Sensitivity Analysis of Surface Deposition in a Numerical Model of Atmospheric Dispersion

Jackie Lewis
Utah Career College

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SENSITIVITY ANALYSIS OF SURFACE DEPOSITION IN A
NUMERICAL MODEL OF ATMOSPHERIC DISPERSION

by

Jackie Lewis

A thesis submitted in partial fulfillment of the requirements for the degree of
MASTER OF SCIENCE
in
Physical Ecology
(Biometeorology)

UTAH STATE UNIVERSITY
Logan, Utah

1976
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The Utah Agricultural Experiment Station supported this research under project 00403. My gratitude is extended to Dr. Gene Wooldridge for arranging for my support and for his guidance and patience during the course of this study. I want to thank Dr. Inge Dirmhirn and Dr. James MacMahon for serving on my committee. My thanks go to Betty Smith for typing the manuscript and Joy Call for her help in preparing the figures. I would also like to thank my mom and dad and sister, Marty, for their "you can do it" attitude.

Jackie Lewis
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ABSTRACT

Sensitivity Analysis of Surface Deposition in a Numerical Model of Atmospheric Dispersion

by

Jackie Lewis, Master of Science
Utah State University, 1976

Major Professor: Dr. Gene L. Wooldridge
Department: Soil Science and Biometeorology

Profiles of height-dependent diffusion which accommodate site-specific diffusivities were produced. A numerical model was adapted to incorporate the profiles. The model represented three-dimensional steady-state advection and diffusion of aerosols from an elevated point source. Sorption effects were simulated with surface attachment coefficients greater than unity. This proved effective in depleting the plume differentially upward from the surface.

(60 pages)
### NOTATIONS AND SYMBOLS

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<td>B</td>
<td>Distance from source in valley to the farthest wall</td>
</tr>
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<td>$B_T$</td>
<td>Half width of ridge</td>
</tr>
<tr>
<td>C</td>
<td>Distance from source in valley to the closest wall</td>
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<td>h</td>
<td>Effective height of source</td>
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<td>K</td>
<td>Eddy diffusivity; subscript denotes reference axis</td>
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<td>$Z_M$</td>
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<td>$Z_T$</td>
<td>Height at the top of the Ekman layer</td>
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<td>$(1 - \alpha)$</td>
<td>Attachment coefficient</td>
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<td>$\Delta_2$</td>
<td>Finite approximation of first derivative</td>
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<td>Variance</td>
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<tr>
<td>$\phi$</td>
<td>Slope of valley walls</td>
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<td>$\chi$</td>
<td>Local concentration (mass per unit volume)</td>
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INTRODUCTION

Atmospheric dispersion models have been developed and refined in several forms over the past two decades, due to increased aerosol production and a heightened concern over the toxic effects of some aerosols on humans, animals, and plants. The models provide estimates of ambient aerosol concentrations and fallout; they aid in decisions on site selection for effluent sources (Priestley, McCormick, and Pasquill, 1958).

Dispersion models generally represent solutions of a differential equation which contains terms for advection and diffusion. The more basic solution in common use is the "plume" model, with a number of restrictive assumptions on atmospheric conditions. More sophisticated three-dimensional models, developed over the past few years, incorporate characteristic wind systems, height-dependent diffusivity coefficients, chemical and radioactive rate constants, and particulate fallout.

A variety of processes remove aerosols from the atmosphere, although they are incompletely understood. Deposition by precipitation scavenging accounts for some removal, but it occurs infrequently in time and space. Reaction, or sorption, with soil or plant surfaces probably removes the largest percentage of the aerosols; vegetation should be considered as a major "sink" since plant life covers 90 percent of the land surface of the United States (Hill, 1971).
Representation of sorption of aerosols on plants presents several problems. Wells and Chamberlain (1967) suggested that the degree and nature of the roughness of the plant canopy was a major factor in determining the turbulent intensity on the small scale. Ventilation depends upon the plant surface area, canopy density and height, and stomatal response. The atmospheric turbulence near the ground differs significantly from the mesoscale eddy turbulence usually used for dispersion calculations (Pasquill, 1974). Diffusivity coefficients in mountainous regions, computed from superpressure balloon flights (Wooldridge, 1974) exhibit marked differences when compared to reference values from plains areas.

The research work and aerosol tracer studies performed to date suggest the efficacy of a parametric approach to the question of surface sorption of aerosols. The research described here was designed to measure the effect of surface attachment in a mountain valley plume model; the model uses height-dependent diffusivities and a parameterization of the attachment processes.
LITERATURE REVIEW

Plume theory

The starting point of most mathematical treatments of diffusion from sources is a generalization of the classical differential equation of heat conduction in a solid. Assuming an incompressible fluid and eddy flux of the simplest gradient-transfer form (Pasquill, 1974), the equation becomes:

$$\frac{dx}{dt} = \frac{\partial}{\partial x} \left( K_x \frac{\partial x}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial x}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial x}{\partial z} \right). \quad [1]$$

Neglecting diffusion along the wind (along-wind diffusion is much less than advection), Roberts (1923) gave the solution for a steady-state continuous point source as:

$$\chi \left( x, y, z \right) = \frac{1}{4\pi^2 (K_x K_y K_z)^{3/2}} \exp \left[ -\overline{U} \left( \frac{y^2}{4xK_y} + \frac{z^2}{4xK_z} \right) \right]. \quad [2]$$

This not only allows for anisotropic diffusion, but for spatial variations as well. The mathematical device which represents perfect reflecting boundaries (valley walls and floor) is the introduction of "mirror-image" sources of strength equal to the source at its origin (Csanyi, 1973). For an elevated source, the equation becomes:

$$\chi \left( x, y, z \right) = \frac{1}{4\pi^2 (K_x K_y K_z)^{3/2}} \left[ \exp \left( \frac{-\overline{U}^2}{4xK_y} \right) + \exp \left( \frac{-\overline{U}(2C+y)^2}{4xK_y} \right) + \exp \left( \frac{-\overline{U}(2B-y)^2}{4xK_y} \right) \right]$$

$$\times \left[ \exp \left( \frac{-\overline{U}(z-h)^2}{4xK_z} \right) + \exp \left( \frac{-\overline{U}(z+h)^2}{4xK_z} \right) \right], \quad [3]$$
where $B$ is the distance to $(x,y,z)$ from one wall and $C$ is the distance from the other (see Figure 1). The classical plume models now in use substitute $\sigma^2 = 2Kt$ into the above equations resulting in height-independent diffusion. Estimates of $\sigma$ are tabulated on graphs as functions of downwind distance for broad stability categories (Pasquill, 1961; Bultynck, 1972). This approach yields reasonable concentration estimates when numerous assumptions are met. The terrain must be flat and open with a perfectly reflecting surface. Local disturbances are assumed to be smaller than the diffusing cloud (Pasquill, 1974). The wind and turbulence are represented as homogeneous horizontally and vertically with steady state conditions persisting. The pollutant is considered passive with crosswind and vertical concentrations following a Gaussian distribution (Munn et al., 1972). In mountainous topography, vertical diffusion cannot be accurately estimated by using standard $\sigma$ values; vertical plume growth is not the same as in flat open areas. Pollution concentrations were observed by Hinds (1970) to be lower on valley floors than predicted by classical models.

**Diffusivity**

Sutton (1953) recognized that constant eddy diffusivity is unacceptable in problems of diffusion in a turbulent atmosphere. Dispersion coefficients depend upon height above the surface, surface roughness, the scale of motion, wind speed and fluctuations, thermal and horizontal pressure gradients, and stability (Turner, 1969; Agee et al., 1973). Diffusivity cannot be treated independent of height above the ground if the boundary layer flow in the first several hundred meters is to be represented. There exists no
Figure 1. Simulated topography and ideal plume position for a continuous point source in a mountain valley: (a) side view, (b) top view, (c) cross-section.
convenient method for determining the relationship between the aerodynamic roughness of the surface and the dispersion coefficients (Ragland and Dennis, 1975). Estimates of diffusivities from Pasquill stability categories only give crude indications of the diffusion characteristics (Reiter, 1973).

Lettau (1973) concluded that eddy diffusivities are generally unique to any given experimental situation and have very little extrapolative value to other experimental situations.

Leahey (1974) derived diffusion coefficients from bivane wind data over irregular terrain. He found concentrations predicted in a Gaussian plume model using his derived values gave better agreement with observations than did Pasquill's standard coefficients. Using superpressure mylar balloons, measurement of lateral and vertical diffusivities as functions of height can be made. From the tracking data, the coefficients are calculated as functions of the variance of the Lagrangian velocity components and Lagrangian time constants. Wooldridge and Orgill (1975) used this technique in the Eagle River Valley of Colorado. Wooldridge (1974) determined height profiles of diffusivities in Cache Valley of northern Utah from balloon data. Computations, using calculated diffusivity profiles for these two valleys showed concentration distributions quite different from each other and from the standard model (Wooldridge and Lewis, 1975).

The estimation of diffusivity determined by various researchers covers a large range of values. Priestley (1959) reports that values of $K$ around 0.25 m$^2$ sec$^{-1}$ are typical at 1.5 meters over grassland in winds of 4 m sec$^{-1}$ and slight to moderate instability. This is
comparable to Pasquill's (1974) typical value of 0.5 m$^2$sec$^{-1}$ at 2 m over long grasses. For more stable conditions, $K$ is as much as an order of magnitude smaller. Maxima occur in the lowest few hundred meters and vary from 10$^2$ m$^2$sec$^{-1}$ for unstable conditions to about 5 x 10$^{-1}$ m$^2$sec$^{-1}$ for stable conditions. Koper and Sadeh (1975) calculated diffusivities of consistent orders of magnitude. The maximum of $K_z$ given by Egan and Mahoney (1972b) in the lowest few hundred meters was close to 7 m$^2$sec$^{-1}$. A crude estimate of the average transverse coefficient is around 47 m$^2$sec$^{-1}$. Pandolfo's (1971) profiles predict maxima at 100 meters between 1 and 10 m$^2$sec$^{-1}$ dropping off to 0.4 to 0.8 m$^2$sec$^{-1}$ at the surface. Wooldridge (1974) computed diffusivity coefficients between about 960 m and 2900 m above the surface of a valley 1200 m deep. The wind, and possibly the stability, were different for each data collection day. The vertical diffusivity was as high as 4 x 10$^2$ m$^2$sec$^{-1}$ at the top of the profile and decreased to 20 m$^2$sec$^{-1}$ at 960 meters. The lateral coefficients over the same height span range from 9 x 10$^2$ m$^2$sec$^{-1}$ down to 8 m$^2$sec$^{-1}$.

The general shape of the vertical distribution of diffusivity shows a near-linear increase in $K$ with height close to the ground, a local maximum at the top of the surface boundary layer and then an exponential type of decrease to the top of the planetary boundary layer (Blackadar, 1962; Agee et al., 1973; Egan and Mahoney, 1972a; Whippem, 1973; O'Brien, 1970). The following exponential function was developed by Agee et al. (1973):

$$K(z) = a \left[ \exp \left( -bz/Z_T \right) - \exp \left( -bcz/Z_T \right) \right], \quad [4]$$

where $a, b, c$ are arbitrarily chosen parameters that primarily affect
the magnitude of K, the height scale, and the ratio of the maximum diffusivity to the diffusivity at the top of the Ekman layer, respectively. The model was successfully used to fit profiles derived by Pandolfo (1971) using BOMEX data. O'Brien (1970) suggested the use of a Hermite cubic polynomial to define the diffusivity-height relationship. This generates profiles much like equation [4]. Sasamori (1970) used O'Brien's formulation and found it to compare favorably with observations. Egan and Mahoney (1972b) also adopted forms of height-dependent diffusivity which look much like equation [4].

Buettner and Thyer's (1965) study of valley flow shows that circulation in valleys is separate from the gradient wind above the ridge line. Circulation separation between Cache Valley and above was found by Ellis and Wooldridge (1973). Studies of diffusivities in valleys by Wooldridge (1974) and Wooldridge and Orgill (1975) demonstrate increasing K values throughout the valley and just above the ridge (the upper limit of their profiles). This indicates that the entire valley is within the surface boundary layer and that the diffusivities probably decrease in the gradient flow above this point.

**Deposition**

Small particles may be deposited on the ground at a rate much faster than can be explained by the gravitational fall velocity or by precipitation scavanging. Meetham (1950) found surface adsorption to be about five times as great as washout. The other mechanisms of transport to the surface include surface impaction, electrostatic attraction, chemical interactions, and diffusion (Slade, 1968; Wells
and Chamberlain, 1967). The physics of particle-surface interactions is quite complicated. Natural surfaces may be good reflectors or good adsorbers, but rarely perfect. The exact behavior at the interface depends upon the properties of the surface and the diffusing particles (Csanady, 1973). The EPA's Meteorology Division has developed numerous numerical models to represent atmospheric dispersion. The assumption is made that there is no deposition or reaction at the surface (Turner, 1969). Future efforts, however, will include parameterization of surface deposition (Hosler, 1975).

Depending on the vegetation type, the area of leaf surface per unit area of ground may vary by a factor of two to a factor of ten. The cellular surface area surrounding the intercellular air spaces within the leaf is considerably higher than the leaf surface area (Hill, 1971; Spedding, 1969). Therefore, the effective adsorbing surface may be many times greater than the total surface area. Elliott (1961) made very rough estimates of $SO_2$ deposition in a 100 meter arc from the source using Project Prairie Grass data. He could not state conclusively whether there was deposition or not, but he preferred to believe that there was none. Slade (1968) reported that Simpson (1961) computed deposition of 90 percent within 3200 meters of the source. Martin and Barber (1971) found a reduction of 75 percent in $SO_2$ concentration between 15 cm and 50 cm above a hedge. Hill (1971) measured uptake of $CO_2$ and $O_3$ by alfalfa and oats in a laboratory chamber and in the field. He found it to vary from 86 percent to 95 percent depending upon the wind speed, canopy, and light. On soil with no plants the uptake was only 7 percent for dry soil and 19 percent for wet soil.
Experimenters investigating particle deposition, however, generally isolate one or two mechanisms to study under ideal, controlled conditions. The parameter usually measured is the velocity of deposition on the microscale (Wells and Chamberlain, 1967; Forney and Spielman, 1974; Spedding, 1969; Möller and Schumann, 1970; Pasquill, 1974; Slade, 1968). Incorporating these values into the steady-state model of the present study would not result in reducing the plume concentrations above the surface as is physically realistic.
METHODS OF PROCEDURE

A model of advection and diffusion of a steady-state plume and a model of general diffusion were developed to simulate aerosol movement in a mountain valley. Height-dependent diffusion coefficients were included. Surface attachment was parameterized by considering an attachment coefficient equivalent to the percentage of aerosols allowed to remain in the air space so the effect of an increased surface gradient caused by removal could be simulated, i.e., reduction of the plume differentially with height.

Simulated topography

The topography simulated for this study was a long, narrow, symmetric valley with steep sloping sides. The sloping walls were approximated in a step-like mode (see Figure 1c). This was done by increasing the distance from the valley center \((y = 0)\) to the walls for each increase in height according to

\[ B = Y_t - B_t + \frac{z}{\tan \phi} \]  

[5]

where the slope of the walls, \(\phi\), was 30° from horizontal. Because the valley is symmetric \(C\) is equal to \(B\). At ridge height \((z = 1000 \text{ m})\) the half width of the valley, \(Y_t\), was 2000 m. The valley floor was 534 m wide, flat and non-sloping. There were no obstructions to airflow within the valley as far as the calculations proceeded. The continuous point source was 100 m above the ground surface and in the center of the valley. The mean wind was along the valley at 3 m sec\(^{-1}\). All ground surfaces were assumed to be covered with vegetation.
Two models were used for the simulation of diffusion and surface deposition. The plume model is steady-state and incorporates a parameterization of surface deposition. The second model, based on a time-dependent diffusion equation, was used to compare with the steady-state solution.

**Plume model.** The steady state plume represented by equation [3] was modified for this study to include height-dependent diffusivities and parameterization of surface deposition. Vertical profiles of the diffusivities were determined according to equation [4]. Surface attachment was parameterized by multiplying each reflective term of equation [3] by an attachment coefficient, \((1 - \alpha)\). The equation of advection and diffusion for this model is:

\[
\frac{\chi}{Q(x,y,z)} = \left(\frac{K_y(z)K_z(z)}{4\pi x}\right)^{1/2} \left\{ \exp \left[ -\frac{\bar{u}^2}{4xK_y(z)} \right] + (1 - \alpha) \left\{ \exp \left[ -\frac{(2B+y)^2}{4xK_y(z)} \right] \right\} \right. \\
+ \left. \exp \left[ -\frac{(z+h)^2}{4xK_z(z)} \right] \right\} \left[ \exp \left[ -\frac{\bar{u}(z-h)^2}{4xK_y(z)} \right] + (1 - \alpha) \exp \left[ -\frac{\bar{u}(z+h)^2}{4xK_z(z)} \right] \right],
\]

where \(\alpha\) is the percentage of the reflected plume material that is removed at each point in a three-dimensional grid within the simulated valley. Computations of the values for the normalized concentration, \(\chi/Q\), were done on a Burroughs 7600 computer using the Fortran language to reduce equation [6] to machine-sensible instructions.

**Diffusion model.** Diffusion of plume material was also simulated, for comparative purposes, according to equation [1] with \(\chi/Q\) substituted.
for $\chi$. Since downwind diffusion is negligible, the first term of equation [1] is zero. The following finite center-differencing form was used for each of the other terms (y substituted for $z$ for the lateral term):

$$\Delta \left( \frac{\chi}{Q} \right)_{m,t} = \frac{\Delta t}{2\Delta z} \left[ K(z)z_{m+1} \left( \frac{\chi_{m+2}}{2\Delta z} \right) - K(z)z_{m-1} \left( \frac{\chi_{m-2}}{2\Delta z} \right) \right],$$

[7]

where subscript $t$ indicates the time step and subscript $m$ is the relative position in the grid. $\chi/Q$ at each time step was computed according to

$$\left( \frac{\chi}{Q} \right)_{t+\Delta t} = \left( \frac{\chi}{Q} \right)_t + \Delta \left( \frac{\chi}{Q} \right)_t$$

[8]

An initial set of $\chi/Q$ values are needed for this formulation. These were computed by the plume model some distance downstream from the source. Therefore, comparisons can be made between the two models further downstream. On the top of the volume, the value of $\Delta(\chi/Q)_{m,t}$ was determined by forward differencing. The surface value of $\Delta(\chi/Q)_{m,t}$ was equal to the flux at the surface (terms of equation [7] in square brackets). A steep gradient was set up at the sides by using a point just behind the walls equal to zero. This outside point was used in the finite differencing and there was no surface attachment on the sides. Within this model, surface attachment was accomplished by reducing the ground surface concentration at each time
step by 20 percent. The same vertical profiles of diffusivities as those in the plume model were used.

**Diffusivity profiles**

Three separate diffusion situations were simulated, so three pairs of lateral and vertical diffusion profiles were computed from equation [4]. For each profile a set of the constants $a$, $b$, and $c$ is required. Agee et al. (1973) obtained the following equations for $a$, $b$, and $c$.

$$a = \frac{K_T c \left[ \frac{(Z_T/Z_M)/(c-1)}{1-c(-Z_T/Z_M)} \right]}{K_T}$$  \hspace{1cm} [9]

$$b = \frac{(\ln c)Z_T}{(c-1)Z_M}$$  \hspace{1cm} [10]

$$\frac{K_M}{K_T} = \left[ 1 - \exp \left[ -\frac{(Z_T/Z_M)\ln c}{1}\right] \right] * \left[ \exp \left[ \frac{((Z_T - Z_M)\ln c)/[Z_M(c-1)]}{Z_M(c-1)} \right] \right]$$

Equations [9]-[11] are a solvable system for determining $a$, $b$, and $c$ when values of $K_M$, $K_T$, $Z_M$, and $Z_T$ are given. The height of the maximum diffusivity, $Z_M$, is taken to be just above the ridge height at 1200 m as this is considered to be the top of the surface boundary layer. Because the top of the Ekman layer is likely to be found in a zone around twice the ridge height, 2400 m was taken as the top of the profile, $Z_T$, for this model to simplify the solution of $c$. $K_M$ and $K_T$ were different for each profile and are given in Table 1. The Newton-Raphson numerical technique was used to solve for $c$. This requires the differentiation of equation [11] (Stark, 1970). The
<table>
<thead>
<tr>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
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<tbody>
<tr>
<td>(K_z)</td>
<td>(K_y)</td>
<td>(K_z)</td>
</tr>
<tr>
<td>3.2</td>
<td>4.7</td>
<td>12.3</td>
</tr>
<tr>
<td>1.9</td>
<td>2.8</td>
<td>7.3</td>
</tr>
</tbody>
</table>

Newton-Raphson formulation was translated into Fortran code and convergence was to within \(10^{-2}\) of the chosen \(K_M/K_T\). With the resulting value for \(c\), it is then a simple matter to specify \(a\) and \(b\). The diffusivity profiles were estimated by calculating \(K(z)\) at each computational height. Diffusion at the surface was not allowed to go to zero as per equation [4]. The diffusivity was assumed to be constant from \(z = 10\) m to the surface and equal to the value of 10 m.

**Surface attachment**

A perfectly reflecting surface is represented by equation [6] with \(\alpha = 0\). At any given point in the grid, the reflected amount represents a smaller percentage of the total concentration than the amount contributed by the original source. With \(\alpha = 1\), there would be no reflection of plume material. The unreflected plume would still be within the surface layer and available for removal by the multiple-layered plant canopy. Further removal can be parameterized by increasing the value of \(\alpha\) greater than 1. This would result in removal of not only the reflected amount, but some fraction of the original plume. Values of \(\alpha\) between 1.5 and 4.0 were used in this study. The vegetation on all surfaces was assumed to have similar adsorption capabilities.
RESULTS AND DISCUSSION

Diffusivity profiles

For this study, three sets of $K_y$ and $K_z$ profiles were constructed from equation [4]. A set of the parameters $a$, $b$, and $c$ were determined for each function according to the previously discussed method. The values are listed in Table 2.

Table 2. $a$, $b$, $c$ for each $K_y$ and $K_z$ profile

<table>
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<tr>
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<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_y$</td>
<td>$K_z$</td>
<td>$K_y$</td>
<td>$K_z$</td>
</tr>
<tr>
<td>----------</td>
<td>----------</td>
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</tr>
<tr>
<td>$a$</td>
<td>190.38</td>
<td>-104.68</td>
<td>506.7</td>
</tr>
<tr>
<td>$b$</td>
<td>1.933</td>
<td>2.085</td>
<td>1.92</td>
</tr>
<tr>
<td>$c$</td>
<td>1.07</td>
<td>0.92</td>
<td>1.0865</td>
</tr>
</tbody>
</table>

The diffusivities were assumed constant in the last 10 meters above the surface; resulting profiles are shown in Figure 2. $K_y$ and $K_z$ for Case 1 were chosen to represent very stable conditions. The second and third sets closely represent values typically found in mountain valleys. The profiles were compared with Pasquill's height-independent $\sigma$ values which are related to the diffusivities by

$$\sigma^2 = 2Kx/\bar{U}$$

[12]

Since the diffusivity is a function of height for this study, $K_i$ values at different heights were used to compute a range of $\sigma_i$ values.
Figure 2. Height-dependent diffusivity profiles; $K_z$ is the vertical diffusivity; $K_y$ is the cross-valley diffusivity.
for each profile. The results of this collation are shown in Figure 3; the diffusivities fit well into the range of the Pasquill estimations. Although the slopes vary, the most significant difference is the height dependence of the profiles employed here.

**Surface attachment**

For each of the three diffusivity profile pairs, there were four modes of plume-surface interactions parameterized. This was accomplished by applying $\alpha$ values of 0.0, 1.0, 2.5, and 4.0. The parameter $\alpha$ determines the influence of the imaginary source (see Figures 1a and 1b) on the total concentration. The contribution of the imaginary source is either included in the total or some factor of it is subtracted from the total. For $\alpha$ equal to 0.0, 100 percent of the imaginary source is included in the total concentration in the airspace. In other words, the surface is reflecting all of the material that contacts it. A perfectly adsorbing single surface is represented when $\alpha$ equals 1.0, that is, none of the imaginary source is included in the calculations. Values of $\alpha$ greater than 1.0 are used to parameterize surface adsorption by multiple-layered plant cover. Computationally, this amounts to taking the $\alpha$ equal 1.0 situation and subtracting some factor of the imaginary plume from the airspace where the reflecting portion exists in the $\alpha$ equals 0 mode. Therefore, the removal is not only within the plant canopy, but, to a decreasing degree, up into the airspace above the plant cover perpendicular to the floor and walls of the valley. This is illustrated in Figure 4. The differences in the concentration are much greater in the lowest layers and decrease upward.
Figure 3. Height-dependent diffusivities used in sensitivity tests for three profiles, superimposed on Pasquill standard dispersion graphs.
Figure 4. $\chi/Q$ vs. height at 5 km downstream along centerline for Case 2 diffusivities.
It is physically realistic for surface removal to have an effect on the distribution in the remaining airspace. As material is removed from the lowest layers, the gradient of concentration increases. The result would be transport from above into the lowest region where further removal could take place. In this model, simple removal from the surface layer would not be as realistic since only the ground layer would be affected. With \( \alpha \) equal to 2.5 the reflected plume is not included, and 1.5 times the imaginary plume is subtracted from the original plume. This means that 250 percent of the imaginary plume is subtracted from the \( \alpha = 0 \) situation. For an \( \alpha \) value of 4.0, the \( \alpha = 0 \) concentrations are reduced by 400 percent in the region of the reflected plume.

**Plume Model**

The plume model approximated advection and diffusion of source material according to equation [5]. Three diffusion situations (Cases 1, 2, and 3) are used (refer to Table 1 for parameters). Case 1 represented a very stable situation where the diffusion was small. Case 2 considered more rapid diffusion typical of calm mountain valleys. Case 3's very strong diffusion was representative of mountain valleys during windy conditions. Four surface-plume interactions were parameterized by using values of \( \alpha \) equal to 0, 1, 2.5, and 4.0. The figures referred to in describing the case study results are in the Appendix.
Case 1

For the very stable situations of Case 1, the diffusivity values both laterally and vertically were extremely small. This resulted in very slow spreading of the source material. The distribution was fairly uniform downstream above the source height \( z = 100 \text{ m} \) with the gradient increasing below this. Up to one kilometer downstream \( (x = 1 \text{ km}) \) the maximum was at the source height; beyond 1 km it dropped to around 80 m. Figure 5 shows this along the centerline \( (y = 0) \) of the plume. Figures 6a and 6b illustrate this behavior of the plume near the walls and ground. It should be noted in these figures that the vertical and horizontal scales are not equal so the slope of the walls appears to be greater than the actual 30°. The normalized concentration at the walls was small but slightly increased downstream as the plume had more time to spread out. Concentrations and the gradient of concentration increased near the ground downstream. The gradient of concentration increased near the walls, but was weaker than in the lowest few tens of meters from the ground. While Figures 5 and 6a,b are for \( \alpha = 0 \) values, they represent what occurred for other \( \alpha \) values because only the concentrations on the ground are altered by varying \( \alpha \).

\( \alpha = 0, \alpha = 1 \). The difference between full reflection \( (\alpha = 0) \) and complete adsorption by a single layer \( (\alpha = 1) \) was only at the ground surface \( (z = 0) \). The adsorption situation predicted concentrations that were only an average factor of 1.7 smaller than those of the reflection condition. This amount of difference is so slight that it is not significant.
\( \alpha = 2.5, \alpha = 4.0 \). There was no difference between the \( \alpha = 2.5 \) and the \( \alpha = 4.0 \) adsorption situations with these small diffusivities. The only difference between the concentrations predicted using these \( \alpha \) values and those predicted with \( \alpha = 0 \) or \( \alpha = 1 \) was at the ground. As is shown in Figure 7, all of the material was removed from the ground in this case. This resulted in a much stronger gradient in the lowest 20 meters above the ground. The distribution in the rest of the airspace remained much the same.

**Case 2**

The diffusion simulated in this case was more rapid than in the first case so the plume spread further in both the horizontal and vertical directions. However, the general shape of the iso-concentration lines was the same. The concentrations across the valley were higher with a more uniform gradient. The vertical gradient became weaker downstream as the plume spread out horizontally.

\( \alpha = 0, \alpha = 1 \). The \( \alpha = 0 \) and the \( \alpha = 1 \) situations differ most close to the source and near the walls and floor. Figures 8a,b, 9a,b, and 10a,b represent the plume distribution under these conditions. Near the absorbing surfaces within 6 km of the source, the \( \alpha = 1 \) concentrations were an average of 1.4 times smaller than those predicted with a perfectly reflecting surface (\( \alpha = 0 \)). The greatest difference was within a few tens of meters of the source, but this was still less than a factor of 2 (see Figures 8a and 8b). As demonstrated by Figures 9a and 9b, at 9 km downstream the concentration close to the sloping walls was almost an order of magnitude less near the adsorbing surfaces (\( \alpha = 1 \)). Figures 10a and 10b offer a comparison
along the centerline \((y = 0)\). For the perfectly reflecting surface the concentration was higher in the lowest 40 m above the surface. Above this height the differences were not significant. The maximum concentration for both situations was at stack height at 1 km downstream and downward to 20 m height at 10 km from the source.

\[ \alpha = 2.5. \] Removal by a plant canopy was parameterized in this situation. The largest deviation from the \(\alpha = 0\) or \(\alpha = 1\) simulation was near the surfaces; all the plume material had been removed. This resulted in a sharp gradient of concentration in the lowest 40 m, as can be seen in Figures 11a,b and 12. Figures 11a and 11b exhibit the substantial decrease of gradient across the valley downstream. Comparison between Figures 10a and 12 reveal the affect of the \(\alpha = 2.5\) removal on the \(\alpha = 0\) distribution. The average amount removed from the perfectly reflecting situation \((\alpha = 0)\) at 3 km downstream was 30 percent; at 10 km it had increased to 69 percent. The resulting concentrations were about an order of magnitude less for the parameterized adsorption. The maximum concentration was at the source height at 1 km downstream and became increasingly lower downstream to 20 m at 10 km.

\[ \alpha = 4.0. \] The removal parameterized with \(\alpha = 4.0\) resulted in the largest deviation from the full reflection situation. As depicted in Figures 13a,b and 14, all the plume material was removed from the surface areas and there was nothing left at 10 km downstream. At 9 km downstream there was no plume material below 180 m. The gradients near the edges of the plume were strong and became much weaker vertically upward into the plume. The maximum behaved quite differently in this
situation. It moved from the source height at 1 km downstream to 40 m at 7 km, then upward to the top of the computation area downstream.

Case 3

The diffusion in this case was much more rapid than for the previous case. The concentrations were greatly reduced throughout the airspace considered and the concentration gradients were weaker. The plume spread out faster so the concentrations were generally higher throughout the computational airspace and there was no noticeable low-concentration edge to the plume.

\( \alpha = 0, \alpha = 1 \). Plume material spread out laterally and vertically very rapidly, resulting in an even distribution. Figures 15a,b and 16a,b, when compared with Figures 6a,b and 8a,b, illustrate how rapidly the lateral dispersion occurred. Concentrations that were typical of the middle of the Case 1 and Case 2 plumes were found at the walls in this situation. The maximum concentration at 1 km occurs at 80 m above the surface; by 3 km downstream it was at the surface and remained there (refer to Figure 17a and 17b). Concentrations predicted by the \( \alpha = 1 \) situation were between a factor of 1.4 and 2.0 less than those in the perfectly reflecting \( (\alpha = 0) \) case. This compares with the differences between the \( \alpha = 0 \) and \( \alpha = 1 \) situations for Case 1 and Case 2.

\( \alpha = 2.5, \alpha = 4.0 \). Adsorption parameterized using \( \alpha = 2.5 \) and \( \alpha = 4.0 \) was very effective. The plume spread rapidly toward the valley boundaries. Figure 18 shows the complete removal of plume material within the surface layer. For the \( \alpha = 2.5 \) situation, there was no
plume material left beyond 3 km from the source; nothing existed beyond 1 km for $\alpha = 4.0$. This abrupt ending of the plume is demonstrated in Figures 19a and 19b. The maximum concentration along the centerline occurred at 20 m above the surface, but on either side of the centerline the maximum was above the stack height. This emphasized the effect of surface adsorption up into the plume.

### Diffusion Model

**Case 2**

The diffusion model calculations (based on equation [6]) started at 3 km downstream from the source. The initial conditions used were the concentrations computed by the plume model for Case 2, $\alpha = 2.5$ at 3 km. Case 2 was chosen for this comparison because the results from the plume model were more significant than Case 1 and not as immoderate as Case 3. The forward integration with a time interval of 30 seconds and $\overline{U}$ equal to 3 m sec$^{-1}$ was performed for 23 time steps to a distance of 5070 m downstream. The ground values were reduced by 20 percent at each time step to simulate attachment. In this time-dependent model, attachment at the surface has an effect into the plume away from the surface because of the modification with time of the concentration gradient at the surface. Figure 20 shows the resulting distribution. If this is compared with Figures 11b and 13a, it can be seen how closely the steady-state plume model represents the diffusion equation. The surface values for the diffusion model were not zero as they were for the plume model. The isopleths of concentration have the same basic shape, illustrating the similarity of the two distributions. This
emphasizes that the parameterization used for surface adsorption in the plume model had a realistic effect on the predicted distribution.
CONCLUSIONS

The elimination of surface reflection in steady-state plume models is not a sufficient method for representing surface attachment; the resulting depletion of plume concentrations is much less than surface attachment measurements indicate. Predicted concentrations using the standard plume model with reflection at the surface differed from those with no reflection by less than 50 percent. Measurements have shown, however, that plants remove greater than 75 percent of the aerosols available. With this amount of plume material removed, the high surface concentrations determined by the standard calculations could not exist.

It is important that prediction models for plume dispersion include enhanced surface attachment. Parameterizing surface attachment by increasing the attachment coefficient beyond unity successfully simulated plume distributions that would result from expected physical processes. Using this method, the plume was significantly depleted both at the surface and within the airspace if the diffusivities were not excessively small. The sensitivity of the plume model to the increased surface attachment parameterization depended upon the diffusivity values used. For low values of diffusivity, the plume spread out very slowly towards the surfaces, making less plume material available for removal. In this situation, the predicted distributions varied very little throughout the airspace. The ground concentrations were altered by the parameterization of surface attachment, but the
degree of the attachment made little difference in the predicted concentrations. For moderately large diffusivities, the predicted distributions varied sharply according to the changing rates of surface adsorption. For very high diffusivities, differences in the concentrations due to varying the attachment parameter was only apparent close to the surface; the plume was practically eliminated before it moved very far downstream.

As an operational tool to represent plume dispersion, this model could be easily implemented for a variety of situations. The simulation of surface adsorption produces realistic results without unnecessarily complicating the formulation of the problem or the equations describing it, and without a substantial increase in computational time.

A three-dimensional, time-dependent model for surface attachment using a complete wind field and height-dependent diffusivities is under development by the author. This will result in a more realistic representation of the physical processes operating during dispersion and will require a greater amount of programming effort and computational time. Many more detailed field measurements will be required.
LITERATURE CITED


APPENDIX

(Figures referred to in Results and Discussion)
Figure 5. Isopleths of concentration along plume centerline ($y = 0$) for Case 1, $\alpha = 0$. 
Figure 6. Isopleths of concentration at 3000 m (a) and 9000 m (b) downwind for half of valley crosssection (symmetric around \( y = 0 \)). Case 1, \( \alpha = 0 \).
Figure 7. Isopleths of concentration at 3000 m downstream. Case 1, $\alpha = 2.5$, $\alpha' = 4.0$. 

$\alpha = 2.5, \alpha' = 4.0$ 

$x = 3000 \text{ m}$
Figure 8. Isopleths of concentration at 5000 m downstream. Case 2. (a) \( \alpha = 0 \). (b) \( \alpha = 1.0 \).
Figure 9. Isopleths of concentration at 9000 m downstream. Case 2. (a) $\alpha = 0$. (b) $\alpha = 1.0$. 
Figure 10. Isopleths of concentration along centerline (y = 0).
Case 2. (a) $\alpha = 0$. (b) $\alpha = 1$. 
Figure 11. Isopleths of concentration. Case 2. $\alpha = 2.5$. (a) 3000 m downstream. (b) 5000 m downstream.
Figure 12. Isopleths of concentration along centerline. Case 2. $\alpha = 2.5$. 
Figure 13. Isopleths of concentration along centerline. Case 2, $\alpha = 4$. (a) 5000 m downstream. (b) 9000 m downstream.
Figure 14. Isopleths of concentration along centerline. Case 2, $\alpha = 4$. 
Figure 15. Isopleths of concentration. Case 3. $\alpha = 0$. (a) 3000 m downstream. (b) 5000 m downstream.
Figure 16. Isopleths of concentration. Case 3, $\alpha = 1$. (a) 3000 m downstream, (b) 5000 m downstream.
Figure 17. Isopleths of concentration along centerline (y = 0).
Case 3, (a) $\alpha = 0$. (b) $\alpha = 1$. 
Figure 18. Isopleths of concentration 3000 m downstream. Case 3. \(\alpha = 2.5\).
Figure 19. Isopleths of concentration. Case 3. $\alpha = 2.5$. (a) along centerline ($y = 0$). (b) across valley at 100 m height (symmetric around $x$ axis).
Figure 20. Isopleths of concentration at 4980 m downstream. Case 2. Diffusion model. Surface concentrations reduced 20 percent at each time step.
VITA

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