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PLUME CONCENTRATION ALGORITHMS WITH DEPOSITION,
SEDIMENTATION, AND CHEMICAL TRANSFORMATION

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analytically solved using Green's functions. This analytical
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in a physically realistic and straightforward manner. For
practical application of the model, the eddy diffusivity
coefficients in the analytical solutions are expressed in
terms of the widely-used Gaussian plume dispersion
parameters. The latter can be specified as functions of the
downwind distance and the atmospheric stability class within
the framework of the standard turbulence-typing schemes. The
new point-source algorithms are applied to study the
atmospheric transport and transformation of SO2 to SO4(-2),
and deposition of these species. The work described in this
report was undertaken to develop concentration algorithms
for the Pollution Episodic Model (PEM).

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## SYMBOLS AND ABBREVIATIONS

### SYMBOLS

$C_1, C_2$      mean concentrations of primary and secondary pollutants for point source

$C_{A1}, C_{A2}$      mean concentrations of primary and secondary pollutants for area source

$D_1, D_2$      surface deposition fluxes of primary and secondary pollutants

$F_1, F_2$      Weighting functions in secondary pollutant concentration algorithms

$G_1, G_2, G_3$      Green's functions

$H$      effective height of source

$k_t$      chemical transformation rate

$K_y, K_z$      eddy diffusivities in y and z directions

$L$      height of the inversion lid

$L_y, L_z$      length scales of concentration distribution in y and z directions

$p$      probability density of concentration distribution in y direction

$Q_1, Q_2$      source strengths or emission rates of primary and secondary pollutants

$q_1, q_2$      probability densities of concentration distributions of primary and secondary pollutants in z direction

$U$      mean wind speed

$V_{d1}, V_{d2}$      dry deposition velocities of primary and secondary pollutants

$V_{11}$      $V_{d1} - W_1/2$

$V_{12}$      $V_{d2} - W_2/2$

$V_{13}$      $V_{11} - (W_1 - W_2)/2$

| | |
|---|---|
| $V_{21}$ | $V_{d1} - W_1$ |
| $V_{22}$ | $V_{d2} - W_2$ |
| $W_1, W_2$ | gravitational settling velocities of primary and secondary pollutant particles |
| $x, y, z$ | horizontal downwind, horizontal crosswind, and vertical coordinates |
| $x_m$ | downwind distance at which $\sigma_z = 0.47L$ |
| $\sigma_y, \sigma_z$ | Gausssian dispersion parameters in $y$ and $z$ directions |
| $\tau_c$ | characteristic time scale of chemical transformation |

## NONDIMENSIONAL QUANTITIES

| | |
|---|---|
| $g_1$ | crosswind diffusion function |
| $g_2$ | vertical diffusion function for point source when $x \leq x_m$ |
| $g_{21}', g_{22}'$ | $g_2$ modified (for deposition and chemical transformation) for primary and secondary pollutants |
| $g_3$ | vertical diffusion function for point source in plume-trapping region ($x_m < x < 2 x_m$) |
| $g_{31}', g_{32}'$ | $g_3$ modified (for deposition and chemical transformation) for primary and secondary pollutants |
| $g_4$ | vertical diffusion function for point source in well-mixed region ($x \geq 2 x_m$) |
| $g_{41}', g_{42}'$ | $g_4$ modified (for deposition and chemical transformation) for primary and secondary pollutants |
| $\hat{H}$ | $H/\sqrt{2}\ \sigma_z$ |
| $\hat{L}$ | $L/\sqrt{2}\ \sigma_z$ |
| $\hat{V}_{d1}, \hat{V}_{d2}$ | $V_{d1}/U$ , $V_{d2}/U$ |
| $\hat{V}_{11}, \hat{V}_{12}$ | $V_{11}/U$ , $V_{12}/U$ |

$\hat{V}_{13}$          $V_{13}/U$

$\hat{V}_{21}$ , $\hat{V}_{22}$          $V_{21}/U$  ,  $V_{22}/U$

$\hat{W}_1$ , $\hat{W}_2$          $W_1/U$    ,  $W_2/U$

$\hat{x}$, $\hat{z}$          $x/\sqrt{2}\ \sigma_z$,  $z/\sqrt{2}\ \sigma_z$

$\hat{y}$          $y/\sqrt{2}\ \sigma_y$

$\hat{\tau}_c$          $\tau_c U/\sqrt{2}\ \sigma_z$

$\gamma$          ratio of molecular weight of secondary pollutant
                   to molecular weight of primary pollutant


ABBREVIATIONS

ATDL          Atmospheric Turbulence and Diffusion Laboratory

EPA          Environmental Protection Agency

GLC          Ground-level concentration

KST          Atmospheric stability class index

P-G          Pasquill-Gifford

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ABSTRACT


A gradient-transfer model for the atmospheric transport, diffusion, deposition, and first-order chemical transformation of gaseous and particulate pollutants emitted from an elevated continuous point source is formulated and analytically solved using Green's functions. This analytical plume model treats gravitational settling and dry deposition in a physically realistic and straightforward manner. For practical application of the model, the eddy diffusivity coefficients in the analytical solutions are expressed in terms of the widely-used Gaussian plume dispersion parameters. The latter can be specified as functions of the downwind distance and the atmospheric stability class within the framework of the standard turbulence-typing schemes.

The analytical plume algorithms for the primary (reactant) and the secondary (product) pollutants are presented for various stability and mixing conditions. In the limit when deposition and settling velocities and the chemical transformation rate are zero, these equations reduce to the well-known Gaussian plume diffusion algorithms presently used in EPA dispersion models for assessment of air quality. Thus the analytical model for estimating deposition and chemical transformation described here retains the ease of application associated with Gaussian plume models, and is subject to the same basic assumptions and limitations as the latter.

A new mathematical approach, based on mass budgets of the species, is outlined to derive simple expressions for ground-level concentrations of the primary and secondary pollutants resulting from distributed area-source emissions. These expressions, which involve only the point-source algorithms for the well-mixed region, permit one to use the same program subroutines for both point and area sources. Thus the area-source concentration equations developed in this report are simple, efficient, and accurate.

The new point-source algorithms are applied to study the atmospheric transport and transformation of $SO_2$ to $SO_4^-$, and deposition of these species. Calculated variations of the ground-level concentrations are presented and discussed. The results of a sensitivity analysis of the concentration algorithm for the secondary pollutant are given. The specification of gravitational settling and deposition velocities in the model is discussed.

The work described in this report was undertaken to develop concentration algorithms for the Pollution Episodic Model (PEM). This report was submitted by NOAA's Atmospheric Turbulence and Diffusion Division in partial fulfillment of Interagency Agreement No. AD-13-F-1-707-0 with the U. S. Environmental Protection Agency. This work, covering the period September 1981 to March 1983, was completed as of March 31, 1983.

# SECTION 1

## INTRODUCTION

Pollutant gases and suspended particles released into the atmosphere are transported by the wind, diffused and diluted by turbulence, and removed by several natural processes. An important removal mechanism is dry deposition of pollutants on the earth's surface by gravitational settling, eddy impaction, chemical absorption, and other effects. Another significant removal mechanism is chemical transformation in the atmosphere. Depletion of airborne pollutant material by these natural processes affects pollutant concentrations and residence times in the atmosphere. Moreover, the product of a chemical reaction may be the pollutant of primary concern, rather than the reactant itself. Surface deposition of acidic and toxic pollutants may adversely impact on local ecology, human health, biological life, structures, and ancient monuments. Furthermore, large concentrations of particulate products resulting from chemical reactions may lead to significant deterioration of atmospheric visibility. It is important, therefore, to obtain reliable estimates of the effects of dry deposition and chemical transformation.

This report presents an analytical plume model for diffusion, dry deposition, and first-order chemical transformation of gaseous or particulate pollutants released from an elevated continuous point source, based on gradient-transfer or K-theory. The method solves the atmospheric advection-diffusion

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equation subject to a deposition boundary condition. The model includes

similar and complementary sets of equations for the primary (reactant)

and the secondary (product) pollutants. These equations are analytically

solved using Green's functions.

In order to facilitate practical application of the model to air pollution

problems, the K-coefficients are expressed in this report in terms of the

widely-used Gaussian plume dispersion parameters which can be easily obtained

from standard turbulence-typing schemes. The parameterized diffusion-deposi-

tion-transformation algorithms for various atmospheric stability and mixing

conditions are simplified, and presented as analytical extensions of the well-

known Gaussian plume-diffusion algorithms presently used in EPA models for air ·

quality assessment.

For practical application of the model to urban air pollution problems,

a new mathematical approach, based on mass balance considerations, is developed

to derive simple expressions for ground-level concentrations of the reactant

and the product pollutants resulting from distributed area-source emissions.

These novel expressions for area sources involve only the point-source algorithms

of the well-mixed region, thus allowing one to use the same program subroutines

for both point and area sources. In the limit when deposition rates approach

zero, the concentrations calculated by these expressions agree with the corres-

ponding values given by the area-source algorithms without deposition, currently

used in urban air pollution models.

This report gives a brief review of the literature on gradient-transfer

models with chemical transformation. Details of the mathematical formulations

and analytical solutions of the present model with deposition, sedimentation, and chemical transformation are given, and the parameterized concentration algorithms for the primary and the secondary pollutants are listed. Calculated variations of the ground-level concentrations and results of a sensitivity analysis are presented and discussed. Some guidance is provided for the specification of the settling and deposition velocities in the model.

SECTION 2


LITERATURE SURVEY


Applied air pollution models used in industry and regulation are generally based on the Gaussian plume formulation. These models have been extensively modified over the years to include pollutant removal mechanisms such as dry and wet deposition, and chemical decay. Rao (1981) gave a brief review of the existing methodologies of Gaussian diffusion-deposition models, including a comprehensive literature survey of gradient-transfer (K-theory) models. For the latter case, Rao (1981) also gave the mathematical formulations (for a non-reactive pollutant), analytical solutions, parameterized concentration algorithms for various atmospheric stability and mixing conditions, and expressions for net deposition and suspension rates of the pollutant.


In this section, we briefly review the literature on K-theory or Gaussian models for chemically reactive pollutants. Only a first-order chemical trans-formation is considered, and expressions for both the primary (reactant) and secondary (product) pollutants are given in the references cited.


Heines and Peters (1973) studied the diffusion and transformation of pollutants from a continuous point or infinite line source. The effect of a temperature inversion aloft was also included through multiple eddy reflec-tions. The eddy diffusion coefficients were assumed to be power functions of the downwind distance. The expression for concentration of the secondary

pollutant was derived from a simple component mass balance. The concentrations of the reactant and product were presented in terms of dimensionless plots. Deposition and sedimentation were not considered for either species.

Rao (1975) adapted the analytical solution of Monin (1959) to study the dispersion, deposition, and chemical transformation of the $SO_2$ plume from a power plant stack represented by an elevated continuous point source. The eddy diffusivities were expressed in terms of the Gaussian dispersion parameters. A constant first-order transformation rate of $SO_2$ to $SO_4^=$ was assumed. Concentrations of both species were calculated, and compared with observations at several downwind receptors. Izrael, Mikhailova, and Pressman (1979) used Monin's (1959) instantaneous source solution to estimate the long-range transport of sulfur dioxide and sulfates, assuming constant eddy diffusivities and non-equal deposition velocities for the two species.

Ermak (1978) described a multiple point-source dispersion model which considered a chain of up to three first-order chemical transformations. The source-depletion approach (e.g., Van der Hoven, 1968) was used to include ground deposition. The gradient-transfer plume model of Ermak (1977) was used to incorporate the effects of gravitational settling of particles. For the latter case, however, the chemical-transformtion option could not be used, and the effects of an inversion layer were assumed to be negligible.

Lee (1980) gave analytical solutions of a gradient-transfer model similar to that described in this report, in terms of constant eddy diffusivity coefficients. These solutions apply only to gases or very small particles emitted from an elevated continuous point source, since the gravitational settling

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effects were not considered. A first-order chemical transformation was con-
sidered, and direct emission of the secondary pollutant was assumed to be zero.
Lee used this model, which included wet deposition processes, to study the
atmospheric transport and transformation of $SO_2$ to $SO_4^=$, assuming $K_y = K_z = 5 \text{ m}^2/\text{s}$.
Details of the analytical solutions were not available.

# SECTION 3

## THE GRADIENT-TRANSFER DEPOSITION MODEL

This section gives the mathematical formulations and analytical solutions of the gradient-transfer (K-theory) model for the most general case that includes transport, diffusion, deposition, sedimentation, and first-order chemical transformation of pollutants. We consider two chemically-coupled gaseous or particulate pollutant species; the primary (species-1 or reactant) pollutant is assumed to transform into the secondary (species-2 or reaction product) pollutant at a known constant rate. For generality, the two species are assumed to have known non-equal deposition and settling velocities.

. First, we derive analytical solutions for concentrations of the two pollutant species emitted from an elevated continuous point source. Then we express the K-coefficients in these solutions in terms of the widely used Gaussian plume dispersion parameters. The resulting expressions are parameterized, simplified, and presented as extensions of the Gaussian plume algorithms currently used in EPA air quality models for various atmospheric stability and mixing conditions. Further simplifications of the new algorithms are indicated for gaseous or fine suspended particulate pollutants with negligible settling, and for ground-level sources and/or receptors. Limiting expressions of the algorithms are derived for large particles, when gravitational settling is

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the dominant deposition mechanism. Finally, we utilize these new point source concentration algorithms to derive expressions for the concentrations of the two species due to emissions from area sources, using an innovative approach based on mass balance considerations.

No assumptions are made here regarding the nature of the pollutant species. The formulations and the solutions are, therefore, general enough to be applicable to any two gaseous or particulate pollutants that are coupled through a first-order chemical transformation. Either of the two species may be a gas, or particulate matter with a known average size. Molecular weights of the two species are assumed to be known. Direct emission of the secondary pollutant is permitted from both point and area sources. A direct emission of secondary pollutant, if present, may contribute to its concentration significantly more than the chemical transformation.

In the absence of a chemical coupling, expressions for concentrations of two chemically-independent pollutants, each subject to deposition and/or sedimentation, can be obtained as degenerate cases of the concentration algorithms for the general case. The notation used in this section is similar to that of Rao (1981), which is consistent with the notation presently used in the user's guides for EPA's atmospheric dispersion models.

MATHEMATICAL FORMULATIONS

We consider the steady state form of the three-dimensional atmospheric advection-diffusion equation for the primary pollutant (denoted by subscript 1) with deposition, sedimentation, and first-order chemical transformation:

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$$U \, \partial C_1/\partial x = K_y \, \partial^2 C_1/\partial y^2 + K_z \, \partial^2 C_1/\partial z^2 + W_1 \, \partial C_1/\partial z - C_1/\tau_c \qquad (1a)$$

Here, x, y, z are the horizontal downwind, horizontal crosswind, and vertical coordinates, respectively; U is the constant average wind speed, and $W_1$ is the gravitational settling velocity (taken as positive in the downward or negative z-direction) of the primary pollutant particles, $C_1$ is the primary pollutant concentration at (x, y, z), $K_y$ and $K_z$ are constant eddy diffusivities in the crosswind and vertical directions, respectively, and $\tau_c \equiv 1/k_t$ is the time scale associated with the chemical transformation which proceeds at a given rate $k_t$. The last term of the equation, $- C_1/\tau_c$, represents the chemical sink, or loss of the primary pollutant due to transformation.

For a continuous point source, with an emission rate or strength $Q_1$ of pollutant species-1, located at x = 0, y = 0, z = H, the initial and boundary conditions are given by

$$C_1(0, \, y, \, z) = Q_1/U \cdot \delta(y) \cdot \delta(z-H) \qquad (1b)$$

$$C_1(x, \, \pm\infty, \, z) = 0 \qquad (1c)$$

$$[K_z \cdot \partial C_1/\partial z + W_i \cdot C_1]_{z=0} = [V_{d1} \cdot C_1]_{z=0} \qquad (1d)$$

$$C_1(x, \, y, \, \infty) = 0 \qquad (1e)$$

In the initial condition (1b), which is the limiting form of the mass continuity equation at the source, δ is the Dirac delta function. Boundary condition (1d)

states that, at ground-level, the sum of the turbulent transfer of pollutant down its concentration gradient and the downward settling flux due to the particles' weight is equal to the net flux of pollutant to the surface resulting from an exchange between the atmosphere and the surface; $V_{d1}$ is the deposition velocity which characterizes this exchange of the primary pollutant. When deposition occurs, from Eq. (1d) the turbulent flux at the surface (z=0) is given by

$$-\overline{w'c_1'} = K_z \cdot \partial C_1/\partial z = (V_{d1} - W_1) \cdot C_1 \geq 0,$$

which is in agreement with the standard micrometeorological notation. This obviously requires that $V_{d1} \geq W_1 \geq 0$. If $0 < V_{d1} < W_1$, then the direction of the turbulent flux at the surface is reversed, implying re-entrainment of the particles from the surface into the atmosphere. Thus, the deposition boundary condition (1d), originally suggested by Monin (1959) and discussed by Calder (1961), adequately describes the exchange between the atmosphere and the surface. Eq. (1d) is analogous to the so-called 'radiation' boundary condition used in the theory of heat conduction (see, e.g., Carslaw and Jaeger, 1959, p. 18) to describe the temperature distribution in a body from the boundary of which heat radiates freely into the surrounding medium, when the latter is at zero degrees temperature.

The corresponding formulations for the secondary pollutant (designated by subscript 2) can be written as follows:

$$U \partial C_2/\partial x = K_y \partial^2 C_2/\partial y^2 + K_z \partial^2 C_2/\partial z^2 + W_2 \partial C_2/\partial z + \gamma C_1/\tau_c \quad (2a)$$

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$$C_2(0, y, z) = Q_2/U \cdot \delta(y) \cdot \delta(z-H) \tag{2b}$$

$$C_2(x, \pm\infty, z) = 0 \tag{2c}$$

$$[K_z \cdot \partial C_2/\partial z + W_2 \cdot C_2]_{z=0} = [V_{d2} \cdot C_2]_{z=0} \tag{2d}$$

$$C_2(x, y, \infty) = 0 \tag{2e}$$

In Eq. (2a), $W_2$ is the gravitational settling velocity of the secondary pollutant, and $\gamma$ is the ratio of its molecular weight to that of the primary pollutant; the term $\gamma C_1/\tau_c$ represents the chemical source for the secondary pollutant. Eq. (2b) describes the direct emission of species-2 from the point source, located at x=0, y=0, z=H, with an emission rate or strength $Q_2$. Eq. (2d) is the deposition boundary condition, and $V_{d2}$ is the deposition velocity for the secondary pollutant. For generality, we assume here $V_{d2} \neq V_{d1}$ and $W_2 \neq W_1$.

ANALYTICAL SOLUTIONS

The solution of Eqs. (1) and (2) can be expressed as

$$C_1(x, y, z) = Q_1/U \cdot p(x,y) \cdot q_1(x,z) \tag{3}$$

$$C_2(x, y, z) = Q_1/U \cdot p(x,y) \cdot q_2(x,z) \tag{4}$$

where $p$, $q_1$, and $q_2$ are probability densities of the concentration distributions. It should be noted that the concentration of the secondary pollutant, $C_2$, is

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expressed in terms of the emission rate of the primary pollutant, $Q_1$, in Eq. (4). This is due to the likelihood that, for many practical applications of the model, the direct emission rate $Q_2$ of the secondary pollutant may be zero; $C_2$ would then be zero if $Q_2$ were used instead of $Q_1$ in Eq. (4), thus incorrectly ignoring the non-zero contribution to $C_2$ by the chemical source. The probability density $p(x,y)$ of the concentration distribution in the horizontal crosswind direction is unaffected by deposition, sedimentation, and chemical transformation. Therefore, it is identical for both species.

Substituting Eq. (3) in Eq. (1) and using the separation of variables technique, two independent systems of equations and boundary conditions in $p$ and $q_1$ can be obtained as follows:

$$U\, \partial p/\partial x = K_y\, \partial^2 p/\partial y^2 , \qquad 0 < x < \infty , \; -\infty < y < \infty$$

$$p(0,y) = \delta(y) \tag{5}$$

$$p(x,\pm\infty) = 0$$

and

$$U\, \partial q_1/\partial x = K_z\, \partial^2 q_1/\partial z^2 + W_1\, \partial q_1/\partial z - q_1/\tau_c, \qquad 0 < x , \; z < \infty$$

$$q_1(0,z) = \delta(z-H) = \psi_1(z)$$

$$[K_z \cdot \partial q_1/\partial z + W_1 \cdot q_1]_{z=0} = [V_{d1} \cdot q_1]_{z=0} \tag{6}$$

$$q_1(x,\infty) = 0$$

The analytical solution of (5) can be written as

$$p(x,y) = \frac{g_1(x,y)}{L_y}$$

$$g_1(x,y) = \exp\left\{-\frac{y^2 \, U}{4 \, K_y x}\right\} \tag{7}$$

$$L_y = 2 \sqrt{\pi \, K_y x/U}$$

where $L_y$ is a length scale characteristic of the horizontal crosswind diffusion, and $g_1(x,y)$ is a nondimensional function. This is one of the fundamental solutions of the diffusion or heat conduction equation (e.g., see Carslaw and Jaeger, 1963, p.107); $p(x,y)$ represents the probability that a particle released from a source of unit strength located at $x=0$, $y=0$ will be at a crosswind location $y$ after travelling a distance $x$ downwind with a speed of $U$.

Equation (6) cannot be solved in its present form because of the sedimentation term, $W_1 \, \partial q_1/\partial z$, and the chemical sink term, $-q_1/\tau_c$, in the differential equation. In order to remove these terms, we apply the following transformation:

$$q_1(x,z) = \bar{q}_1(x,z) \cdot \exp\left(-\beta_1^2 - \frac{x}{U\tau_c}\right), \tag{8a}$$

where

$$\beta_1(x,z) = \left[\frac{W_1(z-H)}{2K_z} + \frac{W_1^2 \, x}{4K_z U}\right]^{1/2} \tag{8b}$$

is a nondimensional parameter representing the effect of sedimentation of the primary pollutant particles on the primary pollutant concentration, and $\bar{q}_1(x,z)$

is the transformed new variable. Substituting Eq. (8) in Eq. (6) and simplifying, we obtain the following:

$$U\, \partial\bar{q}_1/\partial x = K_z\, \partial^2\bar{q}_1/\partial z^2\ , \qquad 0 < x\ ,\ z < \infty \tag{9a}$$

$$\bar{q}_1(0,z) = \exp\left\{\frac{W_1(z-H)}{2K_z}\right\} \cdot \delta(z-H) = \bar{\psi}_1(z) \tag{9b}$$

$$[\partial\bar{q}_1/\partial z]_{z=0} = h_1 \cdot [\bar{q}_1]_{z=0} \tag{9c}$$

$$\bar{q}_1(x,\infty) = 0 \tag{9d}$$

where

$$h_1 = V_{11}/K_z\ , \qquad V_{11} = V_{d1} - W_1/2 \tag{9e}$$

The homogeneous boundary condition (9c) expresses the relationship between the variable $\bar{q}_1$ and its normal gradient at the surface. This type of equation is usually referred to as a boundary condition of the third kind; (A more general form of this boundary condition is $\partial\bar{q}_1/\partial z - h_1\bar{q}_1 = f_3$. The Dirichlet boundary condition of type $\bar{q}_1 = f_1$ and the Neumann boundary condition of type $\partial\bar{q}_1/\partial z = f_2$, are boundary conditions of the first and second kind, respectively. Here, $f_1$, $f_2$, and $f_3$ are functions of x given at the boundary, z = 0, of the region in which the solution is sought). Equations (9a, c, d) constitute a homogeneous boundary-value problem of the third kind. The solution of this problem, also known as its Green's function $G(x,z,\xi)$, can be obtained by Laplace transform methods (Carslaw and Jaeger, 1963, p. 115), and written as follows:

$$G_1(x,z,\xi) = \frac{1}{L_z}\left[\exp\left\{\frac{-(z-\xi)^2 U}{4K_z x}\right\} + \exp\left\{\frac{-(z+\xi)^2 U}{4K_z x}\right\}\right.$$

$$\left. - 2h_1 \cdot \int_0^\infty \exp\left\{\frac{-(z+\xi+\eta)^2 U}{4K_z x} - h_1 \cdot \eta\right\} d\eta\right] \tag{10a}$$

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where
$$L_z = 2\sqrt{\pi K_z x/U} \qquad (10b)$$

is a length scale characteristic of the vertical diffusion. Equation (10) describes the stationary diffusion in a semi-infinite region from a unit source located at $x=0$, $z=\xi$. The subscript 1 of the Green's function G corresponds to the subscript of h appearing in Eqs. (9c) and (10a).

The solution of Eq. (9) can be now written in terms of its Green's function (see, e.g., Tychonov and Samarskii, 1964), as follows:

$$\bar{q}_1(x,z) = \int_0^\infty \bar{\psi}_1(\xi) \cdot G_1(x,z,\xi)\,d\xi, \qquad (11)$$

where, from Eq. (9b),

$$\bar{\psi}_1(\xi) = \bar{q}_1(0,\xi) = \exp\left\{\frac{W_1(\xi-H)}{2K_z}\right\} \cdot \delta(\xi-H) \qquad (12)$$

Substituting (10) and (12) in (11), and noting that

$$\int_0^\infty f(\xi) \cdot \delta(\xi-a)\,d\xi = f(a),$$

where $f(\xi)$ is any arbitrary function of $\xi$, term-by-term integration of (11) gives

$$\bar{q}_1(x,z) = \frac{1}{L_z}\left[\exp\left\{\frac{-(z-H)^2 U}{4K_z x}\right\} + \exp\left\{\frac{-(z+H)^2 U}{4K_z x}\right\}\right.$$

$$\left. - L_z h_1 \cdot \exp\left\{h_1(z+H) + h_1^2 K_z x/U\right\} \cdot \text{erfc}\left\{\frac{z+H+2h_1 K_z x/U}{2\sqrt{K_z x/U}}\right\}\right] \qquad (13)$$

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In order to simplify the equations, and considerably reduce the difficulty in typing them, we define the following nondimensional parameters:

$$r = \frac{(z-H)^2 U}{4K_z x} \quad , \quad s = \frac{(z+H)^2 U}{4K_z x}$$

$$\xi_1 = \frac{z+H}{2\sqrt{K_z x/U}} + h_1 \sqrt{K_z x/U} \tag{14}$$

$$\alpha_1 = L_z h_1 e^{\xi_1^2} \text{ erfc } \xi_1$$

Noting that

$$\exp\{h_1(z+H) + h_1^2 K_z x/U\} = \exp(\xi_1^2 - s) = e^{\xi_1^2} \cdot e^{-s},$$

Eq. (13) can be now written as

$$\bar{q}_1(x,z) = \frac{1}{L_z} [e^{-r} + e^{-s} \cdot (1 - \alpha_1)] \tag{15}$$

From Eqs. (8) and (15), the solution of Eq. (6) can be written as

$$q_1(x,z) = g'_{21} / L_z , \tag{16a}$$

where

$$g'_{21}(x,z) = \exp(-\beta_1^2 - x/U\tau_c) \cdot \left[ e^{-r} + e^{-s} \cdot (1 - \alpha_1) \right] \tag{16b}$$

is a nondimensional function. The prime indicates modification of function $g_2(x,z)$ of the primary pollutant (denoted by the second subscript 1) for the effects of deposition, sedimentation, and chemical transformation. In the absence of these effects, i.e., when $\alpha_1 = \beta_1 = 0$ and $k_t = 0$ or $\tau_c = \infty$, Eq. (16b) reduces to

$$g'_{21}(x,z) = e^{-r} + e^{-s} = g_2(x,\dot{z}), \qquad (17)$$

as in the familiar Gaussian plume model. The notation used here is an extension of Rao's (1981) notation for one pollutant, and is consistent with the notation presently used in the user's guides for EPA air quality models.

We now turn our attention to the solution of Eq. (2). Substituting Eqs. (3) and (4) in Eq. (2) and using the separation of variables technique, two independent systems of equations and boundary conditions in $p$ and $q_2$ can be obtained. The p-equations and their solution are the same as those given in Eqs. (5) and (7). The $q_2$-equations can be written as follows:

$$U\, \partial q_2/\partial x = K_z\, \partial^2 q_2/\partial z^2 + W_2\, \partial q_2/\partial z + \gamma\, q_1/\tau_c \;, \quad 0 < x\,,\, z < \infty$$

$$q_2(0,z) = Q_2/Q_1 \cdot \delta(z-H) = \psi_2(z) \qquad (18)$$

$$[K_z \cdot \partial q_2/\partial z + W_2 \cdot q_2]_{z=0} = [V_{d2} \cdot q_2]_{z=0}$$

$$q_2(x,\infty) = 0$$

In order to eliminate the sedimentation term, $W_2\, \partial q_2/\partial z$, from the differential equation, we use the following transformation:

$$q_2(x,z) = \bar{q}_2(x,z) \cdot \exp(-\beta_2^2) \qquad (19a)$$

where

$$\beta_2(x,z) = \left[ \frac{W_2(z-H)}{2K_z} + \frac{W_2^2 \, x}{4K_z U} \right]^{1/2} \qquad (19b)$$

is a nondimensional parameter representing the effect of sedimentation of the secondary pollutant particles on the secondary pollutant concentration, and $\bar{q}_2(x,z)$ is the transformed new variable.  Substituting Eqs. (8) and (19) in Eq. (18), we obtain the following transformed equations:

$$U \, \partial\bar{q}_2/\partial x = K_z \, \partial^2\bar{q}_2/\partial z^2 + \gamma \, \frac{\bar{q}_1}{\tau_c} \cdot \exp\left\{ -(\beta_1^2 - \beta_2^2 + x/U\tau_c) \right\},$$
$$0 < x \, , \, z < \infty \qquad (20a)$$

$$\bar{q}_2(0,z) = Q_2/Q_1 \cdot \exp\left\{ \frac{W_2(z-H)}{2K_z} \right\} \cdot \delta(z-H) = \bar{\psi}_2(z) \qquad (20b)$$

$$[\partial\bar{q}_2/\partial z]_{z=0} = h_2 \cdot [\bar{q}_2]_{z=0} \qquad (20c)$$

$$\bar{q}_2(x,\infty) = 0 \qquad (20d)$$

where

$$h_2 = V_{12}/K_z \, , \qquad V_{12} = V_{d2} - W_2/2 \qquad (20e)$$

Equation (20a) is a nonhomogeneous partial differential equation for the secondary pollutant, coupled to Eq. (9) for the primary pollutant through the chemical source term,

$$f(x,z) = (\gamma/\tau_c) \cdot \bar{q}_1(x,z) \cdot \exp\left\{ -(\beta_1^2 - \beta_2^2 + x/U\tau_c) \right\} \qquad (21)$$

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Unlike $Q_2$, this chemical source is not a constant; in addition to  x and z, it depends on H, U, $K_z$, $V_{d1}$, $W_1$, $W_2$, $\gamma$, and $\tau_c$.  As shown by Budak et al. (1964), the analytical solution of Eq. (20) may be directly obtained as follows:

$$\bar{q}_2(x,z) = \int_0^\infty \bar{\psi}_2(\xi) \cdot G_2(x,z,\xi)\, d\xi$$

$$+ \int_0^x dx' \int_0^\infty f(x',\xi) \cdot G_2(x-x',z,\xi)\, d\xi \qquad (22)$$

Here $\bar{\psi}_2$ and f are the functions defined in Eqs. (20b) and (21), respectively. The first term in Eq. (22) gives the contribution of the initial condition, and the second term gives the contribution of the inhomogeneity in Eq. (20a). $G_2(x,z,\xi)$ is the Green's function of the homogeneous differential equation, subject to the boundary condition (20c) of the third kind; the Green's function is given by

$$G_2(x,z,\xi) = \frac{1}{L_z}\left[\exp\left\{\frac{-(z-\xi)^2 U}{4K_z x}\right\} + \exp\left\{\frac{-(z+\xi)^2 U}{4K_z x}\right\}\right.$$

$$\left. - 2h_2 \cdot \int_0^\infty \exp\left\{\frac{-(z+\xi+\eta)^2 U}{4K_z x} - h_2\cdot\eta\right\} d\eta \right] \qquad (23)$$

$G_2(x-x',z,\xi)$, needed to solve Eq. (22), is the associated source function, obtained by replacing x in the Green's function $G_2(x,z,\xi)$ of Eq. (23) with x-x'.

Though straightforward in principle, the solution given by Eq. (22) is difficult
to derive in practice. This is because the contribution of the inhomogeneity,
given by the second part of Eq. (22), involves evaluation of several integrals
whose integrands are complicated functions of $\xi$. Some of these integrations are
mathematically intractable, thus rendering this direct application of the
Green's function solution to the inhomogenous differential equation fruitless.

In order to remove the inhomogeneity from the differential equation (20a),
we introduce the following transformation:

$$\bar{q}_2(x,z) = \bar{q}_3(x,z) - \gamma \, \bar{\bar{q}}_1(x,z) \qquad (24)$$

where

$$\bar{\bar{q}}_1(x,z) = \bar{q}_1(x,z) \cdot \exp\left\{ -(\beta_1^2 - \beta_2^2 + x/U\tau_c) \right\} \qquad (25)$$

and $\bar{q}_3(x,z)$ is a new (unknown) variable. Substituting (24) in Eq. (20a)
and separating the variables, we obtain two independent homogeneous differential
equations in $\bar{\bar{q}}_1$ and $\bar{q}_3$. The initial and boundary conditions to solve the
differential equation for $\bar{\bar{q}}_1$ are obtained by substituting Eq. (25) in Eqs.
(9b,c,d). The initial and boundary conditions for the $\bar{q}_3$-equation can be
obtained by substituting Eq. (24) in Eqs. (20b,c,d), and using the initial
and boundary conditions for $\bar{\bar{q}}_1$ to simplify the resulting expressions. The
final expressions for the two sets of equations thus obtained can be written
as follows:

$$U \, \partial \bar{\bar{q}}_1 / \partial x = K_z \, \partial^2 \bar{\bar{q}}_1 / \partial z^2 - \bar{\bar{q}}_1 / \tau_c \, , \qquad 0 < x \, , \, z < \infty \qquad (26a)$$

$$\bar{\bar{q}}_1(0,z) = \exp \left\{ \frac{W_2(z-H)}{2K_z} \right\} \cdot \delta(z-H) = \bar{\bar{\psi}}_1(z) \qquad (26b)$$

$$[\partial \bar{\bar{q}}_1 / \partial z]_{z=0} = h_3 \cdot [\bar{\bar{q}}_1]_{z=0} \qquad (26c)$$

$$\bar{\bar{q}}_1(x,\infty) = 0 \qquad (26d)$$

where

$$h_3 = V_{13}/K_z \, , \qquad V_{13} = V_{11} - (W_1 - W_2)/2 \qquad (26e)$$

and

$$U \, \partial \bar{q}_3 / \partial x = K_z \, \partial^2 \bar{q}_3 / \partial z^2 \, , \qquad 0 < x \, , \, z < \infty \qquad (27a)$$

$$\bar{q}_3(0,z) = (Q_2/Q_1 + \gamma) \cdot \exp \left\{ \frac{W_2(z-H)}{2K_z} \right\} \cdot \delta(z-H) = \bar{\psi}_3(z) \qquad (27b)$$

$$[\partial \bar{q}_3 / \partial z - h_2 \cdot \bar{q}_3]_{z=0} = - h_2 \cdot \phi_3(x) \qquad (27c)$$

$$\bar{q}_3(x,\infty) = 0 \qquad (27d)$$

where

$$\phi_3(x) = - \frac{\gamma}{h_2} \left[ h_1 - h_2 - \frac{(W_1 - W_2)}{2K_z} \right] \cdot \bar{\bar{q}}_1(x,0) \qquad (28)$$

is the inhomogeneity in the boundary condition (27c). Thus, the transformation (24), which is used to remove the inhomogeneity in the differential equation (20a), transforms the homogeneous boundary condition, Eq. (20c), into

a nonhomogeneous boundary condition of the third kind. Nevertheless, it will be shown later that, unlike the nonhomogeneous differential equation set (20), we can solve Eq. (27) with relative ease, if $\bar{\bar{q}}_1(x,0)$ in Eq. (28) is given from the solution of Eq. (26).

The solution of Eq. (26) can be now expressed as

$$\bar{\bar{q}}_1(x,z) = \exp(-x/U\tau_c) \cdot \int_0^\infty \bar{\bar{\psi}}_1(\xi) \cdot G_3(x,z,\xi)d\xi, \qquad (29)$$

where $\bar{\bar{\psi}}_1(\xi)$ is obtained from the initial condition (26b), and the Green's function $G_3$ is given by

$$G_3(x,z,\xi) = \frac{1}{L_z} \left[ \exp\left\{ \frac{-(z-\xi)^2 U}{4K_z x} \right\} + \exp\left\{ \frac{-(z+\xi)^2 U}{4K_z x} \right\} \right.$$

$$\left. - 2h_3 \cdot \int_0^\infty \cdot \exp\left\{ \frac{-(z+\xi+\eta)^2 U}{4K_z x} - h_3\eta \right\} d\eta \right] \qquad (30)$$

After term-by-term integration, the final form of the solution, Eq. (29), can be written as

$$\bar{\bar{q}}_1(x,z) = \exp(-x/U\tau_c) \cdot \frac{1}{L_z} [e^{-r} + e^{-s} \cdot (1 - \alpha_3)] \qquad (31)$$

where

$$\alpha_3 = L_z h_3 e^{\xi_3^2} \text{ erfc } \xi_3$$

$$\xi_3 = \frac{z + H}{2\sqrt{K_z x/U}} + h_3 \sqrt{K_z x/U} \qquad (32)$$

and r and s are defined in (14).

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Now we can proceed to solve Eq. (27). First, we set z=0 in Eq. (31) and substitute the resulting equation for $\bar{\bar{q}}_1(x,0)$ in Eq. (28). After simplification, the final expression for the inhomogeneity, $\phi_3(x)$, in the boundary condition (27c) is given by

$$\phi_3(x) = \frac{-\gamma}{h_2} \left[ h_1 - h_2 - \frac{(W_1-W_2)}{2K_z} \right] \cdot \left[ \frac{1}{\sqrt{\pi K_z x/U}} \cdot \exp\left( \frac{-H^2 U}{4K_z x} - \frac{x}{U\tau_c} \right) \right.$$

$$\left. - h_3 \exp\left\{ \frac{h_3^2 K_z x}{U} + h_3 H - \frac{x}{U\tau_c} \right\} \cdot \mathrm{erfc}\left\{ \frac{H + 2h_3 K_z x/U}{2\sqrt{K_z x/U}} \right\} \right] \quad (33)$$

Following Budak et al. (1964), the analytical solution of Eq. (27) can be now written as

$$\bar{q}_3(x,z) = \bar{q}_{3A} + \bar{q}_{3B} \quad (34a)$$

where

$$\bar{q}_{3A}(x,z) = \int_0^\infty \bar{\psi}_3(\xi) \cdot G_2(x,z,\xi) \, d\xi \quad (34b)$$

$$\bar{q}_{3B}(x,z) = h_2 \cdot \left[ \frac{K_z}{\pi U} \right]^{\frac{1}{2}} \cdot \int_0^x \frac{\phi_3(x')}{\sqrt{x-x'}} \left[ \exp\left\{ \frac{-z^2 U}{4K_z(x-x')} \right\} \right.$$

$$\left. - h_2 \cdot \int_0^\infty \exp\left\{ \frac{-(z+\eta)^2 U}{4K_z(x-x')} - h_2\eta \right\} d\eta \right] dx' \quad (34c)$$

Here $G_2$ is the Green's function given in Eq. (23), and $\bar{\psi}_3$ and $\phi_3$ are the functions defined in Eqs. (27b) and (33), respectively. $\bar{q}_{3A}$ gives the contribution of the initial condition (27b), and $\bar{q}_{3B}$ gives the contribution of the inhomogeneity in the boundary condition (27c), to the solution $\bar{q}_3(x,z)$.

The evaluation of $\bar{q}_{3A}$ is straightforward. The final expression can be written as

$$\bar{q}_{3A}(x,z) = (Q_2/Q_1 + \gamma) \cdot \frac{1}{L_z} \left[ e^{-r} + e^{-s} \cdot (1 - \alpha_2) \right] \tag{35a}$$

where

$$\alpha_2 = L_z h_2 e^{\xi_2^2} \text{ erfc } \xi_2 \tag{35b}$$

$$\xi_2 = \frac{z+H}{2\sqrt{K_z x/U}} + h_2 \sqrt{K_z x/U}$$

To solve for $\bar{q}_{3B}$, first we integrate with respect to $\eta$ in Eq. (34c), substitute for $\phi_3(x')$ from Eq. (33), and considerably rearrange and simplify the resulting equation. The final expression for $\bar{q}_{3B}$ can be written as

$$\bar{q}_{3B}(x, z) = - \gamma \frac{(V_{21} - V_{22})}{K_z} \cdot F_1(x,z) \tag{36a}$$

where

$$V_{21} = V_{d1} - W_1 = V_{11} - W_1/2$$

$$V_{22} = V_{d2} - W_2 = V_{12} - W_2/2 \tag{36b}$$

and $F_1(x,z)$ is a function given by

$$F_1(x,z) = \frac{1}{\pi} \int_0^x \frac{1}{\sqrt{x'(x-x')}} \cdot \exp \left\{ \frac{-z^2 U}{4K_z(x-x')} - \frac{H^2 U}{4K_z x'} - \frac{x'}{U\tau_c} \right\} \cdot$$

$$\left[ 1 - \sqrt{\pi K_z x'/U} \; h_3 \; e^{\xi_4^2} \text{ erfc } \xi_4 \right] \cdot$$

$$\left[ 1 - \sqrt{\pi K_z (x-x')/U} \; h_2 \; e^{\xi_5^2} \text{ erfc } \xi_5 \right] dx' \tag{36c}$$

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Here,

$$\xi_4 = \frac{H + 2h_3 \, K_z x'/U}{2 \, \sqrt{K_z x'/U}}$$

(36d)

$$\xi_5 = \frac{z + 2h_2 \, K_z \, (x-x')/U}{2 \, \sqrt{K_z(x-x')/U}}$$

are nondimensional functions. The integration with respect to x' in Eq. (36c) cannot be done analytically. Therefore, $F_1(x,z)$ needs to be numerically evaluated.

The expression for $\bar{q}_3(x,z)$, from Eqs. (34a), (35a), and (36a), can be now written as

$$\bar{q}_3(x,z) = (Q_2/Q_1 + \gamma) \cdot \frac{1}{L_z} \left[ e^{-r} + e^{-s} \cdot (1 - \alpha_2) \right]$$

$$- \gamma \, \frac{(V_{21} - V_{22})}{K_z} \cdot F_1(x,z)$$

(37)

This is the analytical solution of Eq. (27). From Eqs. (24), (31), and (37), we obtain

$$\bar{q}_2(x,z) = (Q_2/Q_1 + \gamma) \cdot \frac{1}{L_z} \left[ e^{-r} + e^{-s} \cdot (1 - \alpha_2) \right]$$

$$- \gamma \, \exp(-x/U\tau_c) \cdot \frac{1}{L_z} \left[ e^{-r} + e^{-s} \cdot (1 - \alpha_3) \right]$$

$$- \gamma \, \frac{(V_{21} - V_{22})}{K_z} \cdot F_1(x,z)$$

(38)

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This is the analytical solution of Eq. (20). Finally, from Eqs. (19) and (38), the analytical solution of Eq. (18) can be written as

$$q_2(x,z) = g'_{22} / L_z \qquad (39a)$$

where

$$g'_{22}(x,z) = e^{-\beta_2^2} \cdot \left[ (Q_2/Q_1 + \gamma) \cdot \left\{ e^{-r} + e^{-s} \cdot (1 - \alpha_2) \right\} \right.$$

$$- \gamma \exp(-x/U\tau_c) \cdot \left\{ e^{-r} + e^{-s} \cdot (1 - \alpha_3) \right\}$$

$$\left. - \gamma (V_{21} - V_{22})(L_z/K_z) \cdot F_1(x,z) \right] \qquad (39b)$$

is a nondimensional function. The prime indicates the modification of function $g_2(x,z)$ of the secondary pollutant (denoted by the second subscript 2) for the effects of deposition, sedimentation, and chemical transformation.

The physical meaning of the various terms in Eq. (39b) is as follows: The first term has contributions from $Q_2/Q_1$ and $\gamma$; the $Q_2/Q_1$ part of this term accounts for the direct emission of the secondary pollutant, and the $\gamma$ part of this term assumes that all the primary pollutant is transformed into the secondary pollutant. The second term corrects this spurious assumption by subtracting the equivalent of the primary pollutant still available for transformation at any given location $(x,z)$. The third (last) term accounts for the effect of differences in the removal rates of the two pollutant species by deposition and sedimentation; $F_1(x,z)$ in this term essentially represents a weighting function such that $0 \le F_1 \le 1$, as will be shown later. It can be easily seen the contribution of this term is zero when $V_{21} = V_{22} \ge 0$, i.e., when the deposition and sedimentation velocities of the two pollutants are equal.

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In the absence of a chemical coupling between the two species, all the terms with $\gamma$ will be identically zero, and Eq. (39b) reduces to

$$g'_{22}(x,z) \;=\; Q_2/Q_1 \;\cdot\; e^{-\beta_2^2} \left[\; e^{-r} \;+\; e^{-s} \cdot (1 - \alpha_2) \;\right] \qquad (39c)$$

which is the concentration algorithm for a chemically-independent, non-reactive pollutant produced only by direct emission from a source of strength $Q_2$. For <u>this</u> case alone, we can rewrite Eqs. (4) and (39c) as

$$C_2(x,y,z) \;=\; Q_2/U \;\cdot\; p(x,y) \;\cdot\; q_2(x,z)$$

$$g'_{22}(x,z) \;=\; e^{-\beta_2^2} \left[\; e^{-r} \;+\; e^{-s} \cdot (1 - \alpha_2) \;\right] \qquad (40a)$$

where $p$ and $q_2$ are given by Eqs. (7) and (39a), respectively. This expression for $g'_{22}$ is similar in form to that of $g'_{21}$ given in Eq. (16b) for the primary pollutant.

For $W_1 = W_2 = 0$ and $Q_2 = 0$, Eq. (39b) reduces to

$$g'_{22}(x,z) = \gamma \left[ \left\{ e^{-r} + e^{-s} (1 - \alpha_1) \right\} \left\{ 1 - \exp(-x/U\tau_c) \right\} \right.$$

$$\left. + e^{-s} (\alpha_1 - \alpha_2) - (V_{d1} - V_{d2})(L_z/K_z) \cdot F_1(x,z) \right] \qquad (40b)$$

This equation agrees with the corresponding expression given by Lee (1980), except that the latter paper incorrectly shows $2H/K_z$ instead of $L_z/K_z$ in the last term.

For $V_{d1} = V_{d2} = V_d$ and $W_1 = W_2 = W$, Eq. (39b) reduces to

$$g'_{22}(x,z) = e^{-\beta^2} \cdot \left\{ e^{-r} + e^{-s} (1 - \alpha) \right\} \cdot$$

$$\left[ Q_2/Q_1 + \gamma \left\{ 1 - \exp(-x/U\tau_c) \right\} \right] \tag{40c}$$

This agrees with the expression given by Rao (1975), who assumed equal non-zero deposition and sedimentation velocities for the two species for simplicity. For $V_d = 0$ and $W = 0$, Eq. (40c) reduces to

$$g'_{22}(x,z) = (e^{-r} + e^{-s}) \left[ Q_2/Q_1 + \gamma \left\{ 1 - \exp(-x/U\tau_c) \right\} \right] \tag{40d}$$

which agrees with the expression given by Heines and Peters (1973), who considered only chemical transformation and derived this result based on a simple component mass balance. Thus, we can obtain all the known solutions for simpler problems from the analytical solution (39b) of the general problem considered here.

PARAMETERIZATION OF CONCENTRATIONS

In order to facilitate the practical application of the analytical solutions, the eddy diffusivities $K_y$ and $K_z$ are expressed here in terms of $\sigma_y$ and $\sigma_z$, the standard deviations of the crosswind and vertical Gaussian concentration distributions, respectively, as follows:

$$K_y = \frac{U}{2} \frac{d\sigma_y^2}{dx} \quad , \quad K_z = \frac{U}{2} \frac{d\sigma_z^2}{dx} \tag{41}$$

Thus, for Fickian diffusion, $K_y$ and $K_z$ can be expressed by the relations

$$K_y = \sigma_y^2 \cdot U/2x \quad , \quad K_z = \sigma_z^2 \cdot U/2x, \tag{42}$$

in order to utilize the vast amount of empirical data on the Gaussian plume

parameters $\sigma_y$ and $\sigma_z$ available in the literature for a variety of meteorological

and terrain conditions. An excellent review and summary of these data can be

found in Gifford (1976). Equation (42), in combination with the Gaussian

assumption (see, e.g., Gifford, 1968), forms the basis for the practical

plume diffusion formulas that are found in the applications literature.


In order to parameterize the expressions for concentrations under

various stability conditions and to considerably reduce the difficulty in

typing the equations, we adopt the following nondimensionalization scheme:

All velocities are nondimensionalized by U, the constant mean wind speed.

The horizontal downwind distance x and all vertical height quantities are

nondimensionalized by $\sqrt{2}\,\sigma_z$; the transformation time scale $\tau_c$ is nondimen-

sionalized by $\sqrt{2}\,\sigma_z/U$. The horizontal crosswind distance y is nondimen-

sionalized by $\sqrt{2}\,\sigma_y$. Thus, we define

$$\hat{V}_{d1} = V_{d1}/U \qquad , \qquad \hat{V}_{d2} = V_{d2}/U$$

$$\hat{W}_1 = W_1/U \qquad , \qquad \hat{W}_2 = W_2/U$$

$$\hat{V}_{11} = \hat{V}_{d1} - \hat{W}_1/2 \quad , \quad \hat{V}_{12} = \hat{V}_{d2} - \hat{W}_2/2$$

$$\hat{V}_{13} = \hat{V}_{11} - (\hat{W}_1 - \hat{W}_2)/2$$

$$\hat{V}_{21} = \hat{V}_{d1} - \hat{W}_1 \quad , \quad \hat{V}_{22} = \hat{V}_{d2} - \hat{W}_2 \tag{43}$$

$$\hat{x} = x/\sqrt{2}\,\sigma_z \qquad , \qquad \hat{z} = z/\sqrt{2}\,\sigma_z$$

$$\hat{H} = H/\sqrt{2}\,\sigma_z \qquad , \qquad \hat{L} = L/\sqrt{2}\,\sigma_z$$

$$\hat{\tau}_c = \tau_c U/\sqrt{2}\,\sigma_z \quad , \quad \hat{y} = y/\sqrt{2}\,\sigma_y$$

where the capped quantities denote the nondimensionalized variables, and L is the mixing height.

From Eqs. (3), (7), (8), (14), (16), (42), and (43), we can now rewrite the expression for the primary pollutant concentration as follows:

$$C_1(\hat{x}, \hat{y}, \hat{z}) = \frac{Q_1}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g'_{21}}{L_z} \tag{44a}$$

$$g_1(\hat{x}, \hat{y}) = \exp(-\hat{y}^2) \tag{44b}$$

$$g'_{21}(\hat{x}, \hat{z}) = \exp(-\beta_1^2 - \hat{x}/\hat{\tau}_c) \left[ e^{-r} + e^{-s} \cdot (1 - \alpha_1) \right] \tag{44c}$$

$$L_y = \sqrt{2\pi}\, \sigma_y \quad , \quad L_z = \sqrt{2\pi}\, \sigma_z \tag{44d}$$

where

$$r = (\hat{z} - \hat{H})^2 \quad , \quad s = (\hat{z} + \hat{H})^2$$

$$\beta_1^2 = 2\hat{W}_1(\hat{z} - \hat{H})\,\hat{x} + \hat{W}_1^2\,\hat{x}^2 \tag{44e}$$

$$\alpha_1 = 4\sqrt{\pi}\,\hat{V}_{11}\,\hat{x}\, e^{\xi_1^2}\, \text{erfc}\, \xi_1$$

$$\xi_1 = \hat{z} + \hat{H} + 2\,\hat{V}_{11}\,\hat{x}$$

Equation (44) clearly shows that concentration $C_1$ depends on the ratios $W_1/U$ and $V_{d1}/U$, not on $W_1$ and $V_{d1}$ per se. Thus, the effect on $C_1$ of large values of $W_1$ and $V_{d1}$ at high wind speeds is the same as that of small values of $W_1$ and $V_{d1}$ at low wind speeds, provided $W_1/U$ and $V_{d1}/U$ remain constant. The effect of deposition can be seen as a multiplication of the contribution

of the image-source or reflection term, $e^{-s}$, by a factor $-1 \leq (1 - \alpha_1) \leq 1$.
In the absence of chemical decay ($\hat{\tau}_c = \infty$), Eq. (44) agrees with the expression
for concentration given by Rao (1981). In the trivial case of negligible
deposition and chemical decay ($\hat{W}_1 = 0$, $\hat{V}_{d1} = 0$, $\hat{\tau}_c = \infty$), this equation reduces
to the well-known Gaussian plume model with $g'_{21} = g_2$, where $g_2(x,z)$ is defined
in Eq. (17).

For a ground-level receptor ($\hat{z}=0$), the concentration algorithm for the
primary pollutant reduces to

$$g'_{21}(\hat{x},0) = \exp(-\beta_1^2 - \hat{H}^2 - \hat{x}/\hat{\tau}_c) \cdot (2 - \alpha_1) \qquad (45a)$$

where 
$$\beta_1^2 = - 2 \hat{W}_1 \hat{x} \hat{H} + \hat{W}_1^2 \hat{x}^2$$

$$\alpha_1 = 4\sqrt{\pi} \hat{V}_{11} \hat{x} \ e^{\xi_1^2} \ \text{erfc} \ \xi_1 \qquad (45b)$$

$$\xi_1 = \hat{H} + 2 \hat{V}_{11} \hat{x}$$

Further simplifications of this equation are possible by setting $\hat{H} = 0$ for
ground-level sources, and $\hat{W} = 0$ and $\hat{V}_{11} = \hat{V}_{d1}$ for gases and small particles
with negligible settling.

From Eqs. (4), (7), (19b), (32), (35b), (39), (42), and (43), the
parameterized expression for the secondary pollutant concentration can be
written as follows:

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$$C_2(\hat{x},\hat{y},\hat{z}) = \frac{Q_1}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g_{22}'}{L_z} \tag{46a}$$

$$g_{22}'(\hat{x},\hat{z}) = e^{-\beta_2^2} \left[ (Q_2/Q_1 + \gamma) \left\{ e^{-r} + e^{-s} \cdot (1 - \alpha_2) \right\} \right.$$

$$-\gamma \exp(-\hat{x}/\hat{t}_c) \left\{ e^{-r} + e^{-s} \cdot (1 - \alpha_3) \right\}$$

$$\left. -\gamma 4\sqrt{\pi} \, (\hat{V}_{21} - \hat{V}_{22}) \, \hat{x} \cdot F_1(\hat{x},\hat{z}) \right] \tag{46b}$$

where $g_1(\hat{x},\hat{y})$, $L_y$, $L_z$, $r$, and $s$ are defined in Eq. (44), and the remaining quantities are as follows:

$$\beta_2^2 = 2 \hat{W}_2 \, (\hat{z} - \hat{H}) \, \hat{x} + \hat{W}_2^2 \, \hat{x}^2$$

$$\alpha_2 = 4\sqrt{\pi} \, \hat{V}_{12} \, \hat{x} \, e^{\xi_2^2} \, \text{erfc} \, \xi_2$$

$$\xi_2 = \hat{z} + \hat{H} + 2 \hat{V}_{12} \, \hat{x} \tag{46c}$$

$$\alpha_3 = 4\sqrt{\pi} \, \hat{V}_{13} \, \hat{x} \, e^{\xi_3^2} \, \text{erfc} \, \xi_3$$

$$\xi_3 = \hat{z} + \hat{H} + 2 \hat{V}_{13} \, \hat{x}$$

From Eqs. (36c), (36d), (42), and (43), the nondimensional function $F_1(\hat{x},\hat{z})$ in Eq. (46b) can be parameterized as

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$$F_1(\hat{x},\hat{z}) = \frac{1}{\pi}\int_0^1 \frac{1}{\sqrt{t(1-t)}} \exp\left(\frac{-\hat{z}^2}{1-t} - \frac{\hat{H}^2}{t} - \frac{\hat{x}t}{\hat{\tau}_c}\right) \cdot$$

$$\left[1 - 2\hat{V}_{13}\hat{x}\sqrt{\pi t}\, e^{\xi_4^2}\, \text{erfc}\,\xi_4\right] \cdot$$

$$\left[1 - 2\hat{V}_{12}\hat{x}\sqrt{\pi(1-t)}\, e^{\xi_5^2}\, \text{erfc}\,\xi_5\right] dt \qquad (46d)$$

where
$$\xi_4 = \hat{H}/\sqrt{t} + 2\hat{V}_{13}\hat{x}\sqrt{t} \qquad (46e)$$

$$\xi_5 = \hat{z}/\sqrt{1-t} + 2\hat{V}_{12}\hat{x}\sqrt{1-t}$$

and $t = \hat{x}'/\hat{x}$ is the normalized integration variable.

Equation (46b) calculates $g'_{22}$ as the sum of contributions from the three major terms on the right-hand side of this equation. The physical significance of these terms has been already explained in the discussion following Eq. (39b). In the absence of a direct emission of the secondary pollutant (i.e., $Q_2 = 0$), a delicate balance exists between these three terms, as shown in the next section. The third term, which arises due to the differences in the deposition rates of the two pollutant species, becomes important at large x and, therefore, cannot be ignored. The weighting function in this term $F_1(\hat{x},\hat{z})$, given by Eq. (46d), should be evaluated by numerical integration to a sufficiently high degree of accuracy.

For a ground-level receptor ($\hat{z}=0$), the concentration algorithm for the secondary pollutant reduces to:

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$$g'_{22}(\hat{x},0) = e^{-\beta_2^2} \left[ (Q_2/Q_1 + \gamma) \; e^{-\hat{H}^2} \cdot (2 - \alpha_2) \right.$$

$$-\gamma \exp(-\hat{H}^2 - \hat{x}/\hat{\tau}_c) \cdot (2 - \alpha_3)$$

$$\left. -\gamma \, 4\sqrt{\pi} \, (\hat{V}_{21} - \hat{V}_{22}) \, \hat{x} \cdot F_1(\hat{x},0) \right] \tag{47a}$$

where

$$\beta_2^2 = -2 \, \hat{W}_2 \, \hat{x} \, \hat{H} + \hat{W}_2^2 \, \hat{x}^2$$

$$\alpha_2 = 4\sqrt{\pi} \, \hat{V}_{12} \, \hat{x} \; e^{\xi_2^2} \; \text{erfc} \; \xi_2$$

$$\alpha_3 = 4\sqrt{\pi} \, \hat{V}_{13} \, \hat{x} \; e^{\xi_3^2} \; \text{erfc} \; \xi_3 \tag{47b}$$

$$\xi_2 = \hat{H} + 2 \, \hat{V}_{12} \, \hat{x} \; , \quad \xi_3 = \hat{H} + 2 \, \hat{V}_{13} \, \hat{x}$$

and

$$F_1(\hat{x},0) = \frac{1}{\pi} \int_0^1 \frac{1}{\sqrt{t(1-t)}} \quad \exp\left( \frac{-\hat{H}^2}{t} - \frac{\hat{x}t}{\hat{\tau}_c} \right) \cdot$$

$$\left[ 1 - \sqrt{\pi} \, (\xi_4 - \hat{H}/\sqrt{t}) \; e^{\xi_4^2} \; \text{erfc} \; \xi_4 \right]$$

$$\left[ 1 - \sqrt{\pi} \, \xi_5 \; e^{\xi_5^2} \; \text{erfc} \; \xi_5 \right] \; dt \tag{47c}$$

where

$$\xi_4 = \hat{H}/\sqrt{t} + 2 \, \hat{V}_{13} \, \hat{x} \, \sqrt{t}$$

$$\tag{47d}$$

$$\xi_5 = 2 \, \hat{V}_{12} \, \hat{x} \, \sqrt{1 - t}$$

Further simplifications of Eq. (47) are possible by setting $\hat{H} = 0$ for ground-level sources, and $\hat{W}_1 = \hat{W}_2 = 0$, $\hat{V}_{13} = \hat{V}_{d1}$, and $\hat{V}_{12} = \hat{V}_{d2}$ when both species are gases or small particles with negligible settling.

WELL-MIXED REGION

Under unstable or neutral atmospheric conditions, when the plume travels sufficiently far away from the source, the pollutant is generally well-mixed by atmospheric turbulence, resulting in a uniform vertical concentration profile between the ground and the stable layer aloft at a height L. This concentration, which is independent of source height as well as the receptor height, can be calculated as the average concentration in a mixed layer of depth L. Following Turner (1970), we assume that the plume is well-mixed for $x \geq 2\, x_m$, where $x_m$ is the downwind distance at which $\sigma_z(x_m)=0.47\, L$.

The primary pollutant concentration in the well-mixed region can be calculated as follows:

$$C_1(\hat{x},\hat{y},\hat{z}) = \frac{Q_1}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g'_{41}}{L} \tag{48a}$$

$$g_1(\hat{x},\hat{y}) = \exp(-\hat{y}^2) \tag{48b}$$

$$g'_{41}(\hat{x}) = \int_0^\infty \left[ \frac{g'_{21}}{L_z} \right]_{H=0} dz = \frac{1}{\sqrt{\pi}} \int_0^\infty \left[ g'_{21}(\hat{x},\hat{z}) \right]_{\hat{H}=0} d\hat{z} \tag{48c}$$

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Substituting for $g'_{21}(\hat{x},\hat{z})$ from Eq. (44) and carrying out the integration in Eq. (48c), we obtain the following:

For $\hat{V}_{d1} \neq \hat{W}_1$ or $\hat{V}_{21} \neq 0$,

$$g'_{41}(\hat{x}) = \exp(-\beta_1^2 - \hat{x}/\hat{\tau}_c) \left[ (\hat{V}_{11}/\hat{V}_{21}) \, e^{\xi_1^2} \, \text{erfc} \, \xi_1 \right.$$

$$\left. - (\hat{W}_1/2\hat{V}_{21}) \, e^{\beta_1^2} \, \text{erfc} \, \beta_1 \right] \qquad (48d)$$

where    $\xi_1 = 2 \hat{V}_{11} \hat{x}$    and    $\beta_1 = \hat{W}_1 \hat{x}$.

This algorithm applies to gases or small particles. This equation is indeterminate when $\hat{V}_{d1} = \hat{W}_1$ or $\hat{V}_{21} = 0$. For this case, $g'_{41}(\hat{x})$ can be determined by setting $\hat{W}_1 = \hat{V}_{d1}$ in the expression for $g'_{21}$ in Eq. (44) and then integrating as indicated in Eq. (48c). Alternately, one can take the limit of Eq. (48d) as $\hat{W}_1 \longrightarrow \hat{V}_{d1}$. Thus, we obtain the limiting expression for $g'_{41}(\hat{x})$ for large particles as follows:

For $\hat{V}_{d1} = \hat{W}_1$ or $\hat{V}_{21} = 0$,

$$g'_{41}(\hat{x}) = \exp(-\xi_1^2 - \hat{x}/\hat{\tau}_c) \left[ (1 + 2 \, \xi_1^2) \, e^{\xi_1^2} \, \text{erfc} \, \xi_1 - 2 \, \xi_1/\sqrt{\pi} \right] \qquad (48e)$$

where    $\xi_1 = 2 \hat{V}_{11} \hat{x} = \hat{V}_{d1} \hat{x} = \hat{W}_1 \hat{x}$.

Equations (48d) and (48e) agree with the corresponding expressions given by Rao (1981) when $\hat{\tau}_c = \infty$.

The secondary pollutant concentration in the well-mixed region can be calculated as follows:

$$C_2(\hat{x},\hat{y},\hat{z}) = \frac{Q_1}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g'_{42}}{L} \qquad (49a)$$

$$g'_{42}(\hat{x}) = \int_0^\infty \left[ \frac{g'_{22}}{L_z} \right]_{H=0} dz = \frac{1}{\sqrt{\pi}} \int_0^\infty \left[ g'_{22}(\hat{x},\hat{z}) \right]_{\hat{H}=0} d\hat{z} \qquad (49b)$$

Substituting for $g'_{22}(\hat{x},\hat{z})$ from Eq. (46) and carrying out the integration in Eq. (49b), we obtain the following:

For $\hat{V}_{21} \neq 0$ and $\hat{V}_{22} \neq 0$,

$$g'_{42}(\hat{x}) = e^{-\beta_2^2} \left[ (Q_2/Q_1 + \gamma) \left\{ (\hat{V}_{12}/\hat{V}_{22}) e^{\xi_2^2} \operatorname{erfc} \xi_2 - (\hat{W}_2/2\hat{V}_{22}) e^{\beta_2^2} \operatorname{erfc} \beta_2 \right\} \right.$$

$$- \gamma e^{-\hat{x}/\hat{\tau}_c} \left\{ (\hat{V}_{13}/\hat{V}_{21}) e^{\xi_3^2} \operatorname{erfc} \xi_3 - (\hat{W}_2/2\hat{V}_{21}) e^{\beta_2^2} \operatorname{erfc} \beta_2 \right\}$$

$$\left. - \gamma 4\sqrt{\pi} (\hat{V}_{21} - \hat{V}_{22}) \hat{x} \cdot F_2(\hat{x}) \right] \qquad (50a)$$

where 
$$\xi_2 = 2 \hat{V}_{12} \hat{x} , \quad \beta_2 = \hat{W}_2 \hat{x}$$

$$\xi_3 = 2 \hat{V}_{13} \hat{x} , \quad \hat{V}_{13} = \hat{V}_{11} - (\hat{W}_1 - \hat{W}_2)/2 \qquad (50b)$$

$$F_2(\hat{x}) = \int_0^\infty \left[ F_1(\hat{x},\hat{z}) \right]_{\hat{H}=0} d\hat{z}$$

Substituting for $F_1(\hat{x}, \hat{z})$ from Eq. (46d) and integrating, we obtain

$$F_2(\hat{x}) = \frac{1}{2\pi} \int_0^1 \frac{1}{\sqrt{t}} \exp(-\hat{x}t/\hat{t}_c) \left[ 1 - \sqrt{\pi} \, \xi_4 \, e^{\xi_4^2} \, \text{erfc} \, \xi_4 \right] \cdot$$

$$\left[ (\hat{V}_{12}/\hat{V}_{22}) \, e^{\xi_5^2} \, \text{erfc} \, \xi_5 - (\hat{W}_2/2\hat{V}_{22}) \, e^{\xi_6^2} \, \text{erfc} \, \xi_6 \right] dt, \qquad (50c)$$

where $\qquad \xi_4 = \xi_3 \sqrt{t}, \quad \xi_5 = \xi_2 \sqrt{1-t}, \quad \xi_6 = \beta_2 \sqrt{1-t}$ $\qquad (50d)$

Equation (50) is applicable when the two pollutant species are either gases or small particles. In the large-particle limit of $\hat{W} \longrightarrow \hat{V}_d$ for one or both of the species, three other forms of this algorithm can be derived as follows:

For $\hat{V}_{21} \neq 0$ and $\hat{V}_{22} = 0$,

$$g'_{42}(\hat{x}) = e^{-\xi_2^2} \left[ (Q_2/Q_1 + \gamma) \left\{ (1 + 2\xi_2^2) \, e^{\xi_2^2} \, \text{erfc} \, \xi_2 - 2\xi_2/\sqrt{\pi} \right\} \right.$$

$$- \gamma \, e^{-\hat{x}/\hat{t}_c} \left\{ (\hat{V}_{13}/\hat{V}_{21}) \, e^{\xi_3^2} \, \text{erfc} \, \xi_3 - (\hat{W}_2/2\hat{V}_{21}) \, e^{\xi_2^2} \, \text{erfc} \, \xi_2 \right\}$$

$$\left. - \gamma \, 4\sqrt{\pi} \, \hat{V}_{21} \, \hat{x} \cdot F_2(\hat{x}) \right] \qquad (51a)$$

where $\qquad \xi_2 = 2 \hat{V}_{12} \, \hat{x} = \hat{V}_{d2} \, \hat{x} = \hat{W}_2 \, \hat{x} = \beta_2$

$$\xi_3 = 2 \hat{V}_{13} \, \hat{x}$$

$$F_2(\hat{x}) = \frac{1}{2\pi}\int_0^1 \frac{1}{\sqrt{t}} \exp\left(-\hat{x}t/\hat{\tau}_c\right) \cdot \left[ 1 - \sqrt{\pi}\ \xi_4\ e^{\xi_4^2}\ \text{erfc}\ \xi_4 \right] \cdot$$

$$\left[ (1 + 2\ \xi_5^2)\ e^{\xi_5^2}\ \text{erfc}\ \xi_5\ -\ 2\ \xi_5/\sqrt{\pi} \right]\ dt, \tag{51b}$$

with $\qquad \xi_4 = \xi_3\ \sqrt{t}\ ,\quad \xi_5 = \xi_2\ \sqrt{1-t}\ \cdot$

Equation (51) is applicable when species-1 is a gaseous or small-particle pollutant, and species-2 consists of large particles.

For $\hat{V}_{21} = 0$ and $\hat{V}_{22} \neq 0$,

$$g'_{42}(\hat{x}) = e^{-\xi_3^2}\left[ (Q_2/Q_1 + \gamma)\left\{ (\hat{V}_{12}/\hat{V}_{22})\ e^{\xi_2^2}\ \text{erfc}\ \xi_2\ -\ (\hat{W}_2/2\hat{V}_{22})\ e^{\xi_3^2}\ \text{erfc}\ \xi_3 \right\} \right.$$

$$-\ \gamma\ e^{-\hat{x}/\hat{\tau}_c}\left\{ (1 + 2\ \xi_3^2)\ e^{\xi_3^2}\ \text{erfc}\ \xi_3\ -\ 2\ \xi_3/\sqrt{\pi} \right\}$$

$$\left. +\ \gamma\ 4\sqrt{\pi}\ \hat{V}_{22}\ \hat{x} \cdot F_2(\hat{x}) \right]. \tag{52}$$

where $\qquad \xi_2 = 2\ \hat{V}_{12}\ \hat{x}\ ,\quad \xi_3 = 2\ \hat{V}_{13}\ \hat{x} = \hat{W}_2\ \hat{x} = \beta_2\ ,$

and $F_2(\hat{x})$ is given by Eq. (50c). This algorithm applies when species-1 consists of large particles, and species-2 is a gaseous or small-particle pollutant.

For $\hat{V}_{21} = 0$ and $\hat{V}_{22} = 0$,

$$g'_{42}(\hat{x}) = \left[ Q_2/Q_1 + \gamma (1 - e^{-\hat{x}/\hat{t}_c}) \right] \cdot$$

$$e^{-\xi_2^2} \left\{ (1 + 2\xi_2^2) e^{\xi_2^2} \operatorname{erfc} \xi_2 - 2\xi_2/\sqrt{\pi} \right\} \qquad (53)$$

where $\qquad \xi_2 = \hat{W}_2 \hat{x} = \beta_2.$

This algorithm applies when both species consist only of large particles.

The physical situations represented by Eqs. (52) and (53) are unlikely to occur in reality, since any primary pollutant consisting only of large particles would not generally reside in the atmosphere long enough to produce significant concentrations of the secondary pollutant by chemical transformation (i.e., $x_{max}/U \ll \tau_c$). These algorithms are included here primarily for completeness of the solutions. Since the well-mixed region concentration algorithms are independent of $\hat{z}$, they apply to all heights $0 \le \hat{z} \le \hat{L}$.

PLUME TRAPPING

For $x_m < x < 2 x_m$, where $x_m$ is the downwind distance at which the plume upper boundary (corresponding to an isopleth representing one-tenth of the plume centerline concentration) extends to the height of the inversion lid, the mixing depth L should be included in the concentration algorithms. This is usually done through calculation of multiple eddy reflections (Turner, 1970) from both the ground and the stable layer aloft, when the plume is trapped between these two surfaces. For the general case which includes deposition, sedimentation, and chemical transformation, the concentration of the species at any height $\hat{z}$ in the plume trapping region can be expressed as

$$C_1(\hat{x},\hat{y},\hat{z}) = \frac{Q_1}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g'_{31}}{L_z} \qquad\qquad (54a)$$

$$C_2(\hat{x},\hat{y},\hat{z}) = \frac{Q_1}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g'_{32}}{L_z} \qquad\qquad (54b)$$

One can write the equations for $g'_{31}(\hat{x},\hat{z})$ and $g'_{32}(\hat{x},\hat{z})$, following Rao (1981). These expressions look similar to those given for $g'_{21}(\hat{x},\hat{z})$ and $g'_{22}(\hat{x},\hat{z})$, respectively, except that the effective plume height $\hat{H}$ will be replaced here by $\hat{H}_1 = \hat{H} + 2N\hat{L}$ and the equations are summed over N from $-\infty$ to $\infty$. In general, a maximum of $N = \pm 10$ eddy reflections are adequate to obtain convergence of the sum within a small tolerance.

A simpler alternate procedure suggested by Turner (1970) may be adopted if one is interested only in ground-level concentrations: We may calculate the ground-level centerline concentrations of each species at $x_m$ and $2x_m$ using the appropriate algorithms given earlier in this section, and then linearly interpolate between these values on a log-log plot of concentration versus downwind distance to obtain the ground-level centerline concentration at any x in the plume-trapping region.

TABLE 1


SUMMARY OF POINT SOURCE CONCENTRATION EQUATIONS:


Applicable Algorithms and Equation Numbers

|  | Primary Pollutant | Secondary Pollutant |
|---|---|---|
| 1. Near-source region $(0 < x \leq x_m)$ | $C_1 = \dfrac{Q_1}{U} \cdot \dfrac{g_1}{L_y} \cdot \dfrac{g'_{21}}{L_z}$ | $C_2 = \dfrac{Q_1}{U} \cdot \dfrac{g_1}{L_y} \cdot \dfrac{g'_{22}}{L_z}$ |
| (a) Elevated receptor $(z > 0)$ | Eq. (44) | Eq. (46) |
| (b) Ground-level receptor $(z = 0)$ | Eq. (45) | Eq. (47) |
| 2. Plume trapping region $(x_m < x < 2x_m)$ | $C_1 = \dfrac{Q_1}{U} \cdot \dfrac{g_1}{L_y} \cdot \dfrac{g'_{31}}{L_z}$ | $C_2 = \dfrac{Q_1}{U} \cdot \dfrac{g_1}{L_y} \cdot \dfrac{g'_{32}}{L_z}$ |
| (a) Elevated receptor $(z > 0)$ | Eq. (54a) | Eq. (54b) |
| (b) Ground-level receptor $(z = 0)$ | Interpolation | Interpolation |
| 3. Well-mixed region $(x \geq 2x_m)$ | $C_1 = \dfrac{Q_1}{U} \cdot \dfrac{g_1}{L_y} \cdot \dfrac{g'_{41}}{L}$ | $C_2 = \dfrac{Q_1}{U} \cdot \dfrac{g_1}{L_y} \cdot \dfrac{g'_{42}}{L}$ |
| any $z \geq 0$ | Eq. (48) | Eqs. (50 to 53) |

## SURFACE DEPOSITION FLUXES

The surface deposition fluxes of the primary and the secondary pollutants at ground-level receptors are calculated directly from Eqs. (1d) and (2d) as

$$D_1(\hat{x},\hat{y}) = V_{d1} \cdot C_1(\hat{x},\hat{y},0) \qquad (55a)$$

$$D_2(\hat{x},\hat{y}) = V_{d2} \cdot C_2(\hat{x},\hat{y},0) \qquad (55b)$$

D gives the amount of pollutant deposited per unit time per unit surface area, and is usually calculated as $kg/km^2$-hr, while seasonal estimates are expressed as $kg/km^2$-month. The estimation of the monthly or yearly surface deposition fluxes at a given downwind distance x from the source in a given wind-directional sector requires the knowledge of the fraction of the time that a mean wind of a given magnitude blows in that direction in a month or a year, respectively. To obtain D in $kg/km^2$-hr when $V_d$ is given in cm/s and C in $g/m^3$, the right-hand side of Eq. (55) should be multiplied by 36000. To obtain D in $\mu g/m^2$-hr when $V_d$ is given in cm/s and C in $\mu g/m^3$, the corresponding multiplication factor is 36. For D calculations, the ground-level receptor is generally defined as any receptor which is not higher than 1 meter above the local ground-level elevation.

## AREA SOURCES

Urban air pollution results from (a) elevated large point sources such as tall stacks of electric power plants and industries, (b) isolated line

sources such as highways, and (c) distributed area sources such as industrial parks, clustered highways, and busy interchanges, parking lots, and airports. Numerous small low-level point sources distributed over a broad area, such as smoke from chimneys of dwellings in an urban residential area, can be treated as an area source. Therefore, an urban diffusion model should be able to account for point, line, and area sources.

The line and area source problems are generally treated by integrating the point-source diffusion algorithms over a crosswind line or over an area. Differences between urban air pollution models occur only in the details of how the area source summation is carried out and in how various meteorological paremeters are included. The simple ATDL Area-Source Model described by Gifford (1970), Gifford and Hanna (1970), and Hanna (1971) is widely used in many of the current practical urban air pollution models, such as the Texas Episodic Model (TACB, 1979). We briefly describe below the derivation of the Gifford-Hanna algorithm for estimating the ground-level concentrations due to urban area sources.

Consider two equal grid squares with side $\Delta x$, one of them containing the ground-level area source emissions (Q), assumed to be located at the center of the square; the second square, also known as the "calculation grid square," contains a ground-level receptor (R) at its center. The wind (U) blows along the line from Q to R, as shown in Figure 1(a). The distances from the receptor R to the downwind and upwind edges of the emission grid square are denoted by $x_1$ and $x_2$, respectively. Since the two grid squares are equal in size, $x_1$ and $x_2$ are identical to the distances measured from Q to the upwind and downwind edges, respectively, of the calculation grid square,
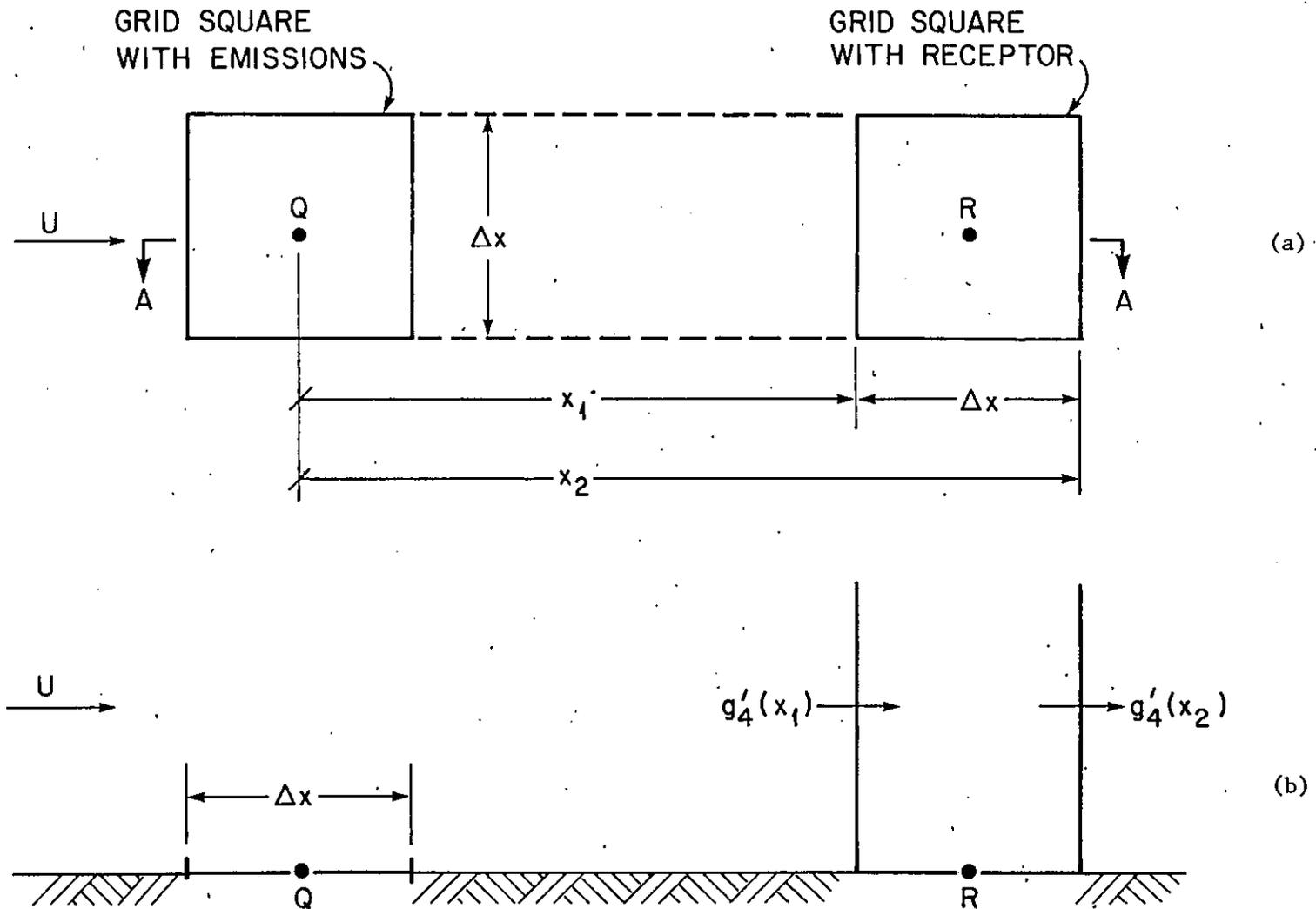
Fig. 1.    Schematic diagram for area-source algorithms showing (a) a grid
square with emissions and a grid square with receptor, and the
distances; (b) a cross-section of the calculation grid square,
and the incoming and outgoing normalized fluxes of pollutant.

as shown in Figure 1(a).

Neglecting deposition, sedimentation, and chemical transformation, the surface (z=0) concentration due to a ground-level (H=0) point source of strength Q (units : $M\ T^{-1}$) is given, from Eq. (44), by

$$C(x,y,0) = \frac{Q}{U} \cdot \frac{g_1}{L_y} \cdot \frac{g_2}{L_z} \qquad\qquad (56a)$$

where

$$g_2(x,0) = 2 \qquad\qquad (56b)$$

The surface concentration due to a crosswind infinite line source can be obtained by integrating Eq. (56a) with respect to y:

$$\bar{C}(x,0) = \int\limits_{-\infty}^{\infty} C(x,y,0)\ dy = \frac{Q}{U} \cdot \frac{g_2}{L_z} = \sqrt{\frac{2}{\pi}}\ \frac{Q}{U\sigma_z} \qquad (57)$$

where Q now has units of $M\ L^{-1}\ T^{-1}$ and represents the emission rate of the line source.

The surface concentration at the receptor R due to an area source Q can be obtained by integrating Eq. (57) with respect to x:

$$C_A = \int\limits_{x_1}^{x_2} \bar{C}(x,0)\ dx = \sqrt{\frac{2}{\pi}}\ \frac{Q}{U} \int\limits_{x_1}^{x_2} \frac{dx}{\sigma_z} \qquad (58)$$

Assuming $\sigma_z$ is given by a power law of the form,

$$\sigma_z(x) = a\,x^b \qquad\qquad (59)$$

where a and b are constants depending only on the atmospheric stability, we obtain

$$C_A = \sqrt{\frac{2}{\pi}}\ \frac{Q}{Ua(1-b)}\left(x_2^{1-b} - x_1^{1-b}\right) \qquad\qquad (60)$$

Here Q has units of $M\,L^{-2}\,T^{-1}$, representing the emission rate of the area source, and $0 \leq x_1 < x_2$. This equation gives the concentration of a single area source Q located upwind of a single receptor R. If the latter were located at the center of the emission grid square itself, then $x_1 = 0$, $x_2 = \Delta x/2$, and Eq. (60) becomes

$$C_A = \sqrt{\frac{2}{\pi}}\ \frac{Q}{Ua(1-b)}\left[\frac{\Delta x}{2}\right]^{1-b} \qquad\qquad (61)$$

If N receptors are located downwind of a single area source $Q_o$, then the concentration at the receptor $R_i$ in the i th grid square (for i = 0, 1, - - -, N) is given by

$$C_{Ai} = \sqrt{\frac{2}{\pi}}\ \frac{Q_o}{Ua(1-b)}\left(x_{2i}^{1-b} - x_{1i}^{1-b}\right) \qquad\qquad (62)$$

where $x_{1i}$ and $x_{2i}$ are the distances measured from $Q_o$ to the upwind and downwind edges, respectively, of the calculation grid square with the i th receptor. Figure 2 illustrates this for N = 4.

If N area sources are located upwind of a single receptor $R_o$, then the contribution to the concentration at the receptor by the source $Q_i$ in the i th
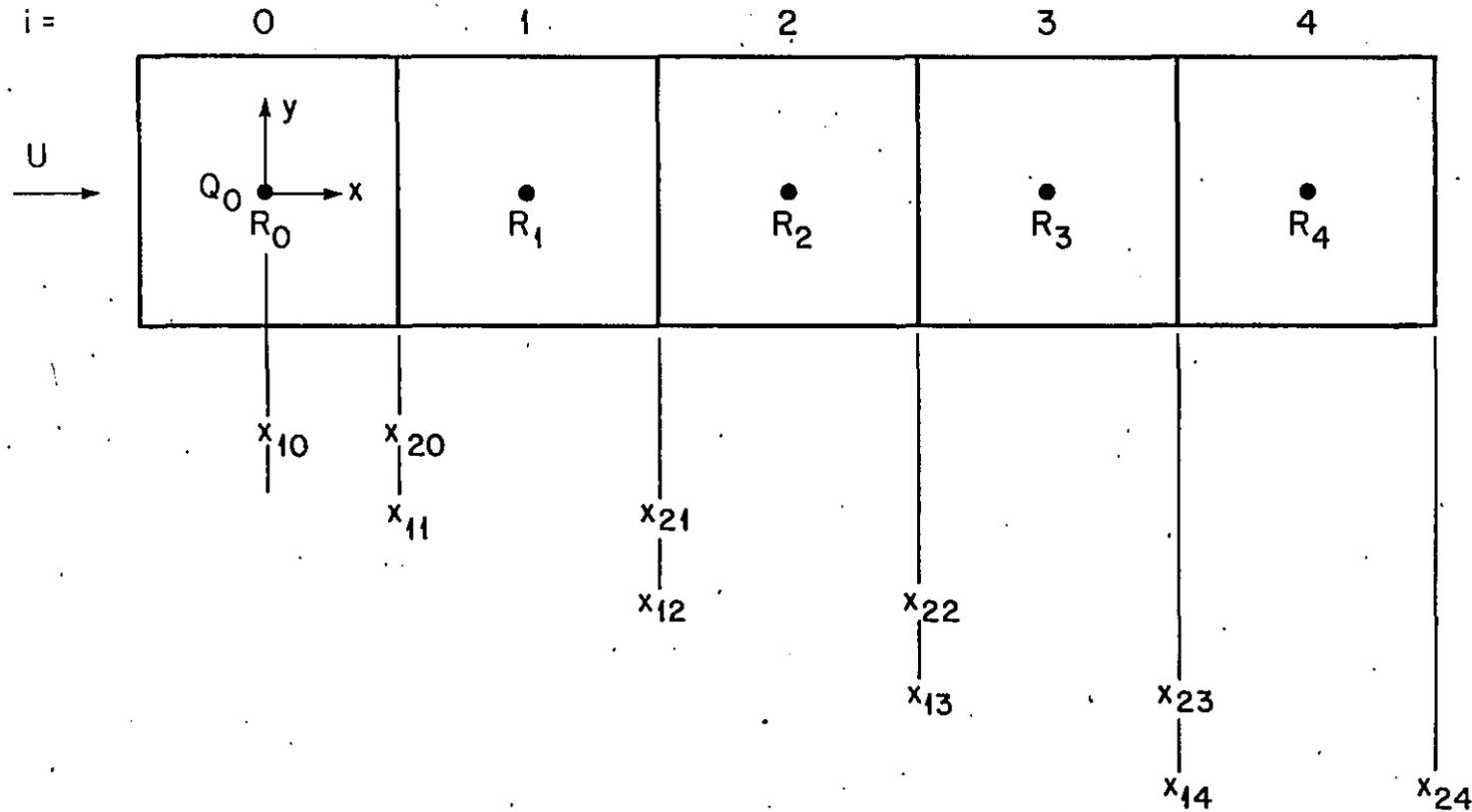
Fig. 2. Schematic diagram showing a single grid square with emissions and four downwind calculation grid squares with receptors, and the distances used in area-source algorithms. These distances are measured downwind from the source $Q_o$.

grid square (for $i = 0, 1, ---, N$) is given by

$$C_{Ai} = \sqrt{\frac{2}{\pi}} \frac{Q_i}{Ua(1-b)} \left( x_{2i}^{1-b} - x_{1i}^{1-b} \right) \tag{63}$$

where $x_{1i}$ and $x_{2i}$ are the distances measured from $R_o$ to the downwind and upwind edges, respectively, of the $i$ th emission grid square. This is illustrated in Figure 3 for $N = 4$. As noted earlier, the distances $x_{1i}$ and $x_{2i}$ in Eq. (63) are identical to those used in Eq. (62), since all grid squares are equal in size. The total surface concentration at the receptor $R_o$ can be obtained by summing up the individual contributions of all N area sources:

$$C_A = \sqrt{\frac{2}{\pi}} \frac{1}{Ua(1-b)} \sum_{i=0}^{N} Q_i \left( x_{2i}^{1-b} - x_{1i}^{1-b} \right) \tag{64}$$

This algorithm for urban area sources was given by Gifford and Hanna (1970) in a slightly different form by using

$$x_{1i} = (2i - 1) \Delta x/2 , \quad x_{2i} = (2i + 1) \Delta x/2 ,$$

$$0 \leq x_{1i} < x_{2i} \tag{65}$$

A more general form of this algorithm was first derived by Gifford (1970), assuming that the mean wind and vertical eddy diffusivity are functions of height given by power laws.

It should be noted that the Gifford - Hanna algorithm, Eq. (64), ignores horizontal diffusion. Gifford (1959) postulated that air pollutant concentration at a receptor due to the distributed area sources depends only on sources located in a rather narrow upwind sector. The angular width of this sector, derived from
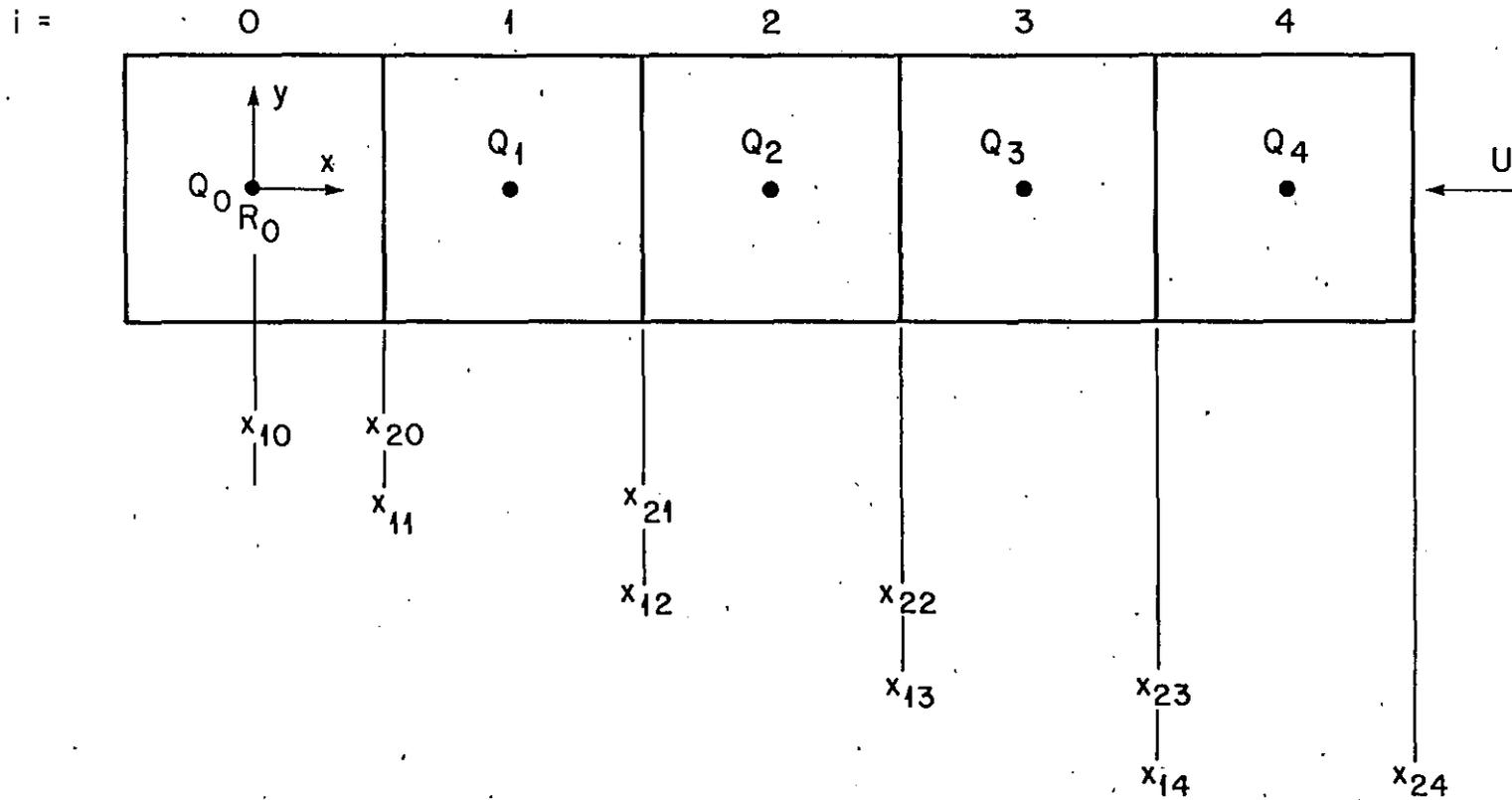
i =    0        1        2        3        4



Fig. 3.    Schematic diagram showing a single grid square with receptor and four upwind grid squares with emissions, and the distances used in area-source algorithms. These distances are measured upwind from the receptor $R_o$.

known values of the horizontal diffusion length scale $L_y$, is less than the usual 22.5° resolution of observed wind directions. Consequently, horizontal diffusion can be ignored. This assumption is referred to as the "narrow plume hypothesis." The crosswind variations in the source-strength patterns can be similarly ignored, since the urban source-inventory box areas are quite large, usually 5 x 5 km or more, and do not vary much in strength from box to box; therefore, the contribution of the source box containing the receptor is generally the dominant one, and the contributions of more remote upwind area sources to this receptor concentration are comparatively small. For this reason, it is generally adequate to consider only four area sources immediately upwind of each receptor grid square, i.e., N = 4 in Eq. (64). For the same reason, a and b are assumed to be independent of the upwind distance x.

Gifford and Hanna (1973) noted that, for the usual case of receptors within a city, the area source component of the urban air pollution is strongly dominated by the source-strength pattern and by transport by the mean wind. Atmospheric diffusion conditions in cities tend to be of the near-neutral type, without the strong diurnal variations found elsewhere. For these reasons, they suggested a simple approximation of the area source formula, Eq. (61), as

$$C_A = k \quad Q/U \qquad (66)$$

where k is given by

$$k = \sqrt{\frac{2}{\pi}} \cdot \frac{x^{1-b}}{a(1-b)} \qquad (67)$$

and x is the distance from a receptor to the upwind edge of the area source. The parameter k is a weak function of city size and should be

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approximately constant. Using a large quantity of air pollution data, average annual emissions, and concentrations of particles for 44 U.S. cities and $SO_2$ data for 20 cities, Gifford and Hanna (1973) found $k = 225$ for particles, and 50 for $SO_2$, with standard deviations of roughly half their magnitude. They noted that Eq. (66) works better for longer averaging periods.

None of the equations given above for area sources consider deposition, sedimentation, and chemical transformation/decay of gaseous or particulate pollutants. However, removal and transformation processes can be important for obtaining reasonable estimates of the pollutant deposition fluxes in urban residential areas. The area source concentration algorithms for the general case that includes deposition, sedimentation, and chemical transformation can be obtained by integrating the point-source concentration algorithms for pollutant species-1 and 2 emitted at ground level, following a procedure similar to that shown in Eqs. (56) to (60), as follows:

$$C_{A1} = \int_{x_1}^{x_2} \int_{-\infty}^{\infty} C_1(x,y,0) \, dy \, dx$$

$$= \frac{Q_1}{U} \int_{x_1}^{x_2} q_1(x,0) \, dx \tag{68a}$$

$$C_{A2} = \int_{x_1}^{x_2} \int_{-\infty}^{\infty} C_2(x,y,0) \, dy \, dx$$

$$= \frac{Q_1}{U} \int_{x_1}^{x_2} q_2(x,0) \, dx \tag{68b}$$

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In the above, we utilized Eqs. (3) and (4), and integrated with respect to y. Though straightforward in principle, the x-integrations required in Eq. (68) are very difficult to carry out in practice, especially for pollutant species-2. This is due to the obvious fact that the integrand functions represented by the probability densities $q_1(x,0)$ and $q_2(x,0)$ are complicated functions of x, unlike the case in the derivation of the Gifford-Hanna algorithm. Even if one is successful in evaluating these difficult integrals analytically, one finds it nearly impossible to physically interpret the terms of the resulting complicated expressions. Following this experience, we started exploring for an alternative to this direct approach for deriving the area source concentration algorithms in the general case that includes deposition, sedimentation, and chemical transformation. These efforts were successful, culminating in the derivation of an elegant alternate approach, which can be physically explained in terms of mass balance considerations, as outlined below.

We rewrite the differential equations and the deposition boundary conditions of Eqs. (6) and (18) as follows:

$$U \, \partial q_1/\partial x = \partial(K_z \, \partial q_1/\partial z + W_1 \, q_1)/\partial z - q_1/\tau_c \tag{69a}$$

$$\left[K_z \, \partial q_1/\partial z + W_1 \, q_1\right]_{z=0} = V_{d1} \, q_1(x,0) \tag{69b}$$

$$U \, \partial q_2/\partial x = \partial(K_z \, \partial q_2/\partial z + W_2 \, q_2)/\partial z + \gamma \cdot q_1/\tau_c \tag{70a}$$

$$\left[K_z \, \partial q_2/\partial z + W_2 \, q_2\right]_{z=0} = V_{d2} \, q_2(x,0) \tag{70b}$$

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Integrating Eqs. (69a) and (70a) with respect to z from 0 to $\infty$, and substituting Eqs. (69b) and (70b), we obtain

$$U \frac{\partial}{\partial x} \int_0^\infty q_1 \, dz = - V_{d1} \, q_1(x,0) - \frac{1}{\tau_c} \int_0^\infty q_1 \, dz \qquad (71a)$$

$$U \frac{\partial}{\partial x} \int_0^\infty q_2 \, dz = - V_{d2} \, q_2(x,0) + \frac{\gamma}{\tau_c} \int_0^\infty q_2 \, dz \qquad (71b)$$

For ground-level sources (H = 0),

$$\int_0^\infty q_1 \, dz = \int_0^\infty \frac{g'_{21}(x,z)}{L_z} \, dz = g'_{41}(x) \qquad (72a)$$

$$\int_0^\infty q_2 \, dz = \int_0^\infty \frac{g'_{22}(x,z)}{L_z} \, dz = g'_{42}(x) \qquad (72b)$$

Substituting Eq. (72) in Eq. (71), and integrating the latter with respect to x from $x_1$ to $x_2$ and rearranging, we obtain

$$V_{d1} \int_{x_1}^{x_2} q_1(x,0) \, dx = U \left[ g'_{41}(x_1) - g'_{41}(x_2) \right] - \frac{1}{\tau_c} \int_{x_1}^{x_2} g'_{41}(x) \, dx \qquad (73a)$$

$$V_{d2} \int_{x_1}^{x_2} q_2(x,0) \, dx = U \left[ g'_{42}(x_1) - g'_{42}(x_2) \right] + \frac{\gamma}{\tau_c} \int_{x_1}^{x_2} g'_{42}(x) \, dx \qquad (73b)$$

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where $V_{d1} \neq 0$ and $V_{d2} \neq 0$.

Noting from Eq. (68) that

$$\int_{x_1}^{x_2} q_i(x,0) \, dx = U \, C_{Ai}/Q_1 \, , \qquad i = 1 \text{ or } 2 \, , \qquad (74)$$

we can now write the area source concentration algorithms for pollutant species-1 and 2 as follows:

$$C_{A1} = \frac{Q_1}{V_{d1}} \left[ g'_{41}(x_1) - g'_{41}(x_2) - \frac{1}{U\tau_c} \int_{x_1}^{x_2} g'_{41}(x) \, dx \right] \qquad (75a)$$

$$C_{A2} = \frac{Q_1}{V_{d2}} \left[ g'_{42}(x_1) - g'_{42}(x_2) + \frac{\gamma}{U\tau_c} \int_{x_1}^{x_2} g'_{41}(x) \, dx \right] \qquad (75a)$$

Here $g'_{41}(x)$ and $g'_{42}(x)$ are the nondimensional algorithms derived for the point-source concentrations (see Table 1) in the well-mixed region. Thus the alternate approach, outlined above, is unique in that it allows one to use the same algorithms (and the same program subroutines) to compute the concentrations due to both point and area sources.

Rao (1981) showed that, for $H = 0$,

$$g'_4(x) \equiv \zeta(x) \qquad (76a)$$

where

$$\zeta(x) = \frac{U}{Q} \int_0^{\infty} \int_{-\infty}^{\infty} C(x,y,z) \, dy \, dz \qquad (76b)$$

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is the suspension ratio, representing the proportion (fraction) of the pollutant released at a rate Q by a source located at $(0,0,H)$ that still remains airborne at downwind distance x. Therefore, $Q_1 \cdot g_4'(x)$ in Eq. (75) represents the flux of pollutant passing through an imaginary vertical plane at downwind distance x. Referring to Figure 1(b), we can now physically interpret the area source concentration algorithms, Eq. (75), as follows: For each calculation grid square box formed by the ground surface and two imaginary vertical planes at $x = x_1$ and $x = x_2$, the pollutant mass balance is given by

Incoming flux - outgoing flux ± flux gain/loss due to chemical

transformation ≡ surface deposition flux

where

Incoming flux = $Q_1 \cdot g_{4i}'(x_1)$,     i = 1 or 2

Outgoing flux = $Q_1 \cdot g_{4i}'(x_2)$,

Flux loss due to chemical transformation (species-1)

$$= \frac{Q_1}{U\tau_c} \int_{x_1}^{x_2} g_{41}'(x) \, dx,$$

Flux gain due to chemical transformation (species-2)

$$= \frac{\gamma Q_1}{U\tau_c} \int_{x_1}^{x_2} g_{41}'(x) \, dx,$$

Surface deposition flux = $V_{di} \cdot C_{Ai}$

The only unknowns in the above are the surface concentrations, $C_{Ai}$, which can be

calculated as shown in Eq. (75). Thus the area source concentration algorithms in the alternate approach, derived mathematically from the governing differential equations and the deposition boundary conditions, can be explained in terms of physically realistic mass budgets of the pollutant species.

Note that the functions $g'_{4i}$ are parameterized and given in terms of $\hat{x} = x/\sqrt{2}\sigma_z$ instead of $x$. Further, we did not specify any particular form of variation for $\sigma_z(x)$ in the derivation of the area source algorithms using the alternate approach. Therefore these algorithms should be valid for any specified type of variation (e.g., power law, exponential, polynomial, etc.) of $\sigma_z(x)$. For a power law of form $\sigma_z = a\,x^b$, used by Gifford and Hanna (1970), the algorithms given by Eq. (75) are valid when the value of $b$ is not significantly different from 0.5. This latter value follows from the relations given in Eq. (42), which allowed us to express the exact analytical solutions in terms of the empirical Gaussian dispersion parameters. For urban area sources, however, Gifford and Hanna (1970) used values of $b$ ranging from 0.91 to 0.71, depending on the atmospheric stability class. These values are based on extensive observational data summarized by Smith (1968) and Slade (1968). Thus when $b$ is significantly different from 0.5, Eq. (75) should be modified for use with a power law variation of $\sigma_z$ as follows:

$$C_{A1} = \frac{Q_1}{2(1-b)V_{d1}} \left[ g'_{41}(x_1) - g'_{41}(x_2) - \frac{1}{U\tau_c} \int_{x_1}^{x_2} g'_{41}(x)\,dx \right] \qquad (77a)$$

$$C_{A2} = \frac{Q_1}{2(1-b)V_{d2}} \left[ g'_{42}(x_1) - g'_{42}(x_2) + \frac{\gamma}{U\tau_c} \int_{x_1}^{x_2} g'_{41}(x)\,dx \right] \qquad (77b)$$

For $V_{di} \longrightarrow 0$ and $\tau_c \longrightarrow \infty$, the concentrations calculated by these algorithms agree with corresponding values given by the Gifford-Hanna algorithm, Eq. (60). The latter can be easily extended for two chemically-coupled pollutants as follows:

$$C_{A1} = \sqrt{\frac{2}{\pi}} \; \frac{Q_1}{Ua} \int_{x_1}^{x_2} x^{-b} \; e^{-x/U\tau_c} \; dx \qquad (78a)$$

$$C_{A2} = \sqrt{\frac{2}{\pi}} \; \frac{Q_1}{Ua(1-b)} \; \cdot \; \left[ \left\{ \frac{Q_2}{Q_1} + \gamma \right\} \left( x_2^{1-b} - x_1^{1-b} \right) \right] - \gamma \, C_{A1} \qquad (78b)$$

For $V_{di} \longrightarrow 0$ and any finite value of $\tau_c$, the concentrations evaluated by Eqs. (77) and (78) show remarkable agreement, even though these two sets of equations are derived using different approaches. This good agreement may be considered as verification of the area source algorithms, Eq. (77), based on the mass balance approach.

Equations (77) can be easily extended, as shown before, to the case of N receptors downwind of a single area source (see Fig. 2); the concentrations at the receptor $R_i$ in the i th grid square can be obtained by using the appropriate downwind distances $x_{1i}$ and $x_{2i}$ in Eq. (77). If N area sources are located upwind of a single receptor $R_o$, as shown in Fig. 3, then the total surface concentrations at the receptor can be obtained by summing up the individual contributions of all N area sources, as follows:

$$C_{A1} = \frac{1}{2(1-b)V_{d1}} \sum_{i=0}^{N} Q_{1i} \left[ g'_{41}(x_{1i}) - g'_{41}(x_{2i}) - \frac{1}{U\tau_c} \int_{x_{1i}}^{x_{2i}} g'_{41}(x) \, dx \right] \qquad (79a)$$

$$C_{A2} = \frac{1}{2(1-b)V_{d2}} \sum_{i=0}^{N} Q_{1i} \left[ g'_{42}(x_{1i}) - g'_{42}(x_{2i}) + \frac{\gamma}{U\tau_c} \int_{x_{1i}}^{x_{2i}} g'_{41}(x) \, dx \right] \qquad (79b)$$

In Eq. (79), it should be noted that for $i = 0$,

$$x_{1i} = 0 \ , \quad g'_{41}(0) = 1 \ , \quad g'_{42}(0) = Q_2/Q_1 \qquad (80a)$$

specify the initial conditions.  Further, we note that for $i > 0$,

$$g'_{41}(x_{1i}) \equiv g'_{41}(x_{2j}) \ , \quad g'_{42}(x_{1i}) \equiv g'_{42}(x_{2j}) \qquad (80b)$$

where $j = i - 1$.

In Eq. (79), therefore, one needs to compute the functions $g'_{41}(x)$ and $g'_{42}(x)$ only at $x = x_{2i}$, $i = 0, 1, \text{---} , N$, since their values at $x = x_{1i}$ are known. The subroutines that compute $g'_{41}$ and $g'_{42}$ are common to both point and area sources.  Thus the area source algorithms, Eq. (79), are simple, accurate, and computationally efficient.

# SECTION 4

## RESULTS AND DISCUSSION

In this section, we consider the well-known problem of the atmospheric transport and transformation of $SO_2$ (species-1 or primary pollutant) to $SO_4^=$ (species-2 or secondary pollutant). The diffusion-deposition algorithms developed in the previous section for various stability and mixing conditions for an elevated rural continuous point source were tested using the following nominal values for the model parameters:

$U = 5$ m/s , $H = 30$ m , KST = 5 (P-G stability class E)

$V_{d1} = 1$ cm/s , $W_1 = 0$ , $Q_1 = 1$ g/s

$V_{d2} = 0.1$ cm/s , $W_2 = 0$ , $Q_2 = 0$

$k_t = 1\%$ per hour ($\tau_c = 36 \times 10^6$ s) , $\gamma = 1.5$

Some of the important results, calculated up to a downwind distance of 20 km from the source, are presented and discussed in this section. Any variations of these nominal values of the model parameters are clearly shown in the figures and noted in the text. The parameters $\sigma_y$ and $\sigma_z$ used in the calculations are the P-G values, which appear as graphs in Turner (1970) and in Gifford (1976, Figure 2). These values, which are widely used for continuous point sources in rural areas, are most applicable to a surface roughness of 0.03 m (Pasquill, 1976).

The diffusion over cities is enhanced, compared to that over rural areas, due to increased mechanical and thermal turbulence resulting from the larger

surface roughness and heat capacity of the cities. This is reflected in the urban dispersion parameter curves based on interpolation formulas given by Briggs (see Gifford, 1976, Figure 7). Some urban air pollution models, such as the Texas Episodic Model (TACB, 1979), simulate the increased surface layer turbulence over urban areas by decreasing the P-G atmospheric stability class index by one, for all classes except Class A. In any case, the algorithms given in the previous section can be applied to sources in urban as well as rural areas by using the appropriate dispersion parameters.

SENSITIVITY ANALYSES

The algorithm for the ground-level concentration of the secondary pollutant given in Eq. (47a) can be written as

$$g_{22}'(\hat{x},0) = \text{Term } 1 + \text{Term } 2 + \text{Term } 3$$

The physical interpretation of these terms was discussed in the previous section. Figure 4 shows the delicate balance that exists between the three terms; Term 2 and Term 3 together nearly balance Term 1. A non-zero concentration for the secondary pollutant results from the small positive imbalance of the three terms. Figure 4 shows that Term 3, which accounts for the differences in the deposition rates of the two pollutant species, becomes increasingly important as x increases.

Because of this tenuous balance between the three terms in $g_{22}'(\hat{x},0)$, the weighting function $F_1(\hat{x},0)$ in Term 3 must be evaluated by numerical integration to a very high degree of accuracy. An examination of $F_1(\hat{x},0)$ in Eq. (47c) shows that the integrand function has singularities at the

KST = 5
H = 30 m
z = 0

$V_{d1}/U = 2 \times 10^{-3}$

$V_{d2}/U = 2 \times 10^{-4}$

——— TERM1

——--- TERM2

· · · · · · TERM3
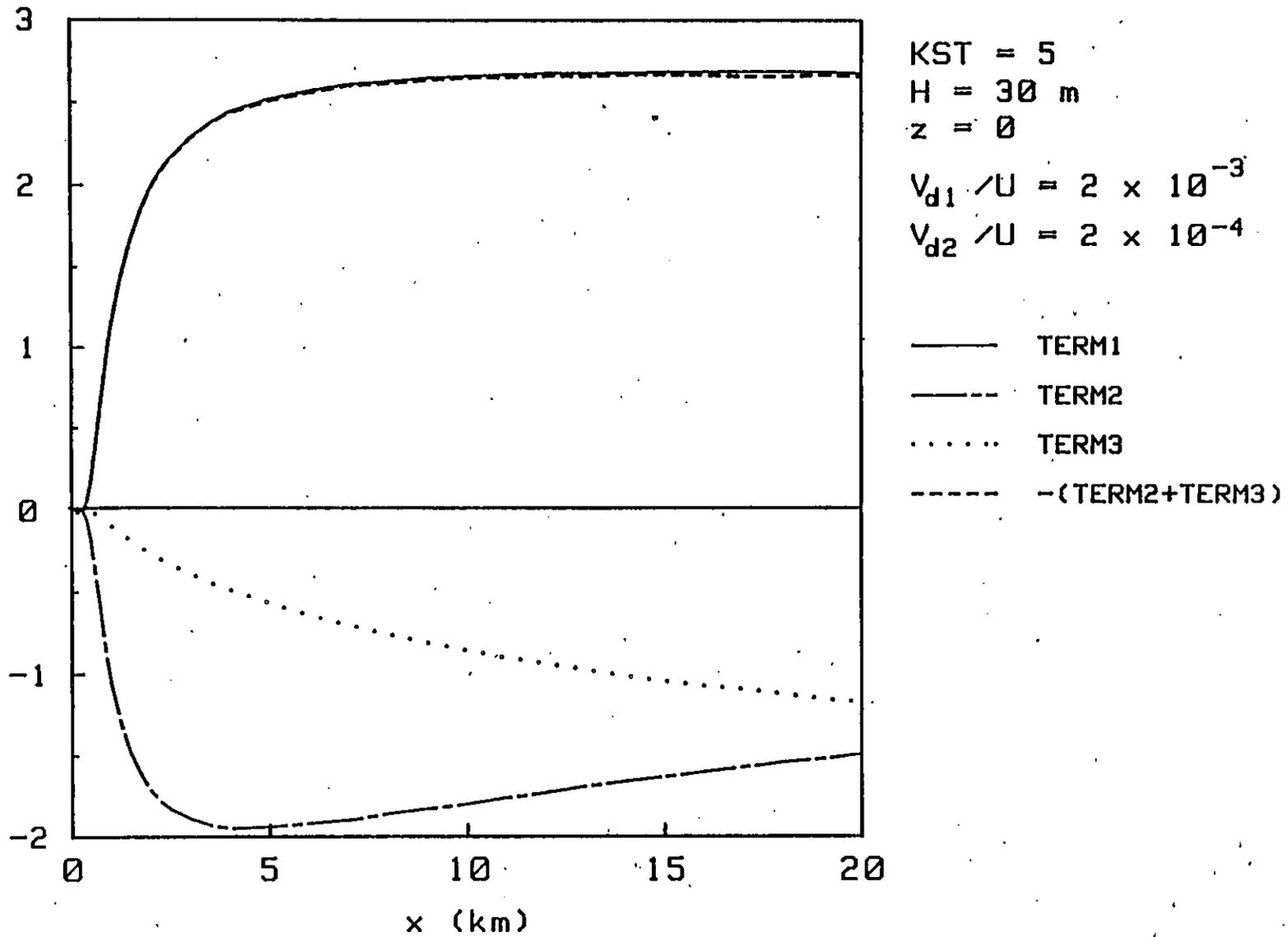
----- −(TERM2+TERM3)

x (km)

Fig. 4.   Variation of the three major terms in the point-source
algorithm for the GLC of the secondary pollutant.  A
non-zero concentration results from the samll positive
imbalance between the terms.

end-points $t = 0$ and $t = 1$ of the integration domain in $t$. A computer-library subroutine named DO1AJF, developed by the Numerical Algorithms Group (NAG), was utilized in this study for the numerical integration. This routine, which is capable of handling the singularities, has been selected because of its accuracy and applicability. It estimates the value of a definite integral of an externally defined function over a finite range to a specified absolute or relative accuracy, using Gauss-Kronrod rules in an adaptive strategy with extrapolation.

The behavior of $F_1(\hat{x},0)$ for four different effective plume heights is explored next. Noting that

$$\frac{1}{\pi} \int_0^1 \frac{1}{\sqrt{t(1-t)}} \, dt = 1,$$

we can easily see from Eq. (46d) that the value of the weighting function $F_1(\hat{x},\hat{z})$ is always between 0 and 1. Figure 5 shows that the value of $F_1(\hat{x},0)$ is close to 1 for ground-level non-buoyant sources (H=0), but decreases rapidly as H increases, especially for small values of x. For all non-zero H values, $F_1(\hat{x},0)$ increases with x as shown in Fig. 5. This clearly illustrates that Term 3 becomes important as x increases.

The behavior of $F_1(\hat{x},\hat{z})$ for four different receptor heights is shown in Fig. 6. The weighting function decreases rapidly as z increases. At large x, the calculated values of $F_1$ are of the same order of magnitude for all z values. Figure 7 shows the variation of $F_1(\hat{x},0)$ for three different values of the deposition parameter $\hat{V}_{11}$ of the primary pollutant. Though $F_1$
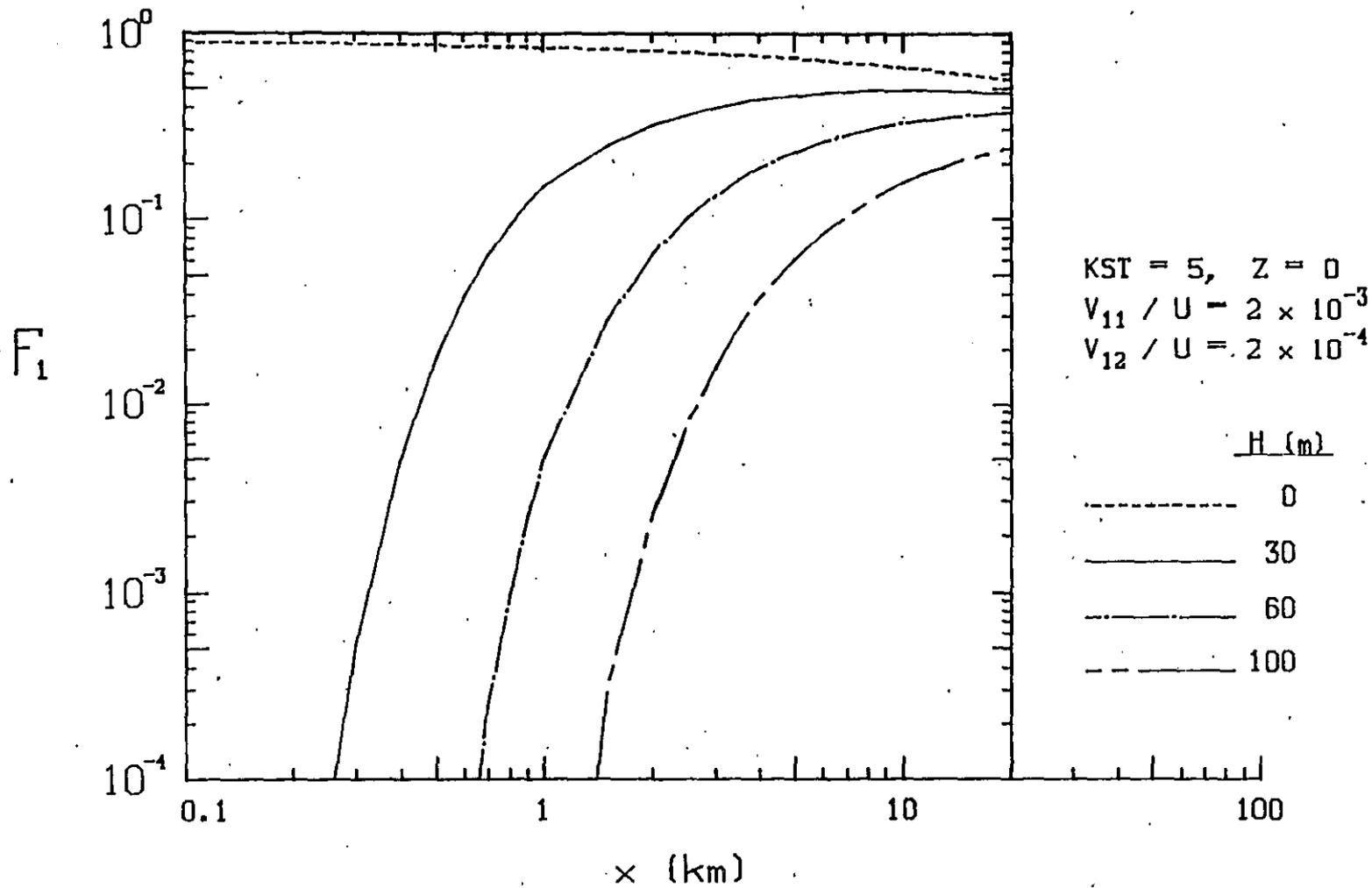
63

Fig. 5.   Variation of the weighting function, in the point-source
          algorithm for the GLC of the secondary pollutant, as a
          function of the effective source height.
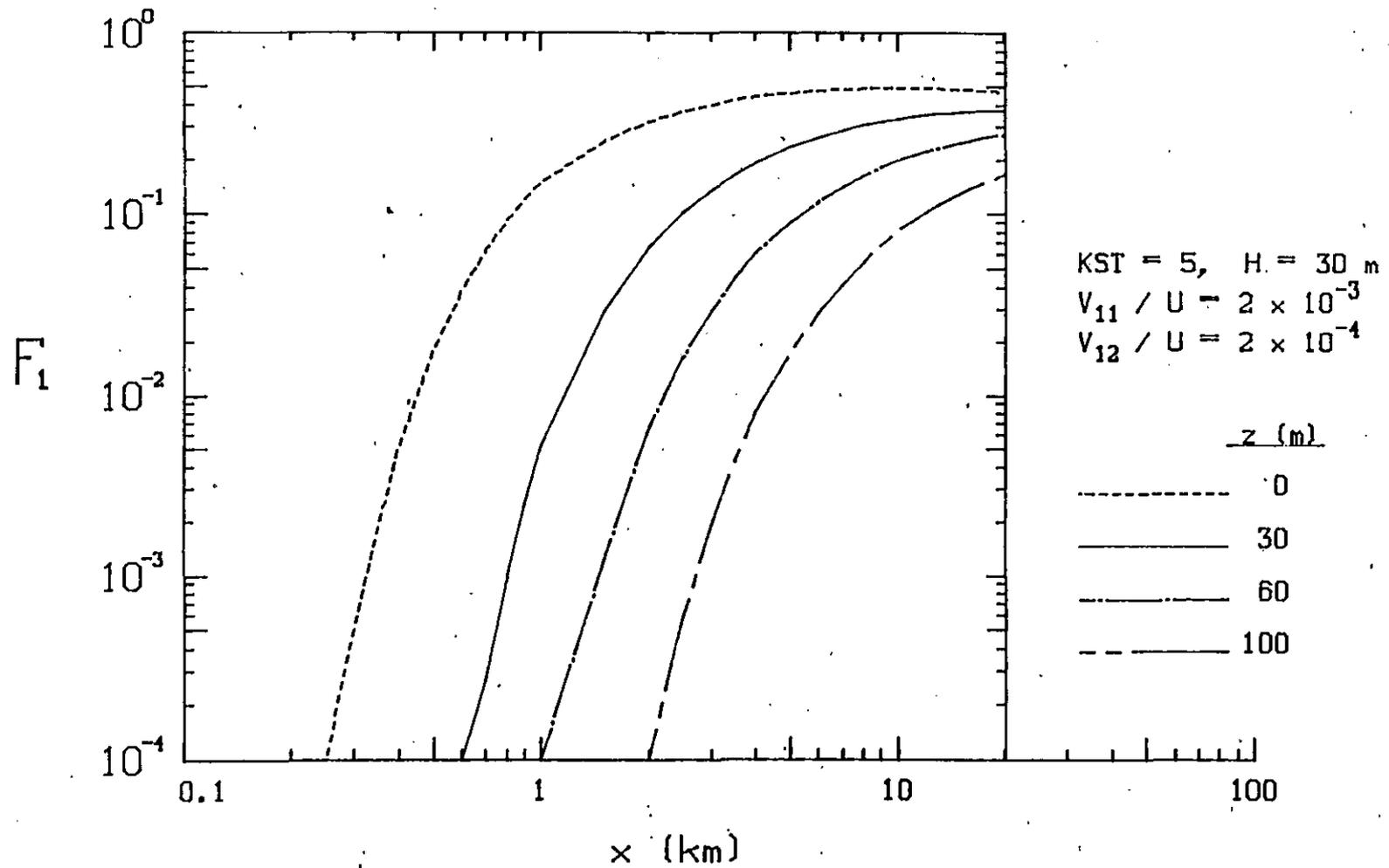
Fig. 6.    Variation of the weighting function, in the point-source
          algorithm for the concentration of the secondary pollutant,
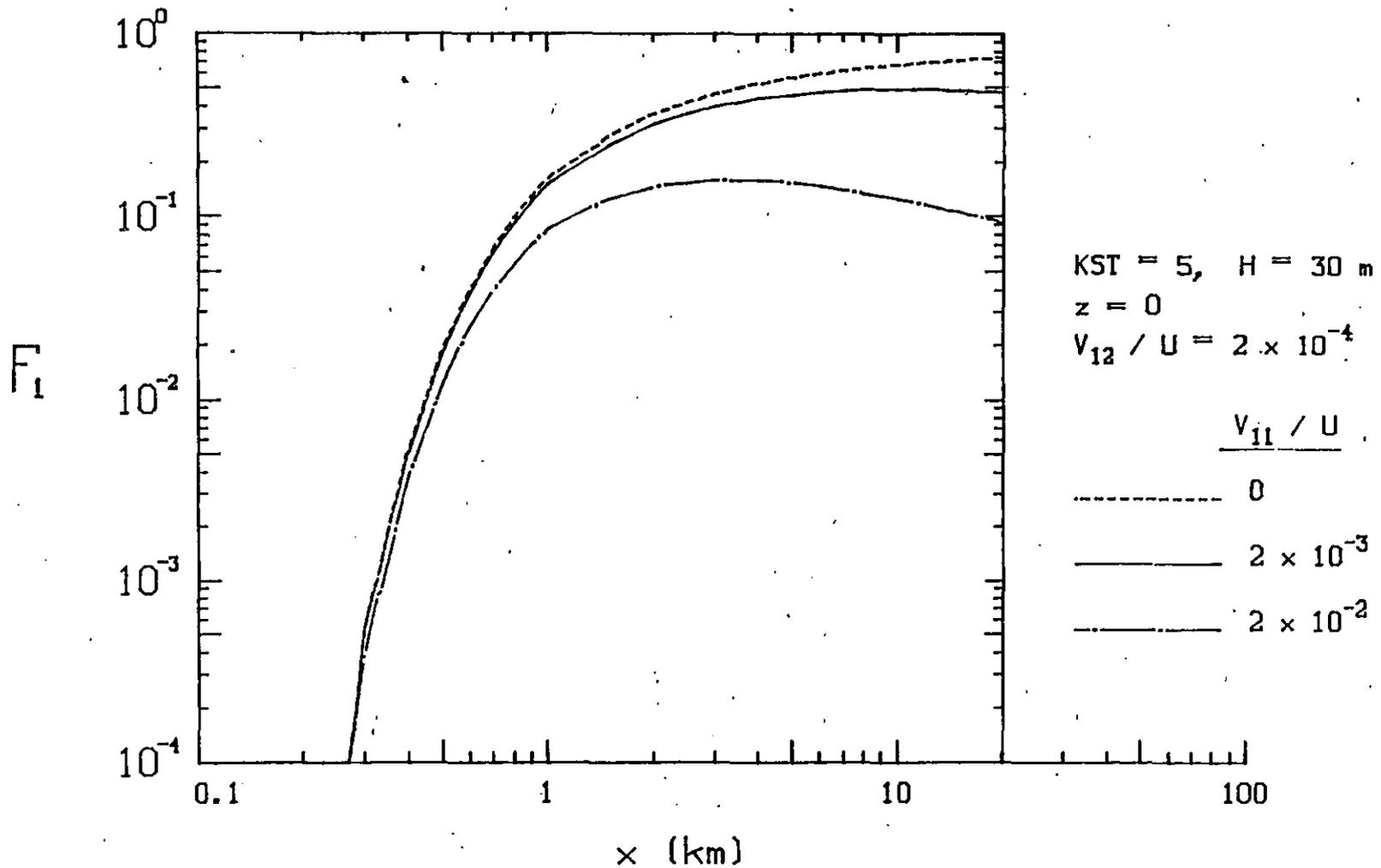          as a function of the receptor height.

Fig. 7. Variation of the weighting function, in the point-source
algorithm for the GLC of the secondary pollutant, as a
function of the deposition velocity of the primary
pollutant.

increases with x initially for all $\hat{V}_{11}$ values, as shown in previous plots, $F_1$ reaches a maximum at a certain value of x, and then starts decreasing as x increases. This is illustrated by an order of magnitude increase in the deposition parameter $\hat{V}_{11}$ in Fig. 7.. A similar behavior is shown in Fig. 8 for the secondary pollutant. This plot suggests that the effects of the deposition parameter in the evaluation of $F_1(\hat{x},0)$ may be ignored if $\hat{V}_{1i} \leq 2 \times 10^{-4}$, i = 1 or 2.


GROUND-LEVEL CONCENTRATIONS (GLC)


The variation of ground-level (z=0) plume-centerline (y=0) relative concentrations, $UC_1(x,0,0)/Q_1$, of the primary pollutant are shown in Fig. 9 for $\hat{V}_{d1}$ = 0, 2 x $10^{-3}$, and 2 x $10^{-2}$; $\hat{W}_1$ = 0 in all three cases. The $\hat{V}_{d1}$ = 0 value corresponds to the zero-deposition case in which the new concentration algorithms reduce to the well-known Gaussian plume algorithms but with a first-order chemical decay of pollutant. This case is included here for comparison. As $\hat{V}_{d1}$ increases, the peak GLC's and the downwind distances where they occur decrease. For $\hat{V}_{d1}$ = 2 x $10^{-2}$, representing moderately strong deposition, the concentration at x = 20 km is about an order of magnitude smaller than the corresponding value for $\hat{V}_{d1}$ = 2 x $10^{-3}$.


Figure 10 shows the GLC variation for the secondary pollutant. Since the direct emission of species-2 is zero, the concentrations shown are entirely due to the chemical transformation. For $k_t$ = 1% per hour, the peak concentration of species-2 is about three orders of magnitude smaller than the corresponding value of species-1, and the downwind-distances of
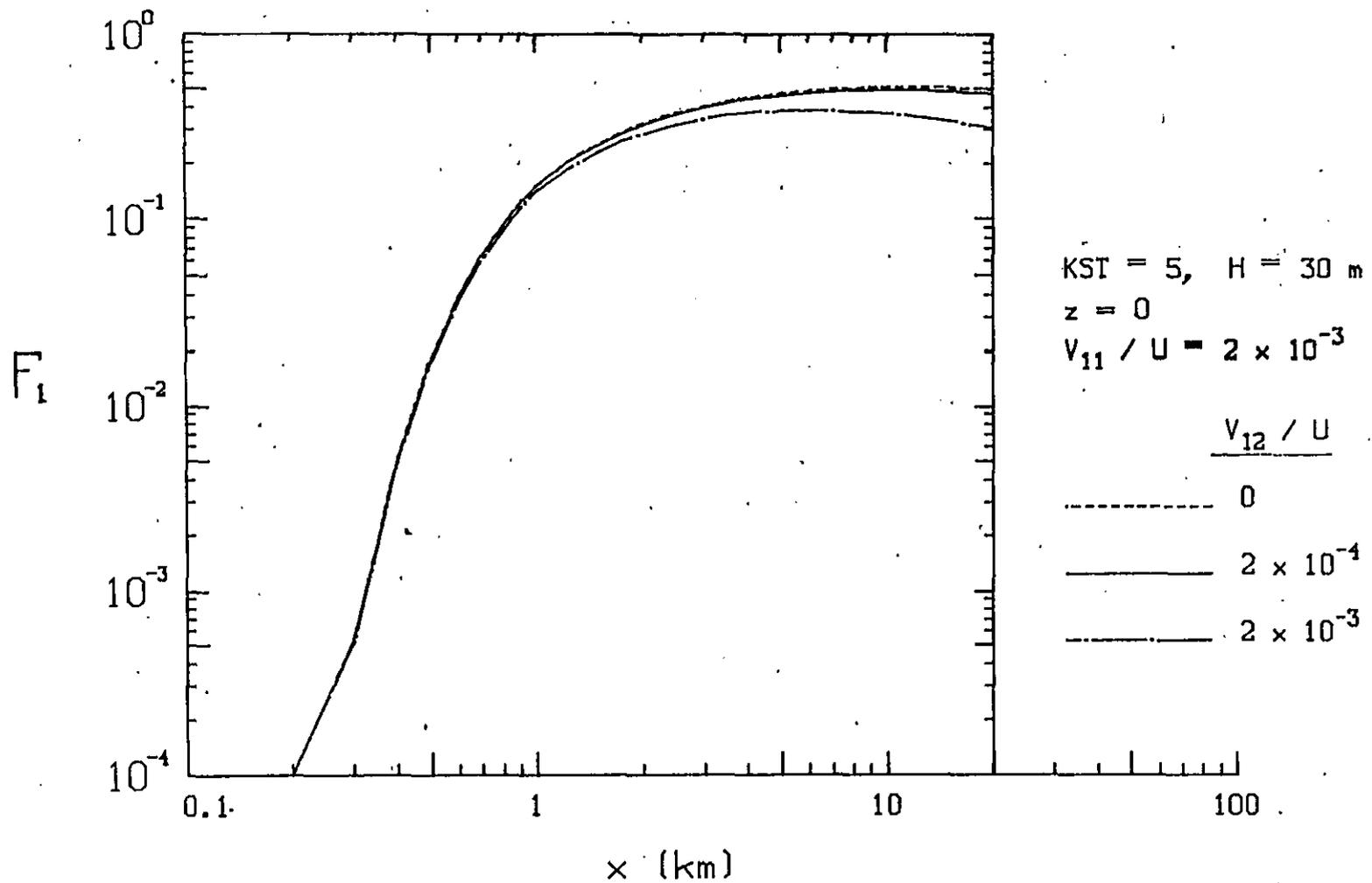
67

Fig. 8.   Variation of the weighting function, in the point-source
algorithm for the GLC of the secondary pollutant, as a
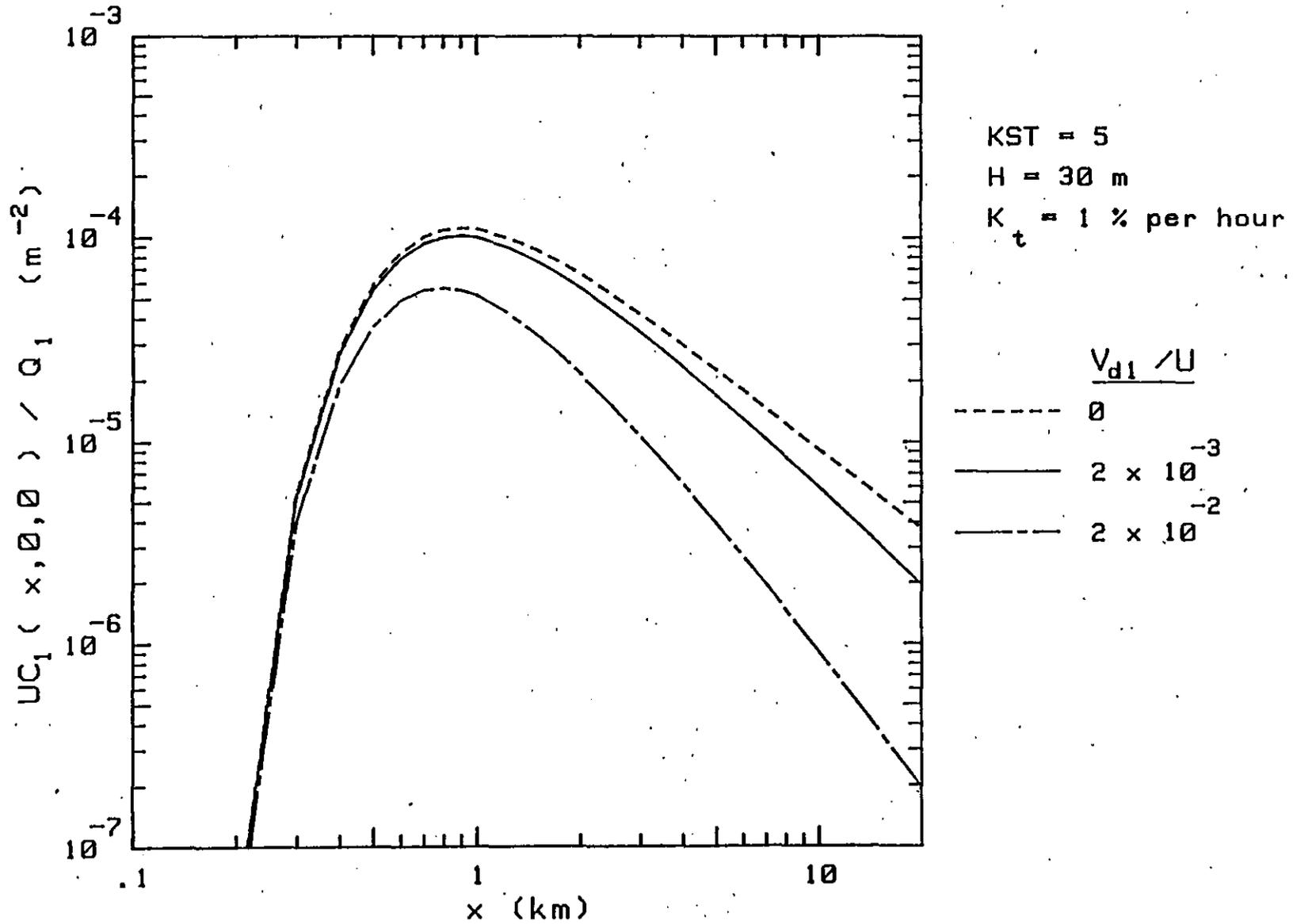function of its deposition velocity.

Fig. 9. Variation of the calculated GLC of the primary pollutant for different values of the paramter $V_{d1}/U$, and $W_1 = 0$.
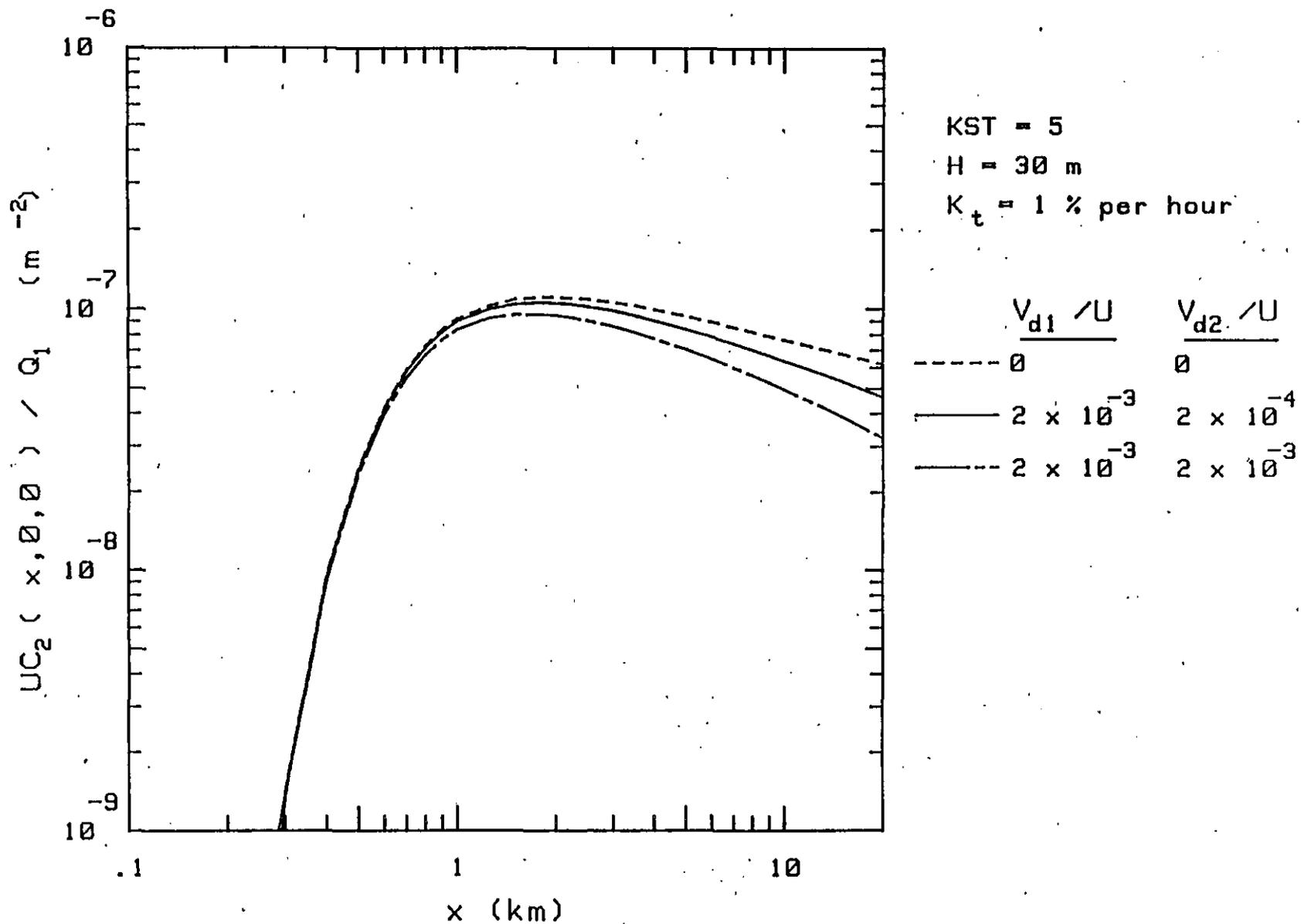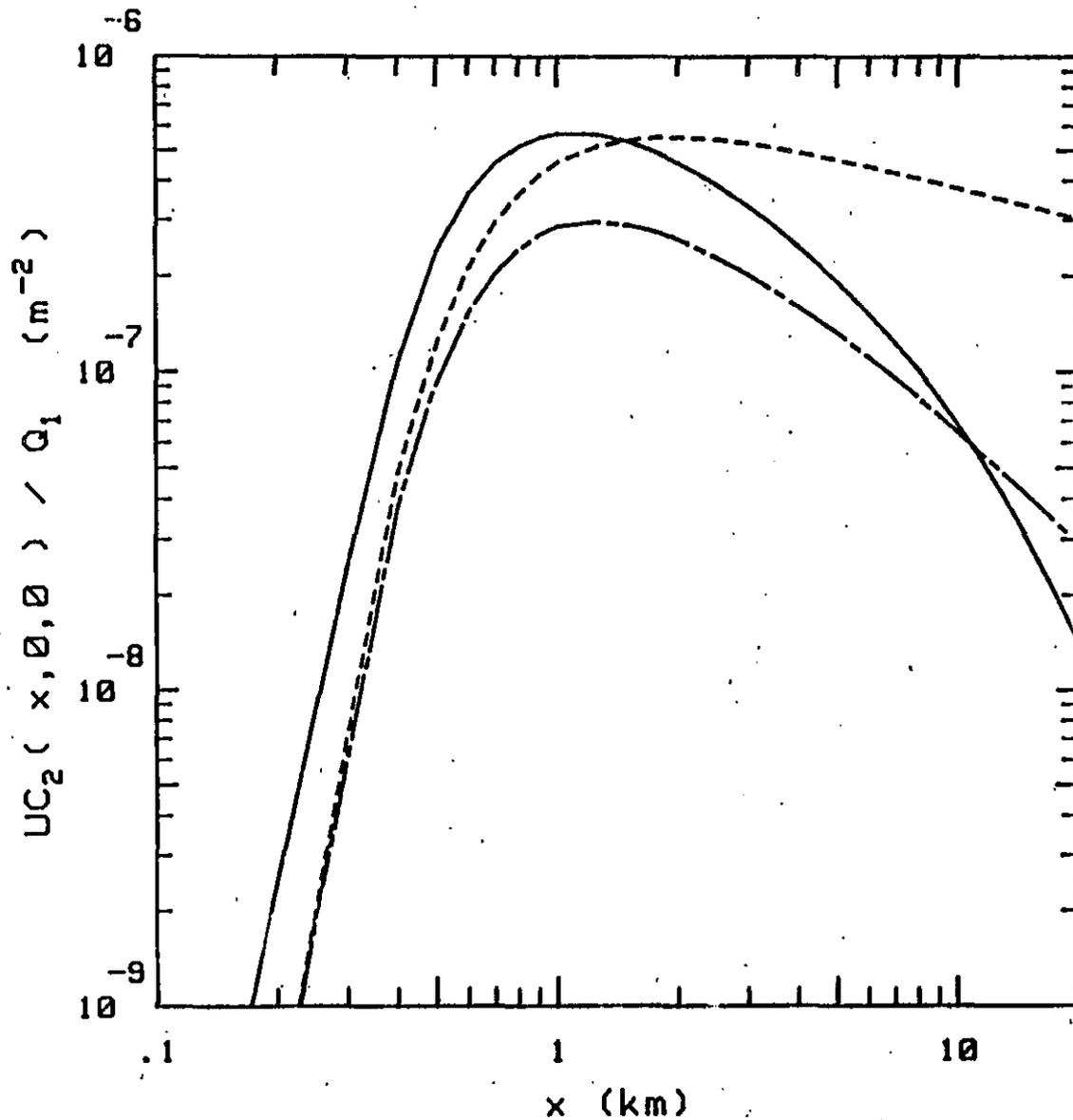
Fig. 10. Variation of the calculated GLC of the secondary pollutant
for different values of the parameter $V_{d2}/U$, and $W_1 = W_2 = 0$.

these peak values are larger than those of species-1. It should be noted that $C_2$ depends on the deposition parameters of both species as well as on the chemical transformation rate.

Figure 11 shows a comparison of calculated ground-level centerline concentrations of the secondary pollutant, when the latter is composed of (a) particulate matter with $V_{d2} = W_2 = 1$ cm/s $(\hat{V}_{12} = 5 \times 10^{-3})$, or (b) gaseous species with $V_{d2} = 1$ cm/s, $W_2 = 0$ $(\hat{V}_{12} = 10^{-2})$. The wind speed U is identical in both cases. The peak GLC for case (a) exceeds the corresponding value for the non-deposition case $(V_{d2} = W_2 = 0)$ and occurs closer to the source. This is a result of gravitational settling of particles which tends to move the plume toward the ground as it travels downwind. The effect of deposition in this case can be seen as an increase of GLC near the source, and a compensating decrease farther downwind. The GLC variation in case (b) for the gaseous pollutant is similar to that shown in the previous figure. These results are consistent with those given by Rao (1981).

CHEMICAL TRANSFORMATION RATE

The effect of varying the chemical transformation rate by two orders of magnitude on the secondary pollutant concentration is shown in Fig. 12. Since $Q_2 = 0$ here, chemical transformation accounts for the entire concentration of species-2. For all $k_t$ values shown, the peak GLC's occur at the same downwind location, since the meteorology and the deposition parameters are kept constant. An order of magnitude increase in $k_t$ increases the

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UC$_2$( x,0,0 ) / Q$_1$  (m$^{-2}$)

x (km)

KST = 5

H = 30 m

K$_t$ = 1 % per hour

| V$_{d1}$ /U | V$_{12}$ /U | |
|---|---|---|
| 0 | 0 | |
| 2 × 10$^{-2}$ | 5 × 10$^{-3}$ | (a) |
| 2 × 10$^{-2}$ | 10$^{-2}$ | (b) |

Fig. 11.  Comparison of the calculated GLC of the secondary pollutant
when it is made of (a) particles with V$_{d2}$ = W$_2$ = 1 cm/s
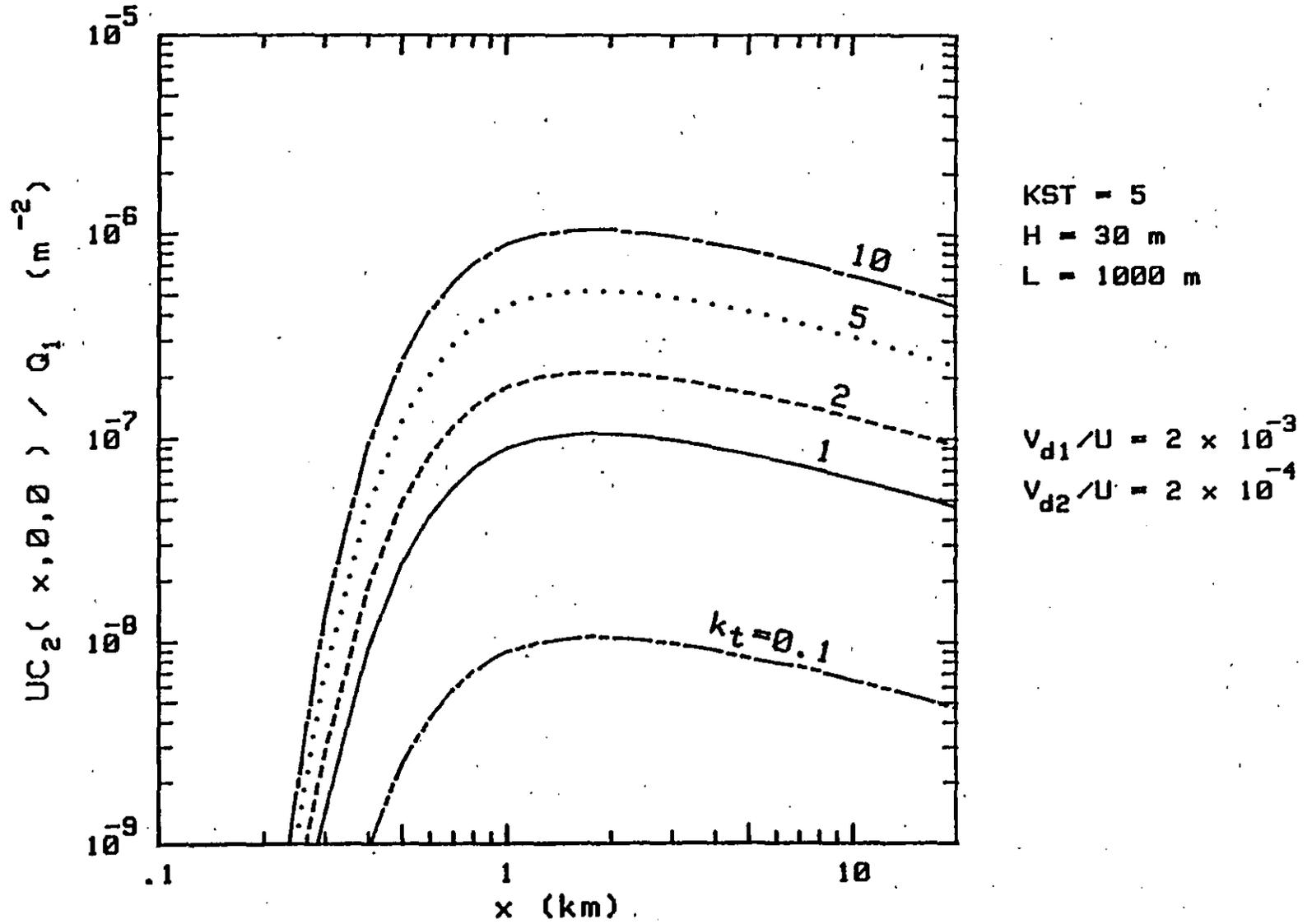or V$_{12}$/U = 5 × 10$^{-3}$, and (b) gas with V$_{d2}$ = 1 cm/s and

Fig. 12. Variation of the calculated GLC of the secondary pollutant for an arbitrary variation of the chemical transformation rate by two orders of magnitude.

concentration by about the same magnitude. The GLC of the secondary pollutant increases sharply with x until its peak value is attained, and then it gradually decreases primarily due to a decrease in the reactant concentration. At small x, the rate of increase in the GLC is directly proportional to $k_t$.

The corresponding plot for the primary pollutant concentrations calculated over the same range of $k_t$ values is shown in Figure 13. The results shows that $C_1$ is not significantly altered by even a value of $k_t = 10\%$ per hour, which corresponds to $\tau_c = 36 \times 10^5$ s. The pollutant-transport time scale, given by x/U, is $4 \times 10^3$ s at x = 20 km; this is much smaller than $\tau_c$, and so $\exp(-x/U\tau_c) \sim 1$. Even for a value of $k_t = 100\%$ per hour, $C_1$ decreases by only about 1.1% at x = 20 km.

EFFECTS OF ATMOSPHERIC STABILITY

Figure 14 shows the primary pollutant concentrations calculated for P-G stability classes A to F (KST = 1 to 6). The peak GLC's decrease slightly with increasing stability, and their downwind locations move farther away from the source. The effects of deposition on the GLC generally increase markedly as the stability increases. However, under convective conditions, atmospheric turbulence enhances the mixing of the plume and, in the well-mixed region, distributes the pollutant uniformly through the entire mixing depth. Therefore, as the stability decreases, the GLC's decrease as shown. For KST = 1, the interpolation for concentration in the plume-trapping region ($1 \lesssim x \lesssim 2$ km) can be clearly seen in the figure.

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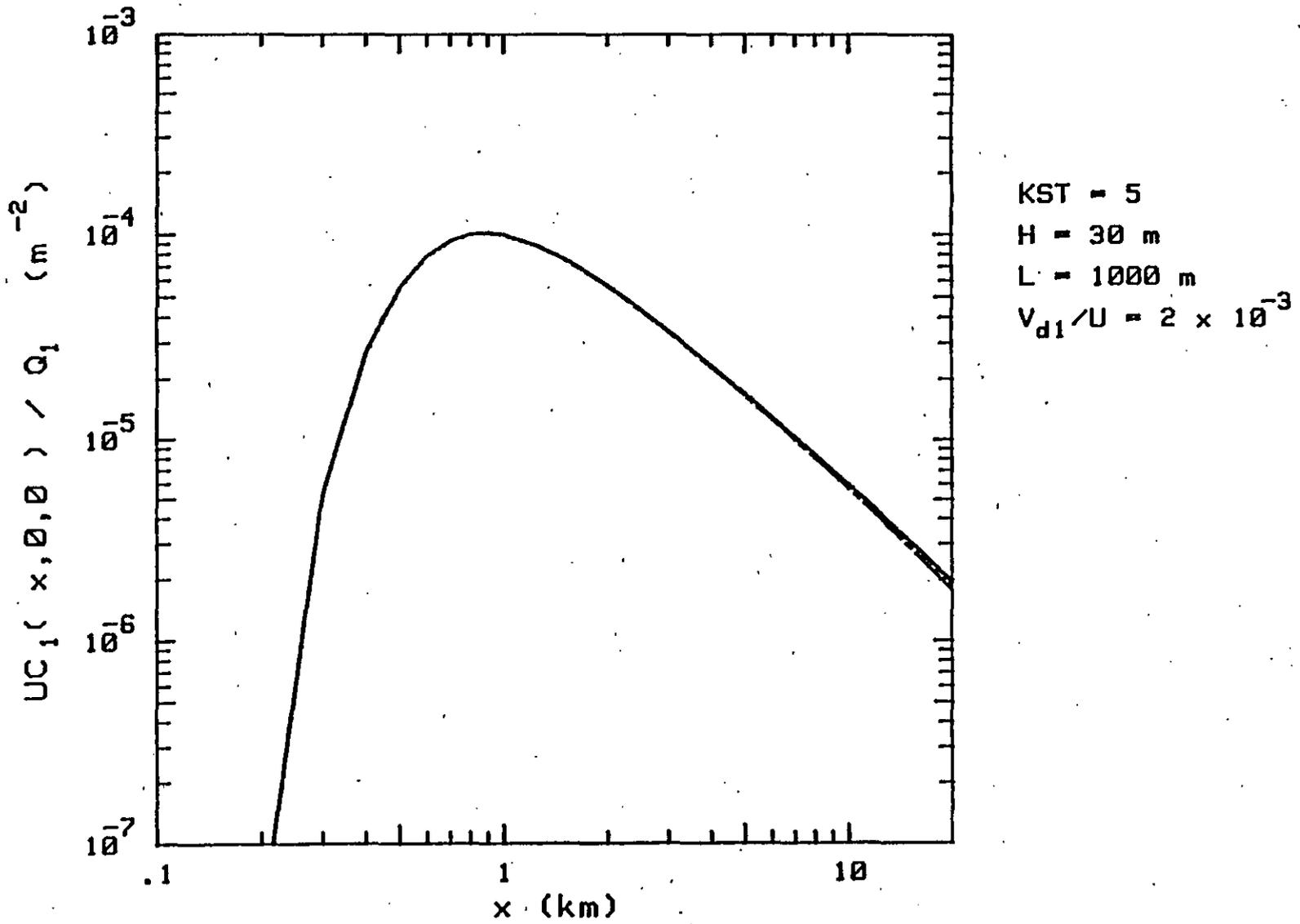KST = 5

H = 30 m

L = 1000 m

$V_{d1}/U = 2 \times 10^{-3}$

Fig. 13. Variation of the calculated GLC of the primary pollutant for an arbitrary variation of the chemical transformation rate by two orders of magnitude.
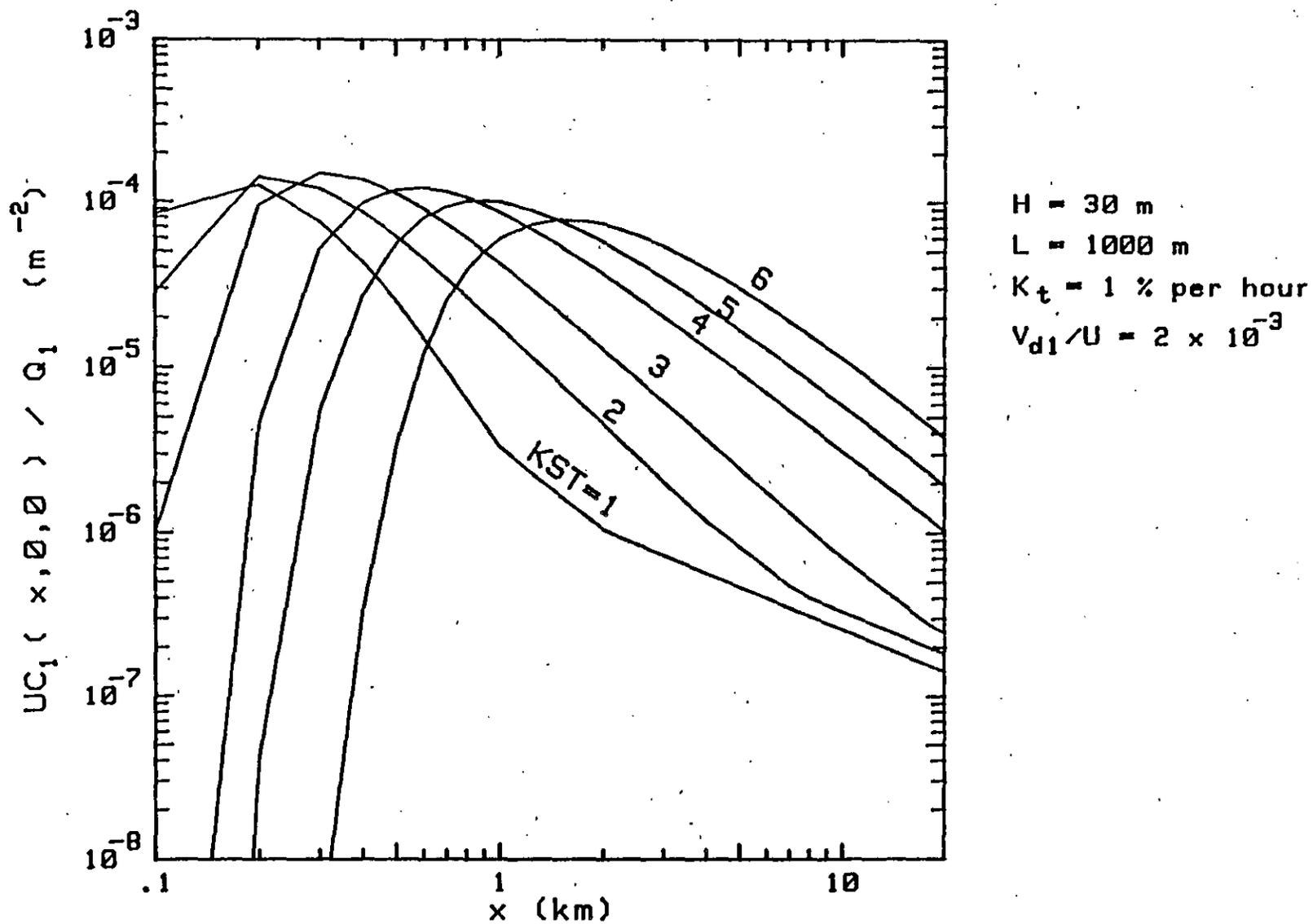
Fig. 14.  Variation of the calculated GLC of the primary pollutant as
a function of the P-G atmospheric stability class.

The corresponding variations of the secondary pollutant concentrations are shown in Fig. 15. It can be seen that the peak GLC's of species-2 increase with increasing stability. Their values are generally about three orders of magnitude smaller than the corresponding values for species-1. The downwind distances of the peak GLC's of the secondary pollutant are generally larger than those for the primary pollutant.

The concentration curves shown in Figs. 14 and 15 do not appear smooth for $x \lesssim 0.5$ km because of the finite steps in x used in the calculations. Smoother curves can be obtained by decreasing the step size $\Delta x$ and increasing the number of steps in this region.
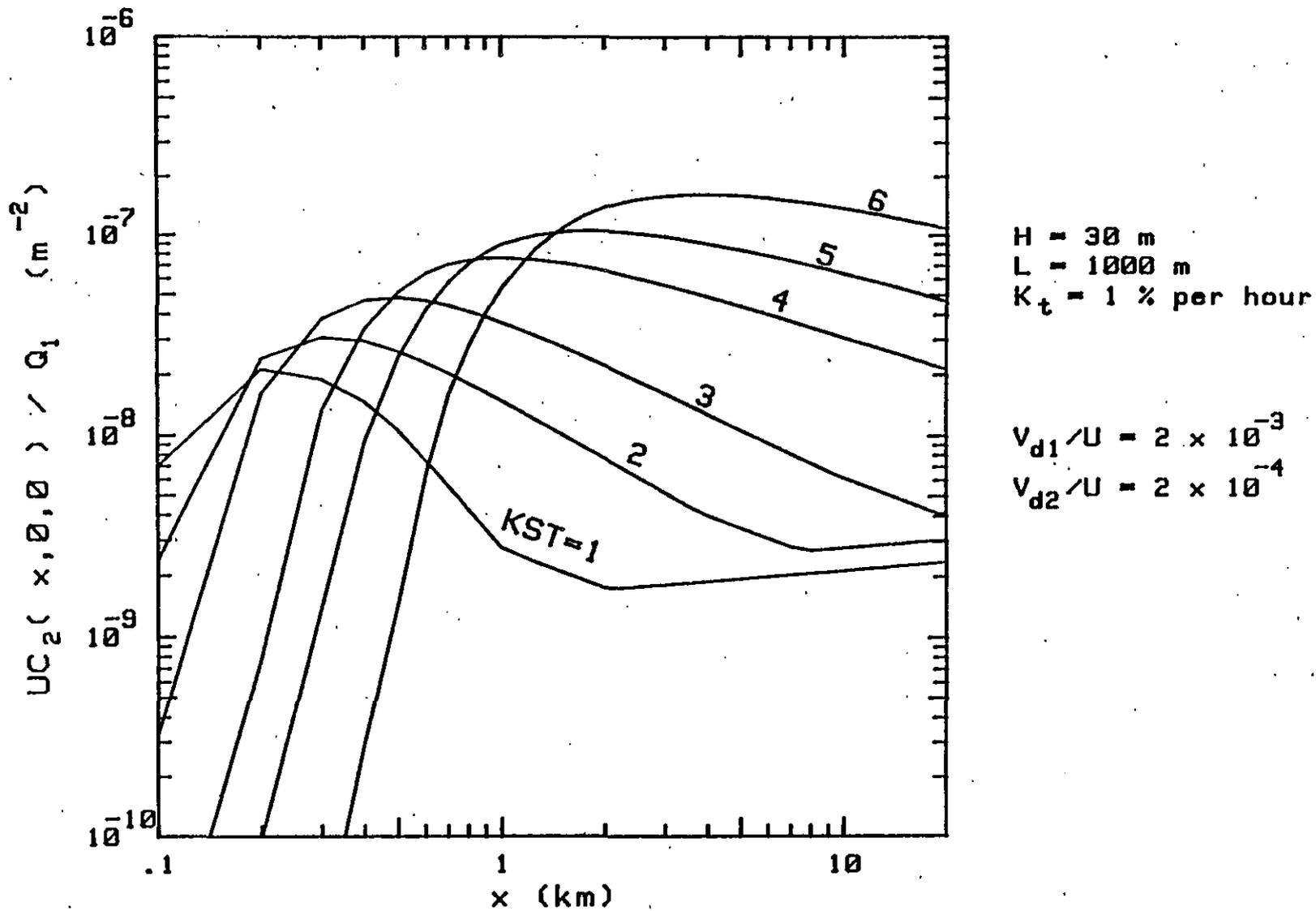
Fig. 15. Variation of the calculated GLC of the secondary pollutant as a function of the P-G atmospheric stability class.

The figure shows curves labeled KST=1, 2, 3, 4, 5, 6 with axes:
- Y-axis: $UC_2(x,0,0)/Q_1$ ($m^{-2}$), ranging from $10^{-10}$ to $10^{-6}$
- X-axis: $x$ (km), ranging from .1 to 10

Parameters shown:
H = 30 m
L = 1000 m
$K_t$ = 1 % per hour

$V_{d1}/U = 2 \times 10^{-3}$
$V_{d2}/U = 2 \times 10^{-4}$

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SECTION 5


SUMMARY AND CONCLUSIONS


A gradient-transfer (K-theory) model that accounts for the atmospheric
diffusion and deposition of two gaseous or particulate pollutant species,
which are coupled through a first-order chemical transformation, has been
formulated. This model, which includes a deposition boundary condition for
each species, treats the pollutant removal mechanisms in a physically realistic
and straightforward manner. The exact analytical solutions for concentrations
of the two pollutants released from an elevated continuous point source have
been derived. For practical application of the model to a variety of atmospheric
stability conditions, the eddy-diffusivity coefficients in the analytical
solutions have been expressed in terms of the widely-used Gaussian plume disper-
sion parameters, which are functions of downwind distance and stability class.
This approximation allows one to utilize the vast amount of empirical data on
these parameters, for a variety of diffusion conditions, within the framework
of the standard turbulence-typing schemes.


In order to facilitate comparison, the new diffusion-deposition-transforma-
tion algorithms for various stability and mixing conditions have been parame-
terized and presented as analytical extensions of the well-known Gaussian plume
dispersion algorithms presently used in EPA air quality models. In the limit
when the deposition and settling velocities and the chemical transformation rate
are zero, the new algorithms reduce to the standard Gaussian plume equations.


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Thus the model outlined here retains the ease of application--and is subject to the same basic assumptions and limitations--associated with Gaussian plume-type models.

The formulations and the solutions are general enough to permit either (or both) of the two pollutant species to be a gas or particulate matter (of a known size). Direct emission of the secondary (reaction product) pollutant from the source is permitted. Simplifications of the new algorithms for ground-level sources and/or receptors, and very slow chemical reactions, are indicated. Limiting expressions of the algorithms for large particles are derived.

An innovative mathematical approach has been outlined to derive elegant expressions for ground-level concentrations of the two species due to emissions from area sources. These simple expressions, derived from the governing equations and the deposition boundary conditions, involve only the point source algorithms for the well-mixed region. This permits one to use the same program subroutines to compute the concentrations due to both point and area sources.

The new area source concentration algorithms are physically explained in terms of the mass budgets for the pollutant species in each calculation grid square. For practical application to urban air pollution models, these algorithms are extended to multiple area sources and receptors. For power-law variation of $\sigma_z(x)$, simple modifications of the algorithms are suggested to establish agreement with the Gifford-Hanna area-source algorithms in the limit when the deposition loss of species is negligible. Thus the area-source

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algorithms, derived here through a new mathematical approach are physically realistic, simple, efficient, and accurate.

A sensitivity analysis of the concentration algorithm for the secondary pollutant is given to illustrate the delicate balance of its terms and the behavior of the numerically-evaluated weighting function in one of the terms. For an elevated point source in a rural area, the variations of the ground-level concentrations of the two species are calculated by varying the assigned nominal values of each of the model parameters. The results are presented and discussed with reference to the Gaussian plume concentrations.

The point and area source concentration algorithms developed in this report may have wide applicability in practical rural and urban air pollution and particulate models, such as the Pollution Episodic Model (Rao and Stevens, 1982), for use in research and regulation.

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# APPENDIX


## SETTLING AND DEPOSITION VELOCITIES


For a monodisperse particulate cloud, the individual particles have a constant gravitational settling velocity. This terminal velocity is given by Stokes' equation (Fuchs, 1964):

$$W = \frac{d^2 \, g \, \rho}{18 \, \mu} \qquad \qquad \text{(A-1)}$$


where d is the diameter of the particle, g is acceleration due to gravity, $\rho$ is the particle density, and $\mu$ is the dynamic viscosity of air. However, for $d > 100$ $\mu$m, the terminal fall velocity is sufficiently great that turbulence in the wake of the particle cannot be neglected, and the drag force on the particle is greater than the viscous drag force given by the Stokes' law, $F_d = 3\pi d\mu W$. For a particle with $d = 400$ $\mu$m, the actual value of W is about one-third the value given by Eq. (A-1). Furthermore, Stokes' expression for the drag force describes the effects of collisions between air molecules and a particle, assuming air to be a continuum. This assumption is not valid for very small particles, since the mean free path between molecular collisions is comparable to the particle size; under these conditions "slippage" occurs, and the particles undergo Brownian motion and diffusion, which give a terminal velocity greater than that predicted by Eq. (A-1). A discussion of the slip correction factor for the Stokes' equation can be found in Fuchs (1964) and Cadle (1975).

The values for the terminal gravitational settling velocities for different

particulate materials are given in a tabular form by Lapple (1961) based on

particle diameter and Reynolds number.  These values, which account for

the deviations from Stokes' equation discussed above, are given for spherical

particles with a specific gravity of 2.0 in air at 25°C and 1 atm. pressure.

This table has been reprinted in Sheehy et al (1969) and Stern (1976).


The dry deposition pollutant-removal mechanisms at the earth's surface

include gravitational settling, turbulent and Brownian diffusion, chemical

absorption, inertial impaction, thermal, and electrical effects.  Some of the

deposited particles may be re-emitted into the atmosphere by mechanical resus-

pension.  Following the concept introduced by Chamberlain (1953), particle

removal rates from a polluted atmosphere to the surface are usually described

by dry deposition velocities which vary with particle size, surface properties

(including surface roughness $z_o$ and moisture), and meteorological conditions.

The latter include wind speed and direction, friction velocity $u_*$, and thermal

stratification of the atmosphere.  Deposition velocities for a wide variety

of substances and surface and atmospheric conditions may be obtained directly

from the literature (e.g., McMahon and Denison, 1979; Sehmel, 1980).  Sehmel and

Hodgson (1974) give plots relating deposition velocity $V_d$ to d, $z_o$, $u_*$, and the

Monin-Obukhov stability length, on the basis of wind tunnel studies.


Considerable care needs to be exercised in choosing a representative

deposition velocity, since it is a function of many factors and can vary by

two orders of magnitude for particles.  Generally, $V_d$ should be defined

relative to the height above the surface at which the concentration measurement

is made.  The particle deposition velocity is approximately a linear function

of wind speed and friction velocity, and its minimum value occurs in the particle diameter range 0.1 - 1 μm.

In the trivial case of $W = V_d = 0$, settling and deposition effects are negligible. For very samll particles (d < 0.1 μm), gravitational settling can be neglected, and dry deposition occurs primarily due to the nongravitational effects mentioned above. In this case, $W = 0$ and $V_d > 0$. For small to medium-sized particles (d = 0.1~50 μm), $0 < W < V_d$; deposition is enhanced here beyond that due to gravitational settling, primarily because of increased turbulent transfer resulting from surface roughness. For larger particles (d > 50 μm), it is generally assumed that $V_d = W > 0$, re-entrainment of the deposited particles from the surface into the atmosphere is implied as, for example, in a dust storm. The first four sets of model parameters given above are widely used in atmospheric dispersion and deposition of particulate material. The deposition of gases is a special case of the particulte problem with $W = 0$.

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