac{Q}{4\pi \sqrt{D_{11} D_{12} t_1}^2} \exp \left[ -\frac{(X_1 - W_1 t_1)^2}{4D_{11} t_1} - \frac{Y_1^2}{4D_{12} t_1} \right] \exp(-k_1 t_1)
$$

The $(X_i,Y_i,z)$ coordinate system is aligned at angle $\theta_i$ to the $(X_2,Y_2,z)$ system. A small element of mass source at $(X_2,Y_2,z) = (\xi,\eta,Z_i)$ at time $t_i$ is given from (11) by

$$
dQ = f(\xi,\eta) d\xi d\eta = \frac{Q}{4\pi \sqrt{D_{21} D_{22} t_1}^2} \exp \left[ -\frac{|\xi \cos(\theta_i - \theta_2) + \eta \sin(\theta_i - \theta_2) - W_1 t_1|^2}{4D_{21} t_i} \right. \\
&\quad \quad \left. -\frac{|-\xi \sin(\theta_i - \theta_2) + \eta \cos(\theta_i - \theta_2)|^2}{4D_{22} t_i} \right] \exp(-k_1 t_1) d\xi d\eta
$$

The total effect of all source elements on the particle concentration in Layer 2 is found by integration of all the small source elements $dQ(\xi,\eta)$ at $(\xi,\eta,Z_i)$ given by (12).

The particle concentration in Layer 2 is then given by:

$$
C(X_2,Y_2,z,t_i) = \int_{\xi=0} \int_{\eta=0} dQ = \int_{\xi=0} \int_{\eta=0} \frac{dQ}{4\pi \sqrt{D_{11} D_{12} t_1}^2} \exp \left[ -\frac{(X_2 - \xi - W_2 (t - t_1))^2}{4D_{12} (t - t_1)} - \frac{(Y_2 - \eta)^2}{4D_{22} (t - t_1)} \right] \exp(-k_2 t_2) \\
\times \delta[z - (Z_i - S_2 (t - t_i))]
$$

Some algebraic manipulation and use of standard integration formulae gives a compact and explicit expression for $C$ at a given position and time, in terms of the various parameters. Proceeding via the same process from layer to layer downwards allows calculation of the concentration within all layers, and thereby the distribution of the deposit on the ground (the bottom of Layer $n$, say, which is at $z = 0$).

The general results for the areal mass distribution at the bottom of any Layer $i \geq 2$ are presented now. Taking $t_0 = 0$, the cohort of particles falls through Layer $i$ between the times $t_{i-1}$ and $t_i$ which, respectively, correspond to their arrival at the top and bottom of that layer. The times may be calculated from:
Note that $Z_{i+1} > Z_i$; the layers are numbered from the top downwards. The areal mass density at the bottom of Layer $i$ (at the level $z = Z_i$) is given by:

$$f(X_i, Y_i, Z_i) = \frac{Q}{4\pi \sqrt{\Delta_i(t_i)}} \exp \left[ -\frac{\sigma_i(t_i)}{4\Delta_i(t_i)} - K_i(t_i) \right], \quad (13)$$

where

$$\sigma_i(t_i) = \sum_{j=1}^{i} (t_j - t_{j-1}) \left\{ D_{ij} \left[ X_j - \sum_{k=1}^{j} W_j(t_k - t_{k-1})c_{ij} \right]^2 + D_{ij} \left[ Y_j - \sum_{k=1}^{j} W_j(t_k - t_{k-1})s_{ij} \right]^2 \right\} \quad (14)$$

with

$$c_{ij} = \cos(\theta_i - \theta_j), \quad s_{ij} = \sin(\theta_i - \theta_j),$$

and the $\Delta_i(t_i)$ are given recursively by the formulae:

$$\Delta_i(t_i) = D_{i1} D_{i1} t_i^2, \quad \Delta_i(t_i) = \Delta_{i-1}(t_{i-1}) + (t_i - t_{i-1}) \sum_{j=1}^{i-1} (t_j - t_{j-1}) P_{ij} + (t_i - t_{i-1})^2 D_{ij} D_{nj} \quad \text{for } i \geq 2,$$

where

$$P_{ij} = s_{ij}^2 (D_{ij} D_{ij} + D_{nj} D_{nj}) + c_{ij}^2 (D_{ij} D_{ij} + D_{ij} D_{ij}).$$

Also,

$$K_i(t_i) = \sum_{j=1}^{i} k_j (t_j - t_{j-1}).$$

The above results are for mass distributions at the bottom of the various layers; formulae for mass fluxes at elevations between layer boundaries are similar in form. If the horizontal dispersion is isotropic ($D_{ij} = D_{nj}$) and there is no trapping ($k_i = 0$), the resulting formulae agree with those given by Lim [2006]. If the dispersion is isotropic and uniform over all elevations ($D_{ij} = D_{nj} = D$) and $k_i = 0$, then the results agree with those given by Bonadonna et al. [2002]. The deposit on the ground (at the bottom of Layer $n$) is given by (13) for $i = n$ at $Z_n = 0$. Note: the $(X_i, Y_i)$ in (14) are given in terms of ground coordinates $(x, y)$ by (10).

## 4. ESTIMATION OF PARAMETERS

The various parameters describing the wind speed and direction, the dominant turbulence length scales and particle settling speeds, all need to be reliably estimated. Wind mean speeds may be found from meteorological simulations or measured data. Particle settling speeds are available from correlations constructed from laboratory experiments.

**Turbulence length scales** – The model above assumes that the particles are spread by mechanical dispersion, caused by the turbulence in the air motion. The turbulence, caused by the wind, varies with height and in part this can be attributed to gradients in wind speed. At a given height, turbulence within the airflow is modelled as having a certain characteristic length; since turbulence has a variety of scales, the length is a typical mean value for the flow. The effect of air turbulence is incorporated using a dispersion tensor $\mathbf{D}$ whose components are constant within each layer.

Experimental observations of turbulence have suggested that the effective dispersion tensor changes with the scale of the dispersing plume. This is not allowed for by Gaussian dispersion in its simplest form. In particular, in an early paper, Sutton [1932] attempts to model dispersion using an empirical formula wherein the effective dispersion rate is given by a fractional power of the distance travelled. Essentially, by implication, this will mean having a dominant length scale that evolves with time. Pasquill [1961] also comments that it is not unreasonable to, locally with respect to height and time, assume a near steady homogeneous structure. His model also allows for a change in length scale with time due
to the spread of the release. Such effects are not excluded from the model of this paper. The particle release falls downwards and so, as the dispersion length scale and velocity constants are varied with height, this effectively allows for changes with time.

**Release/emplacement heights** – If a cohort of particles is released into the air by controlled means (such as from chimney stacks, aerial top-dressing, spraying machines, etc.) then the physical source position is known. In geophysical events such as dust- or sand-storms, or volcanic eruptions, release positions have to be estimated. Estimates of volcanic plume heights, distribution of ash releases from plumes and similar considerations may be found in the volcanological literature – see, for example, Sparks et al. [1997], McKibbin & Smith [2006], Lim et al. [2008a], Bonadonna et al. [2005], Costa et al. [2006]. A brief discussion about plume-type volcanic eruptions is given here.

The collective term for all particles ejected from volcanoes is *tephra*. There are many eruption types, depending on magma composition (rock type), topography, vent history, etc. One event may include several different eruption types (multiple plumes, explosions, dome collapse, pyroclastic flows, etc.); see, for example, Sparks et al. [1997]. The model presented above for particle deposition may be applied to thermally-bouyant plumes of hot gases which lift rock particles of various composition from the eruption site high into the atmosphere, while entraining and heating air. In this process, the plume slows and cools, eventually reaching a maximum height where it spreads laterally. As it slows, the vertical plume speed reduces from the ejection speed \(v_0\) at the eruption vent down to zero at the top of the plume. Observed plume heights of eruptions can be used to estimate the total mass erupted through correlations; e.g., for Plinian eruptions, Carey & Sigurdsson [1989] give:

\[
\log_{10}(M) = \frac{H_{\text{max}} + 60.5}{7.18}
\]

where \(M\) is the total mass released (kg) and \(H_{\text{max}}\) is the maximum observed column height (km).

Treating the column as a vertical line source, at least two approaches can be made to estimate the height at which tephra particles of a certain size are released into the atmosphere. One is from McKibbin & Smith [2006] who calculated the dynamics and shape of entraining plumes using a simplified model, and observed that the calculated vertical speed declined approximately linearly with height above the vent. This allows an estimate of the elevation \(H_s\) at which the plume speed is equal to the settling speed \(S_d\) of a cohort of particles with diameter \(d\). Since the vertical plume speed \(v\) as a function of height \(z\) is given approximately by \(v/v_0 = 1 - z/H_{\text{max}}\), the release height may be estimated by:

\[
H_s = H_{\text{max}} \left(1 - \frac{S_d}{v_0}\right)
\]

An alternative is to use the so-called Suzuki distribution [Suzuki, 1983], which gives a formula for the release density distribution \(\zeta(z)\) of a mass of particles over the total plume height \(0 \leq z \leq H_{\text{max}}\). In terms of the notation used here, the traditional form contains the Suzuki constant \(A\):

\[
\zeta(z) = \frac{A^2}{H_{\text{max}} \left[1 + (A - 1)\exp(-A)\right]} \left(1 - \frac{z}{H_{\text{max}}}\right) \exp\left[-A\left(1 - \frac{z}{H_{\text{max}}}\right)\right]
\]

which has the property that

\[
\int_0^{H_{\text{max}}} \zeta(z) dz = 1
\]

Here the constant has some fixed value \(A \geq 1\), and the maximum density of particle release is at \(z = H_{\text{max}}(1 - 1/A)\). A typical value is \(A = 5\), to give the maximum release at 0.8\(H_{\text{max}}\). However, having fixed the value of \(A\), all particle sizes have the same release distribution up the column.
Perhaps a better approach is to combine the two options above. Note that comparing (16) and the maximum height from the standard Suzuki distribution, the role of \( A \) may be taken by the ratio \( v_0/S_d \). It is reasonable that the maximum release density of a certain size cohort of particles be approximately at the level where the plume speed is the same as the settling speed, i.e., where the particles have neutral buoyancy, and where they may fall out of the plume into the surrounding atmosphere. Substitution for \( A \) into (17) gives:

\[
\zeta_i(z) = \frac{\left(\frac{v_0}{S_d}\right)^2}{H_{max}} \left(1 + \left(\frac{v_0}{S_d} - 1\right) \exp\left(-\frac{v_0}{S_d}\right)\right) \left(1 - \frac{z}{H_{max}} \exp\left(-\frac{v_0}{S_d}\left(1 - \frac{z}{H_{max}}\right)\right)\right) \tag{19}\]

Use of (19) allows each particle size cohort to have its own Suzuki distribution, based on the relevant settling speed. For computation, the line source is partitioned into \( N \) equal sub-intervals \( \{p \Delta z, p \Delta z\} \), \( p = 1, \ldots, N \), each of length \( \Delta z = H_{max}/N \), with corresponding Suzuki density values \( \zeta_i ((p - \frac{1}{2}) \Delta z) / \sum_{i=1}^{N} \zeta_i ((k - \frac{1}{2}) \Delta z) \). Note the normalization to ensure that the discretized distribution has a sum of unity, to maintain the condition (18).

**Particle sizes and settling speeds** – From geological records, volcanic deposits consist of a variety of particle sizes. Their particle size compositions are commonly estimated by sieving a sample, and retrieving size data in the form of \( \phi \) values, which are related to particle diameters by \( d = 2^{-\phi} \) or \( \phi = -\log d \) where \( d \) is measured in mm; a diameter of \( d = 1 \text{ mm} \) corresponds to \( \phi = 0 \). Particles with large diameter \( d \) have small \( \phi \) values and vice versa. Reported results of such sieving are usually stated as a set of data giving either absolute masses or volumes, or sample fraction masses or volumes, of each cohort for integral \( \phi \) values – for typical examples, see Bonadonna et al. [2002]. This distribution is therefore not continuous, but represents a set of "bundled" data for a cohort of particles that are smaller than a certain standard sieve diameter but larger than the next (smaller) size with half the diameter of the first. Diameters \( d \) of particles in the cohort with \( \phi = i \) (\( i \) is an integer) are constrained by \( 2^{-i} < d \leq 2^{-(i+1)} \). The data is therefore coarse, rather than continuous as the sizes in a typical sample are.

One way to deal with this is to use a set of splines, i.e. piecewise continuous smooth functions which connect smoothly (value and slope) at the "knots" \( \phi_i \) and take zero values at the end-points of the data set. Also, for the cohort \( \phi = i \), where the interpolating distribution function is given by \( g(\phi) \), it is required that

\[
\int_{\phi_i}^{\phi_{i+1}} g_i(\phi) d\phi = m_i, \tag{20}\]

where \( m_i \) is the data value [mass or volume (or fraction of either of the total sample)] for that cohort. Quadratic splines are suitable as they require exactly the number of conditions given above.

The smoothed set of data can then be divided as finely as one wishes to use as a set of narrowly-sized cohorts, each with an appropriate settling speed. In this way, a mass release can be modelled as a set of smaller releases, each cohort having similar diameters and hence settling speeds. The deposits from each of these cohorts can be calculated directly from the formulae above and superposed to give the total deposit density at any point on the ground, and, knowing the trapping propensity for differently-sized particles, to calculate the amount left behind on foliage.

The issues of estimating settling speed are discussed by, for example, Bonadonna et al. [2005] and Costa et al. [2006]. It depends on the mass, size and shape of an individual particle, as well as on air density; a suitable correlation that includes the variation of air density with elevation can be easily implemented in the current layered model.
5. EXAMPLES

Because of space restrictions, only two examples can be presented here. The first, in an aerial top-dressing setting, is to illustrate how point sources can be analytically superposed by calculus methods before calculation of deposits. The second illustrates the use of volcanic tephra fallout (ashfall) data to compute ground deposits using the layered-atmosphere model.

**Horizontal line source** – If mass \( Q \) is released uniformly along a straight line between two points of equal height, the total deposit is the sum of deposits of infinitesimal releases along the line; an analytic formula may be found by analytic integration.

From (9), the ground deposit from a mass release \( Q \) from \((X_0,Y_0,H)\) at \( t = 0 \) into a uniform wind of speed \( U \) in the \( x \)-direction, with no trapping, is given by

\[
f(x,y) = \frac{Q}{4\pi \sqrt{D_L D_T t_1^2}} \exp \left[ - \frac{(x-X_0-U t_1)^2}{4 D_L t_1} - \frac{(y-Y_0)^2}{4 D_T t_1} \right]
\]

where \( t_1 = H/S \), and \( S \) is the settling speed. If \( Q \) is now released uniformly along a straight line between \((X_a,Y_a,H)\) and \((X_b,Y_b,H)\), the total deposit is the sum of deposits of infinitesimal releases along the line \((X_a,mX_a+c,H)\) [where \( m = (Y_b - Y_a)/(X_b - X_a) \) and \( c = Y_a - mX_a \)], and is given by:

\[
f_{\text{line}}(x,y) = \int_{x_a}^{x_b} \frac{Q}{4\pi \sqrt{D_L D_T t_1^2}} \exp \left[ - \frac{(x-X_0-U t_1)^2}{4 D_L t_1} - \frac{(y-mX_a - c)^2}{4 D_T t_1} \right] \, dX_a
\]

where

\[
A = \frac{1}{4 D_L t_1} + \frac{m^2}{4 D_T t_1}, \quad B(x,y) = \frac{x-U t_1}{2 D_L t_1} + \frac{m(y-c)}{2 D_T t_1}, \quad C(x,y) = \frac{(x-U t_1)^2}{4 D_L t_1} + \frac{(y-c)^2}{4 D_T t_1}
\]

\[
\alpha(x,y) = \frac{B}{2A}, \quad \beta(x,y) = C - \frac{B^2}{4A}
\]

A suitable modification can be made in the case where \( X_b = X_c \).

In Figure 1, an example where four flight passes are made at an elevation of 200 m, while a 20 m s\(^{-1}\) wind blows from the West; dispersion lengths are taken to be 1 m (dispersion parameters 20 m\(^2\) s\(^{-1}\)), with a particle settling speed of 10 m s\(^{-1}\). The dashed lines are a plan view of the aeroplane’s path while the release is occurring and the contour lines are at intervals of 10 % of the maximum deposit.

Other examples of combining point sources to form a vertical line source and a horizontal disk are provided in Lim et al. [2008b].

**Volcanic ashfall** – Hurst [1994] gave a set of wind and mass release data (titled EX401) which he used for a demonstration of ASHFiLL, a program that calculates estimates of volcanic fallout (tephra deposits) from a vertical ash plume. Input data included the wind speeds and directions over various height intervals, the masses and settling speeds of particle size cohorts, horizontal diffusion (= dispersion) coefficients (with assumed horizontal isotropy), and a Suzuki constant \( (A = 5) \). This data set serves as a good test of the parity of predictions from Hurst’s numerical simulation (which used a finite-difference, time-stepping procedure) and the method described here, where the calculation is direct.
Figure 1. Contours of the deposit from a sequence of aerial top-dressing passes in a wind from the West. Dashed lines are plan views of release paths. See text for parameter values.

The method of this paper produces the contours of ashfall thickness (in mm) as shown in Figure 2. The agreement with the simulation contour plot given by Hurst [1994, Fig. 5] is very good.

Figure 2. Left: Calculated contours of ashfall thickness using the method of this paper. Right: Hurst's [1994, Fig. 5] contour plot. Both are for Hurst's data set EX401.

6. SUMMARY

A mathematical model that allows estimation of deposit distributions from releases of particles in the atmosphere has been described. The solution for a mass release from a single point can be used as a building block for distributed sources, either analytically for some simple geometries such as uniform release along a straight line, or as non-uniform releases in any arrangement by superposition of discrete events. Calculation is by direct evaluation of analytic formulae, so no decisions have to be made about convergence or stability, such as must be considered in numerical solutions of differential equations. Good results rely on satisfactory estimation of the parameters arising in the formulae. Wind conditions, particle sizes and positions of their release, and the trapping characteristics of foliage, all need to be available. However, because the formulae are explicit, the sensitivity with respect to variation of the parameters is readily explored without the re-meshing usually required in numerical schemes. Consideration of the effects of inclusion of vertical dispersion near the ground, the evaporation or condensation of liquid droplets, and appropriate turbulence length scales in forest canopies is continuing.
REFERENCES


