Characteristics of Maximum Concentrations from Multiple Point Sources

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ABSTRACT

A simple quasi-Newton numerical scheme is applied to determine the hypothetical worst-case meteorology that will result in the maximum combined concentrations at any receptor location in air quality modeling over short distances for multiple point sources. Also, a search procedure is suggested to investigate the combination of location and atmospheric conditions of wind direction, wind speed, and stability that produces the highest possible ground-level concentration, the so-called critical concentration. The proposed methodology may help in applications in design of stacks, air quality management, and air pollution episode control planning.

1. Introduction

Air quality models are routinely used to estimate the degree of emission control required to reduce the air quality impact of industrial and other sources to acceptable levels. Multiple point-source plume models are commonly used for mathematical modeling of concentrations of chemically inert pollutants over urban and industrial areas. Although there are many special-purpose computational algorithms currently in use, the basic element that is common to most is the simple plume from a single point-source release. The spatial distribution of pollution is then calculated by simple superposition of the individual plumes from all the elevated point sources.

The most important output of a diffusion model is the maximum concentration, which is related to the air pollution episode concentrations (e.g., Zoumakis et al. 1992). As discussed by Turner (1970), for elevated sources, maximum concentrations for time periods of a few minutes occur with unstable conditions. The distance of this maximum concentration occurs near the stack from one to five stack heights downwind. For time periods of about half an hour, the maximum concentrations can occur with fumigation conditions when an unstable layer increases vertically to mix downward with a plume previously discharged within a stable layer. Under stable conditions, the maximum concentrations at ground level from elevated sources are less than those occurring under unstable conditions and occur at greater distances from the source. On the other hand, as discussed by Hanna et al. (1982), maximum concentrations from tall stacks (with a stack height h of 100 m) generally occur during light wind, daytime convective conditions, while maximum concentrations from short stacks generally occur during high wind, neutral conditions. Moreover, because ground-level concentration is a minimum at low wind speeds (because of large plume rise) and at high wind speeds (because of large rate of dilution), there is a critical wind speed at which the ground-level concentration is a maximum. Therefore, it is often desirable to determine the hypothetical worst-case meteorology that causes a maximum calculated concentration in dispersion prediction and to locate the receptor where the maximum occurs. This is also useful for determining compliance with short-term ambient air quality standards and environmental impact studies (e.g., see Wu 1982). Ragland (1976), Roberts (1980), Bowman (1983), Seinfeld (1986), and others have obtained the worst-case results for a Gaussian type of plume when the dispersion parameters σ_y and σ_z can be expressed as functions of downwind distance from a stack and atmospheric stability category. However, such an approach is limited to a single point source.

For a pollutant regarded as chemically inert, it is assumed that the concentration contributions produced at a receptor from individual plumes combine additively so that the plumes may be simply superimposed to obtain the total effect at the receptor location. The total concentration C is then given by summing the individual contributions C_i from each source,

$$C = \sum_{i=1}^{n} C_i, \tag{1}$$

where n represents the number of stacks. As stated in Turner (1970), it is often difficult to determine the atmospheric conditions of wind direction, wind speed, and

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stability that will result in the maximum combined concentrations from two or more sources. However, as discussed by Wu (1982), computers have become so fast and computer time is so accessible (especially for personal microcomputers) that solving any usual optimization problem is easily accomplished.

Wu (1982) proposed a computer optimization technique to determine the hypothetical worst-case meteorology and receptor location in short-term dispersion modeling for multiple point sources. Meteorological variables included in this search procedure are mean wind speed U; mean wind direction A, expressed as the angle between the positive horizontal axis of an arbitrary coordinate system and the incoming wind; and the Pasquill stability category K. Receptor location variables are polar coordinates (X, AA) with respect to the above-mentioned arbitrary coordinate system (e.g., Turner 1970; Wu 1982). For multiple point-source modeling, it is convenient to consider the receptor as being at the origin of the diffusion coordinate system. The evaluation of the concentration due to a single stack can be conveniently performed by a transformation of the receptor coordinates involving a rotation (to align with the wind direction) and a transition from the arbitrary origin to a new origin–stack location, so that any point-source dispersion formula can be directly applied. The contribution due to a stack is considered zero if the variable receptor is found to be upwind of a stack.

Because of the inherently random character of atmospheric motions, one can never predict with certainty the distribution of concentration of marked particles emitted from a source. However, for the purposes of practical computation, several approximate theories have been used for calculating mean concentrations of species in turbulence. For example, the mean concentration of a species emitted from a continuous, elevated point source has a Gaussian distribution in a stationary and homogeneous Gaussian flow field. Thus, under certain idealized conditions, the expression for the mean concentration, the so-called Gaussian plume equation, can be obtained as a solution of an appropriate form of the atmospheric diffusion equation (e.g., Seinfeld 1986). In developing the search algorithm (Wu 1982), as a working hypothesis, the simple Gaussian plume model for chemically inert pollutants was used for all calculations. In addition, only ground-level receptors were considered.

The methodology suggested by Wu (1982) is applied to determine the hypothetical worst-case meteorology that causes a maximum calculated concentration in dispersion prediction and to locate the receptor where the critical concentration occurs. According to this search algorithm, one starts by searching the full ranges of meteorological and receptor location variables with judiciously chosen step sizes. This search procedure may continue (with smaller step sizes) until a desired degree of accuracy or a stable maximum value is reached after a number of iterations. However, the most important point to be mentioned here is that such a (step by step) screening model approach gives only approximations for an exact solution vector:

$$\boldsymbol{\Theta} \equiv (X, \text{AA}, U, A). \tag{2}$$

A different approach is proposed here to determine the characteristics of maximum concentrations from multiple point sources by using a simple numerical solution technique. The hypothetical worst-case meteorology and the worst receptor location can be determined by extremizing the meteorological variables (i.e., wind speed, wind direction, and stability category) and the receptor location variables with an appropriate numerical method. Therefore, the function to be maximized is the superposition of concentrations (from all the elevated point sources) at a variable receptor due to all stacks. The most important difference from the iterative search procedure suggested by Wu (1982) is that the proposed methodology uses a simple quasi-Newton numerical scheme to solve the relevant optimization problem, giving the exact solution vector ($\boldsymbol{\Theta}$) for the worst-case meteorology and the worst receptor location. On the other hand, compared with the numerical algorithm, results from the screening model approach may be extremely delayed because of the time required to select the successive ''judicious'' step sizes (for the meteorological and receptor location variables) and perform the calculations.

2. Methodology

The characteristics of maximum concentrations from multiple point sources, with respect to ground-level receptor (X, AA) and wind vector (U, A), can be determined by maximizing the superposition of concentrations at a variable receptor due to all stacks.

Differentiating Eq. (1) with respect to X and AA and setting the resulting relations equal to zero yields

$$F(X, \text{AA}, U, A) = \sum_{i=1}^{n} \left(\frac{\partial C_i}{\partial X}\right) = 0 \tag{3}$$

and

$$G(X, \text{AA}, U, A) = \sum_{i=1}^{n} \left(\frac{\partial C_i}{\partial \text{AA}}\right) = 0. \tag{4}$$

The location of the maximum ground-level concentration for any given wind vector (U, A) and atmospheric stability category (e.g., a Pasquill stability class K) can be calculated by solving the pair of nonlinear equations (3) and (4). If (X_m, AA_m) is a point satisfying Eq. (3) and (4) and if Δ is defined by

$$\Delta = \begin{vmatrix} \dfrac{\partial^2 C}{\partial X^2} & \dfrac{\partial^2 C}{\partial X \partial \text{AA}} \\ \dfrac{\partial^2 C}{\partial \text{AA} \partial X} & \dfrac{\partial^2 C}{\partial \text{AA}^2} \end{vmatrix}, \tag{5}$$

then (X_m, AA_m) is called a maximum point if

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$$\Delta > 0 \quad \text{and} \quad \frac{\partial^2 C}{\partial X^2} < 0 \tag{6}$$

or, equivalently,

$$\Delta > 0 \quad \text{and} \quad \frac{\partial^2 C}{\partial \mathrm{AA}^2} < 0. \tag{7}$$

Then, for any given wind vector (U, A), atmospheric stability category (K), and AA $\in [0, 2\pi]$ with AA = AA + step, that is, the interval from 0 to 2π is divided into a number (approximately 2π per step) of subintervals of equal width, Eq. (3) can be solved for X by the Newton–Raphson iterative formula

$$X_{k+1} = X_k - \frac{F_k}{\partial F_k/\partial X}. \tag{8}$$

Successive iterations (for $k = 1, 2, 3, \ldots$) converge if (e.g., see Gerald 1978)

$$-1 < \frac{F_k(\partial^2 F_k/\partial X^2)}{(\partial F_k/\partial X)^2} < +1, \tag{9}$$

on an interval about the root; that is, the numerical method will converge for any initial value X_0 in the interval (in general, the Newton–Raphson method is quadratically convergent). Note that Eq. (9) is a sufficient condition only and requires the usual continuity and existence of $F(X, \mathrm{AA}, U, A)$ and its derivatives. Moreover, the quantity $\partial F_k/\partial X$ must not be zero. Having obtained for AA $\in [0, 2\pi]$ the successive values of X from Eq. (3), one could then proceed to find from Eq. (1) the corresponding ground-level concentrations. Thus, a relative maximum value of $C(X, \mathrm{AA})$ occurring at a point (X_0, AA_0) can be estimated from Eq. (1). Consequently, Newton's method may be used to solve the system of nonlinear equations (3) and (4) by numerical iterations for X and AA to obtain the exact solution vector (X_m, AA_m) in the near neighborhood (e.g., Isaacson and Keller 1966; Gerald 1978; Burden et al. 1981) of the initial approximation (X_0, AA_0). Expanding both functions $F(X, \mathrm{AA}, U, A)$ and $G(X, \mathrm{AA}, U, A)$ as a Taylor series about the initial approximation point (X_0, AA_0) from Eqs. (3) and (4) finally yields

$$\frac{\partial F}{\partial X}\Delta X + \frac{\partial F}{\partial \mathrm{AA}}\Delta \mathrm{AA} = -F(X, \mathrm{AA}, U, A) \tag{10}$$

and

$$\frac{\partial G}{\partial X}\Delta X + \frac{\partial G}{\partial \mathrm{AA}}\Delta \mathrm{AA} = -G(X, \mathrm{AA}, U, A), \tag{11}$$

where ΔX and ΔAA are increments to add to the initial guesses to get an improved estimate of the root of the nonlinear system (i.e., $X = X + \Delta X$ and AA = AA + ΔAA). It is obvious then, in passing from one dimension, that is, from Eq. (8), to two dimensions, that is, to Eqs. (10) and (11), that Newton's method is generalized by replacing tangent lines with tangent planes. Thus, the pair of the linear equations (10) and (11) is solved giving values for the increments ΔX and ΔAA to the initial guesses X_0 and AA_0 that should make them closer to the exact solution vector (X_m, AA_m) of the system of nonlinear equations (3) and (4). Newton's algorithm repeats the procedure until convergence is obtained.

Next consider the effect of mean wind speed U and mean wind direction A on the maximum ground-level concentration. The highest concentration at any receptor location can be determined as a function of wind speed and wind direction. Taking the partial derivatives of C from Eq. (1) with respect to U and A and setting them equal to zero yields

$$\Phi(X, \mathrm{AA}, U, A) = \sum_{i=1}^{n}\left(\frac{\partial C_i}{\partial U}\right) = 0 \tag{12}$$

and

$$\Psi(X, \mathrm{AA}, U, A) = \sum_{i=1}^{n}\left(\frac{\partial C_i}{\partial A}\right) = 0. \tag{13}$$

The ''worst'' wind vector (U_w, A_w), for which the ground-level concentration is the maximum at any given receptor location (X, AA) and atmospheric stability category (e.g., a Pasquill stability class, K), can be calculated by solving the pair of the nonlinear equations (12) and (13). If (U_w, A_w) is a point satisfying Eqs. (12) and (13) and if Δ is defined by

$$\Delta = \begin{vmatrix} \dfrac{\partial^2 C}{\partial U^2} & \dfrac{\partial^2 C}{\partial U \partial A} \\ \dfrac{\partial^2 C}{\partial A \partial U} & \dfrac{\partial^2 C}{\partial A^2} \end{vmatrix}, \tag{14}$$

then (U_w, A_w) is called a maximum point if

$$\Delta > 0 \quad \text{and} \quad \frac{\partial^2 C}{\partial U^2} < 0 \tag{15}$$

or, equivalently,

$$\Delta > 0 \quad \text{and} \quad \frac{\partial^2 C}{\partial A^2} < 0. \tag{16}$$

Having obtained for $A \in [0, 2\pi]$ the successive values of U from Eq. (12) by the Newton–Raphson iterative formula

$$U_{k+1} = U_k - \frac{\Phi_k}{\partial \Phi_k/\partial U}, \tag{17}$$

one could then find from Eq. (1) the corresponding ground-level concentrations. Successive iterations (for $k = 1, 2, 3, \ldots$) converge if (e.g., see Gerald 1978)

$$-1 < \frac{\Phi_k(\partial^2 \Phi_k/\partial U^2)}{(\partial \Phi_k/\partial U)^2} < +1 \tag{18}$$

on an interval about the root (i.e., the numerical method will converge for any initial value U_0 in the interval). Thus, a relative maximum value of $C(U, A)$ occurring

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for a mean wind vector (U_0, A_0) can be estimated from Eq. (1). Consequently, Newton's method may be used to solve the system of nonlinear equations (12) and (13) by numerical iterations for U and A to obtain the exact solution vector (U_w, A_w) in the near neighborhood of the initial approximation (U_0, A_0). Expanding both functions $\Phi(X, \text{AA}, U, A)$ and $\Psi(X, \text{AA}, U, A)$ as a Taylor series about the initial approximation (U_0, A_0), from Eqs. (12) and (13) finally yields

$$\frac{\partial \Phi}{\partial U}\Delta U + \frac{\partial \Phi}{\partial A}\Delta A = -\Phi(X, \text{AA}, U, A) \tag{19}$$

and

$$\frac{\partial \Psi}{\partial U}\Delta U + \frac{\partial \Psi}{\partial A}\Delta A = -\Psi(X, \text{AA}, U, A), \tag{20}$$

where ΔU and ΔA are increments to add to the initial guesses to get an improved estimate of the root of the nonlinear system (i.e., $U = U + \Delta U$ and $A = A + \Delta A$). Thus, the pair of the linear equations (19) and (20) is solved, giving values for the increments ΔU and ΔA to the initial guesses U_0 and A_0 that should make them closer to the exact solution vector (U_w, A_w) of the system of nonlinear equations (12) and (13). Newton's algorithm repeats the procedure until convergence is obtained.

Another point to be investigated is the combination of location, **DIST** = (X, AA), and wind vector, **WIND** = (U, A), which produces the highest possible ground-level concentration, the so-called critical concentration. Differentiating Eq. (1) with respect to $\omega \equiv X$, AA, U, and A, and setting the resulting relation equal to zero, yields

$$\frac{\partial C}{\partial \omega} = \sum_{i=1}^{n}\left(\frac{\partial C_i}{\partial \omega}\right) = 0, \tag{21}$$

and from Eqs. (3), (4), (12), and (13) finally yields

$$F(X, \text{AA}, U, A) = 0, \tag{22}$$

$$G(X, \text{AA}, U, A) = 0, \tag{23}$$

$$\Phi(X, \text{AA}, U, A) = 0, \tag{24}$$

and

$$\Psi(X, \text{AA}, U, A) = 0. \tag{25}$$

Then the critical receptor location $\mathbf{DIST}_{\text{cr}} = (X_{\text{cr}}, \text{AA}_{\text{cr}})$ and the critical wind vector $\mathbf{WIND}_{\text{cr}} = (U_{\text{cr}}, A_{\text{cr}})$ can be calculated by solving the system of nonlinear equations (22)–(25) for day (or for night) conditions (see Wu 1982, 626). If $\mathbf{\Theta}_{\text{cr}} = (X_{\text{cr}}, \text{AA}_{\text{cr}}, U_{\text{cr}}, A_{\text{cr}})$ is a point satisfying Eqs. (22) through (25). And if γ_{ij} is defined by

$$\gamma_{ij} = \frac{\partial^2 C}{\partial \omega_i \partial \omega_j} \quad \text{for } i, j = 1, 2, 3, \text{ and } 4, \tag{26}$$

then $\mathbf{\Theta}_{\text{cr}}$ is called a maximum critical point if

$$\gamma_{11} < 0, \tag{27}$$

$$\begin{vmatrix} \gamma_{11} & \gamma_{12} \\ \gamma_{21} & \gamma_{22} \end{vmatrix} > 0, \tag{28}$$

$$\begin{vmatrix} \gamma_{11} & \gamma_{12} & \gamma_{13} \\ \gamma_{21} & \gamma_{22} & \gamma_{23} \\ \gamma_{31} & \gamma_{32} & \gamma_{33} \end{vmatrix} < 0, \tag{29}$$

and

$$\begin{vmatrix} \gamma_{11} & \gamma_{12} & \gamma_{13} & \gamma_{14} \\ \gamma_{21} & \gamma_{22} & \gamma_{23} & \gamma_{24} \\ \gamma_{31} & \gamma_{32} & \gamma_{33} & \gamma_{34} \\ \gamma_{41} & \gamma_{42} & \gamma_{43} & \gamma_{44} \end{vmatrix} > 0, \tag{30}$$

where $\omega_1 = X$, $\omega_2 = \text{AA}$, $\omega_3 = U$, and $\omega_4 = A$.

Having obtained for $\text{AA} \in [0, 2\pi]$ and $A \in [0, 2\pi]$ an initial approximate solution vector (as mentioned previously),

$$\mathbf{\Theta}_0 \equiv (X_0, \text{AA}_0, U_0, A_0), \tag{31}$$

Newton's method may be used to solve the system of nonlinear equations (22)–(25) by numerical iterations for X, AA, U, and A to obtain the exact solution vector $\mathbf{\Theta}_{\text{cr}}$ in the near neighborhood of the initial approximation $\mathbf{\Theta}_0$. If the Jacobian matrix $\mathbf{J}(X, \text{AA}, U, A)$ associated with the system of nonlinear equations (22)–(25) is nonsingular at the root, $\mathbf{\Theta} = \mathbf{\Theta}_{\text{cr}}$, and differentiable there, then the convergence of Newton's method is quadratic. In addition, the Kantorovich theorem (e.g., see Isaacson and Keller 1966) gives a sufficient condition under which Newton's numerical scheme converges (in fact, the theorem proves the existence of a unique root of a set of nonlinear equations in an appropriate interval about the initial iterate). Expanding the functions F, G, Φ, and Ψ, as a Taylor series about the initial approximation $(X_0, \text{AA}_0, U_0, A_0)$ from Eqs. (22) through (25) finally yields

$$\frac{\partial F}{\partial X}\Delta X + \frac{\partial F}{\partial \text{AA}}\Delta \text{AA} + \frac{\partial F}{\partial U}\Delta U + \frac{\partial F}{\partial A}\Delta A = -F(X, \text{AA}, U, A), \tag{32}$$

$$\frac{\partial G}{\partial X}\Delta X + \frac{\partial G}{\partial \text{AA}}\Delta \text{AA} + \frac{\partial G}{\partial U}\Delta U + \frac{\partial G}{\partial A}\Delta A = -G(X, \text{AA}, U, A), \tag{33}$$

$$\frac{\partial \Phi}{\partial X}\Delta X + \frac{\partial \Phi}{\partial \text{AA}}\Delta \text{AA} + \frac{\partial \Phi}{\partial U}\Delta U + \frac{\partial \Phi}{\partial A}\Delta A = -\Phi(X, \text{AA}, U, A), \tag{34}$$

and

$$\frac{\partial \Psi}{\partial X}\Delta X + \frac{\partial \Psi}{\partial \text{AA}}\Delta \text{AA} + \frac{\partial \Psi}{\partial U}\Delta U + \frac{\partial \Psi}{\partial A}\Delta A = -\Psi(X, \text{AA}, U, A), \tag{35}$$

where ΔX, ΔAA, ΔU, and ΔA are increments to add to

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the initial guesses to get an improved estimate of the root of the nonlinear system (i.e., $X = X + \Delta X$, AA = AA + ΔAA, $U = U + \Delta U$, and $A = A + \Delta A$). It is obvious then, in passing from one dimension to more than two dimensions, that Newton's numerical scheme is generalized by replacing tangent lines with tangent hyperplanes. Thus, the system of the linear equations (32)–(35) is solved giving values for the increments ΔX, ΔAA, ΔU, and ΔA to the initial guesses X_0, AA_0, U_0, and A_0 (for the variables X, AA, U, and A), which should make them closer to the exact solution vector

$$\mathbf{\Theta}_{cr} \equiv (X_{cr}, AA_{cr}, U_{cr}, A_{cr}) \tag{36}$$

of the system of nonlinear equations (22)–(25). Newton's algorithm repeats the procedure until convergence is obtained.

It is interesting to observe that Newton's method, as applied to the set of nonlinear equations (22)–(25), reduces the problem to solving the set of linear equations (32)–(35) in order to determine the values that improve the accuracy of the estimates. However, a significant weakness of Newton's method for solving the system of nonlinear equations (22)–(25) lies in the requirement that, at each iteration, a Jacobian matrix be computed and the linear system of equations (32)–(35) be solved that involves this matrix. It is obvious that, in a computer program, it is awkward to introduce each of the partial derivative functions in order to implement Eqs. (32) through (35). In most situations, the exact evaluation of the Jacobian matrix is inconvenient and in many applications impossible.

An alternative technique (known as a quasi-Newton algorithm) is to replace the Jacobian matrix in Newton's method with an approximation matrix that is updated at each iteration [the disadvantage to this method is that the quadratic convergence of Newton's method is lost, being replaced in general by a super linear convergence; e.g., see Burden et al. (1981)]. According to the proposed quasi-Newton numerical method, the partial derivatives are computed by making a small change in the value of a variable and dividing the change in value of the function by the change in value of the variable; this estimates the derivative by a difference quotient (e.g., see Gerald 1978). After all the partials have been approximated, the numerical method reduces the problem to solving the corresponding linear system (involving the approximate Jacobian matrix) in order to determine the values that improve the accuracy of the estimates. The quasi-Newton numerical scheme repeats the procedure until convergence is obtained.

3. Application and discussion

Since the purpose of this study is to demonstrate a search approach rather than a model development, simple point-source dispersion formulas (e.g., analytical solutions of the *K*-theory atmospheric diffusion equation) were used in developing the proposed methodology. In the special case in which the atmospheric diffusion process is described by the usual Gaussian plume equation (incorporating reflection of the material at the ground to ensure conservation of mass), the ground-level concentration C_i (mg m^{-3}) from each elevated continuous point source at downwind distance (DX) from the stack and crosswind displacement (DY) is then given (see appendix of Wu 1982) by

$$C_i = \frac{Q_i}{\pi\sigma_y\sigma_z U} \exp\left[-V_1\left(\frac{\mathrm{DY}}{\sigma_y}\right)^2\right] \exp\left[-V_2\left(\frac{H}{\sigma_z}\right)^2\right], \tag{37}$$

where Q_i is the pollutant emission rate (g s^{-1}), U is the mean wind speed representative of the diffusing layer (m s^{-1}), σ_y and σ_z are the horizontal and vertical standard deviations of plume spread (m), V_1 and V_2 are constants (that equal 0.5), and H is the effective emission height (m). Input parameters for the Gaussian plume model (for multiple point sources) are stack locations in polar coordinates [(R_1, P_1); (R_2, P_2); . . . ; (R_n, P_n)], stack heights (h_1, h_2, . . . , h_n), plume rise buoyancy fluxes (F_{b1}, F_{b2}, . . . , F_{bn}), emission rates (Q_1, Q_2, . . . , Q_n), and ambient temperature T_a (K). Then, the downwind distance (DX) and the crosswind displacement (DY) in Eq. (37) can be expressed as functions of stack locations variables (R, P), receptor location variables (X, AA), and mean wind direction A (e.g., Wu 1982):

$$\mathrm{DX} \equiv \mathrm{DX}(R, P, X, \mathrm{AA}, A) \tag{38}$$

and

$$\mathrm{DY} \equiv \mathrm{DY}(R, P, X, \mathrm{AA}, A). \tag{39}$$

The effective stack height (H) is taken to be the sum of the actual stack height (h) and the plume rise (Δh), defined as the height at which the plume becomes passive and subsequently follows the ambient air motion (Seinfeld 1986),

$$H = h + \Delta h. \tag{40}$$

The behavior of a plume is generally affected by a number of parameters, including the initial source conditions (e.g., the stack gas exit velocity, the stack diameter, the stack exit temperature at stack height, the ambient temperature at stack height, etc.) and the plume rise buoyancy flux parameter F_b (m^4 s^{-3}), the stratification of the atmosphere, and the mean wind speed. Most of the available plume rise formulas can be expressed in the form (Seinfeld 1986)

$$\Delta h = \frac{E(\mathrm{DX})^b}{U^a}, \tag{41}$$

where a, b, and E are empirically determined constants. As a working hypothesis, it is also assumed that the effective emission height H in the Gaussian plume equation (37) can be estimated by using the plume rise formulas of Briggs (1976). For example, during neutral and unstable conditions, in the case of $F_b < 55$ and

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(DX) $< 49F_b^{5/8}$, the plume rise formula was adopted with $a = 1$, $b = 2/3$, and $E = 1.6F_b^{1/3}$; in the case of $F_b < 55$ and (DX) $\geq 49F_b^{5/8}$, $a = 1$, $b = 0$, and $E = 21.4F_b^{3/4}$; in the case of $F_b \geq 55$ and (DX) $< 119F_b^{2/5}$, $a = 1$, $b = 2/3$, and $E = 1.6F_b^{1/3}$; and in the case in which $F_b \geq 55$ and (DX) $\geq 119F_b^{2/5}$, the plume rise formula was adopted with $a = 1$, $b = 0$, and $E = 38.7F_b^{3/5}$.

Finally, the analysis is based on the assumption that the horizontal $\sigma_y \equiv \sigma_y$(DX) and vertical $\sigma_z \equiv \sigma_z$(DX) dispersion coefficients are functions of atmospheric stability (Pasquill stability classes) and downwind distance (DX) from the source (see appendix of Wu 1982). In addition, there are some constraints between U and K according to the Pasquill stability scheme. For a more detailed description of the input parameters for the Gaussian plume model, the horizontal σ_y and vertical σ_z dispersion coefficients, the effective emission height H, and meteorological and receptor location variables used in the search, see Wu (1982).

If we accept, as a working hypothesis, the usual Gaussian diffusion equation as a valid basis for analysis, Eq. (21), together with Eqs. (37), (40), and (41), implies that

$$\frac{\partial C}{\partial \omega} = -\sum_{i=1}^{n} [C_i(W_Y + W_Z + W_D + W_H)], \quad (42)$$

where

$$W_Y = \frac{1}{\sigma_y}\left(\frac{\partial \sigma_y}{\partial \omega}\right), \quad (43)$$

$$W_Z = \frac{1}{\sigma_z}\left(\frac{\partial \sigma_z}{\partial \omega}\right), \quad (44)$$

$$W_D = 2V_1(\mathrm{DY})\sigma_y^{-2}\left[\frac{\partial(\mathrm{DY})}{\partial \omega} - (\mathrm{DY})W_Y\right], \quad (45)$$

$$W_H = 2V_2 H\sigma_z^{-2}\left[\left(\frac{\partial H}{\partial \omega}\right) - HW_Z\right), \quad (46)$$

and

$$\frac{\partial H}{\partial \omega} = \frac{b}{(\mathrm{DX})}\left[\frac{\partial(\mathrm{DX})}{\partial \omega}\right]\Delta h \quad (47)$$

for $\omega = X$, AA, and A. In the case of $\omega = U$, it yields

$$\frac{\partial C}{\partial U} = -\sum_{i=1}^{n} (C_i W_U) \quad (48)$$

with

$$W_U = \frac{2V_2}{\sigma_z^2}\left(H\frac{\partial H}{\partial U}\right) + \frac{1}{U} \quad (49)$$

and

$$\frac{\partial H}{\partial U} = -\frac{a}{U}\Delta h. \quad (50)$$

Adopting the transformations for the downwind distance (DX) and the crosswind displacement (DY) suggested by Wu (see appendix of Wu 1982),

$$\mathrm{DX} = [R\sin(P) - X\sin(\mathrm{AA})]\cos(\mathrm{AL}) - [R\cos(P) - X\cos(\mathrm{AA})]\sin(\mathrm{AL}) \quad (51)$$

and

$$\mathrm{DY} = [R\cos(P) - X\cos(\mathrm{AA})]\cos(\mathrm{AL}) + [R\sin(P) - X\sin(\mathrm{AA})]\sin(\mathrm{AL}). \quad (52)$$

Equations (51) and (52) yield

$$\frac{\partial(\mathrm{DX})}{\partial X} = \sin(\mathrm{AL} - \mathrm{AA}), \quad (53)$$

$$\frac{\partial(\mathrm{DX})}{\partial \mathrm{AA}} = -X\cos(\mathrm{AL} - \mathrm{AA}), \quad (54)$$

$$\frac{\partial(\mathrm{DX})}{\partial A} = [R\sin(P) - X\sin(\mathrm{AA})]\cos(A) - [R\cos(P) - X\cos(\mathrm{AA})]\sin(A), \quad (55)$$

$$\frac{\partial(\mathrm{DY})}{\partial X} = -\cos(\mathrm{AL} - \mathrm{AA}), \quad (56)$$

$$\frac{\partial(\mathrm{DY})}{\partial \mathrm{AA}} = -X\sin(\mathrm{AL} - \mathrm{AA}), \quad (57)$$

and

$$\frac{\partial(\mathrm{DY})}{\partial A} = [R\cos(P) - X\cos(\mathrm{AA})]\cos(A) + [R\sin(P) - X\sin(\mathrm{AA})]\sin(A), \quad (58)$$

where AL $= A - \pi/2$.

A simple numerical algorithm suitable for execution on a small personal computer was used to perform an exhaustive search for the worst-case meteorology and receptor. A hypothetical five-stack problem was formulated and tested with the methodology presented above on a CYRIX P166+ (6X86 - RAM: 32 MB, EDO) personal computer. The input parameter values for the dispersion model (37)–(58) are described in Table 1.

Based on Eqs. (1) through (36), which require that the atmospheric diffusion process be described by the usual Gaussian plume model in Eqs. (37) through (58) for multiple point sources, Fig. 1 presents the effect of mean wind direction A and receptor location angle AA on the maximum ground-level concentrations C_{MAX}, in polar coordinates (C, J), with

$$C_X = C_{\mathrm{MAX}}\cos(J), \quad (59)$$

$$C_Y = C_{\mathrm{MAX}}\sin(J), \quad (60)$$

and

$$C_{\mathrm{MAX}}^2 = C_X^2 + C_Y^2, \quad (61)$$

where $J \equiv A$ and AA for the worst-case meteorology

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TABLE 1. Input parameters.

Parameter	Stack 1	Stack 2	Stack 3	Stack 4	Stack 5
R (km)	0.1	0.2	0.15	0.12	0.10
P (radian)	0.8	1.8	4.0	1.5	1.7
h (m)	100	75	50	120	150
Q (g s^{-1})	100	200	150	250	50
F_b (m^4 s^{-3})	50	60	70	60	70
T_a (K)	293	293	293	293	293

and worst receptor location search procedure, respectively.

To illustrate a simple calculation, the suggested methodology is used to determine the worst-case meteorology, that is, the worst wind vector **WIND** = (U_w, A_w), which causes maximum concentrations at the receptor location with polar coordinates (X, AA) for the Pasquill stability category K. Having obtained for $A \in [0, 2\pi]$ the successive values of U from Eq. (12), the corresponding ground-level concentrations C_{MAX} (A) are calculated from Eq. (1) at the receptor location with polar coordinates (X, AA). The elliptic curves illustrated in Fig. 1 were constructed by connecting the successive points of (C_X, C_Y) from Eqs. (59) through (61). Geometrically, the major axis of the curve corresponds to a relative maximum concentration. Thus, a relative maximum value of $C(U, A)$, occurring for a mean wind vector, $\mathbf{V}_{\text{WM}} = (U_0, A_0)$, can be estimated from Eq. (1). Having obtained the initial approximate solution vector $\mathbf{V}_{\text{WM}}$, the quasi-Newton numerical algorithm can be used to solve the system of nonlinear equations (12) and (13), by numerical iterations for U and A, to obtain (in the near neighborhood of the initial approximation) the exact solution vector $\mathbf{V}_{\text{WM}} = (U_w, A_w)$, satisfying the conditions (14)–(16) for a relative maximum. Therefore, Eqs. (1), (19), and (20) finally yield the worst wind direction A_w, the worst wind speed U_w, and the worst ground-level concentration C_w. Input parameter values for X, AA, and K, and final values for U_w, A_w, and C_w are described in Table 2 (where the computer time is about 40 s for each of the four separate sets of runs). Furthermore, as an inverse problem, the suggested quasi-Newton numerical scheme is also used (as mentioned previously) to estimate the location **DIST** = (X_m, AA$_m$) of the maximum ground-level concentration, for any given wind vector **WIND** = (U, A) and atmospheric stability category. Therefore, for the wind vectors and stability classes discussed above, Eqs. (1) through (11) finally yield the worst receptor location variables X_m and AA$_m$, and the maximum ground-level concentration C_{MAX}. Input parameter values for U, A, and K, and final values for X_m, AA$_m$, and C_{MAX}, are described in Table 3. Then the critical receptor location **DIST**$_{\text{cr}}$ and the critical wind vector **WIND**$_{\text{cr}}$, for day conditions (see Wu 1982), are calculated by solving the following system of nonlinear equations (22)–(25): $X_{\text{cr}} = 0.988060$ km, AA$_{\text{cr}} = 1.466954$ rad, $U_{\text{cr}} = 1.546178$ m s^{-1}, $A_{\text{cr}} = 4.577571$ rad, and $K_{\text{cr}} = 1$. Finally, Eq. (1) gives the

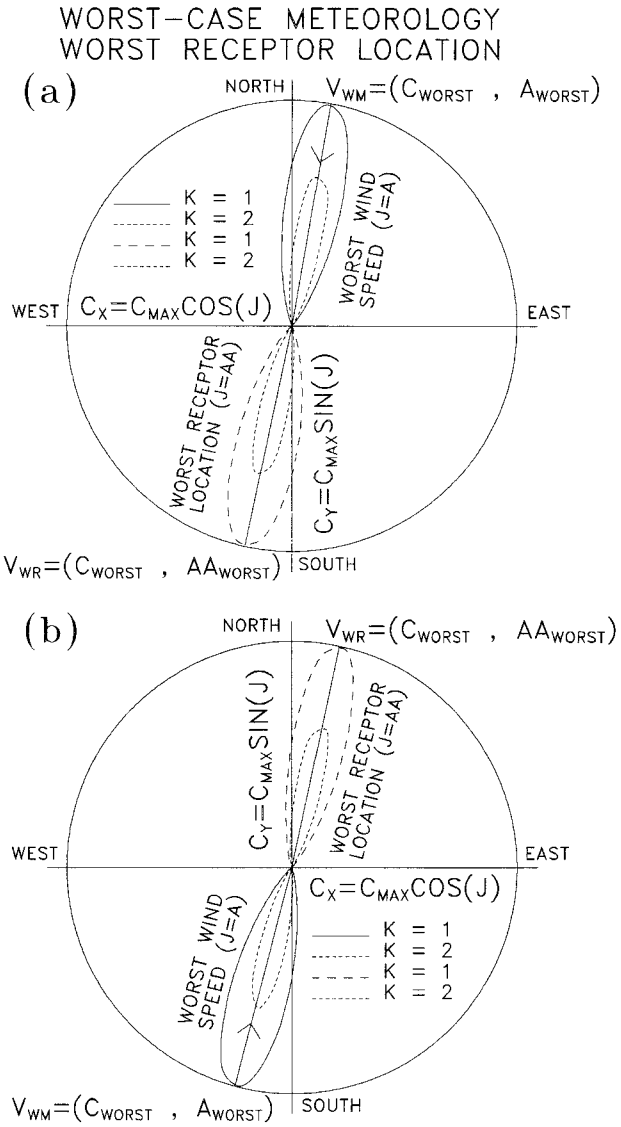

FIG. 1. (a) The maximum concentration C_{MAX} at various receptor locations, **DIST** = (X, AA), as a function of the mean wind direction (A) for the stability classes $K = 1$ and $K = 2$. (b) The maximum concentration C_{MAX} for different wind vectors, **WIND** = (U, A), as a function of the receptor location angle AA for the stability classes $K = 1$ and $K = 2$.

TABLE 2. Worst-case meteorology: A test problem.

X (km)	AA (rad)	K	Initial approximations	U_w (m s^{-1})	A_w (rad)	C_w (mg m^{-3})
0.90	4.50	1	Solid curve, Fig. 1a	1.292	1.398	1.0946
1.50	4.50	2	Dotted curve, Fig. 1a	3.377	1.386	0.7446
0.90	1.36	1	Solid curve, Fig. 1b	2.001	4.453	1.1384
1.50	1.36	2	Dotted curve, Fig. 1b	3.830	4.471	0.7290

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TABLE 3. Worst-receptor location: An inverse test problem.

U (m s^{-1})	A (rad)	K	Initial approximations	X_m (km)	AA_m (rad)	C_{MAX} (mg m^{-3})
1.292	1.398	1	Dashed curve, Fig. 1a	0.90	4.50	1.0946
3.377	1.386	2	Dotted curve, Fig. 1a	1.50	4.50	0.7446
2.001	4.453	1	Dashed curve, Fig. 1b	0.90	1.36	1.1384
3.830	4.471	2	Dotted curve, Fig. 1b	1.50	1.36	0.7290

critical concentration $C_{cr} = 1.152624$ mg m^{-3} (where the computer time is about 50 s for the quasi-Newton numerical scheme to solve the relevant optimization problem).

To assess the validity of the proposed methodology, a comparison of its results with that obtained running the Gaussian model in screening procedure is presented in Table 4. Also, search ranges, step sizes, and final values for all runs are described in Table 4. It is obvious then, compared with the screening model approach, that the numerical algorithm is better able to predict the characteristics of maximum concentrations from multiple point sources. On the other hand, results from the screening model approach may be delayed because of the time required to select the successive ''judicious step sizes'' (Wu 1982) for the meteorological and receptor location variables. Moreover, when using a screening model approach with smaller step sizes, the results may be extremely delayed because of the time required to perform the calculations (e.g., see the computer time for run 6 presented in Table 5).

4. Recommendations for future work

As a working hypothesis, the Gaussian plume model for multiple point sources in Eqs. (37) through (58) was adopted in developing the numerical solution to the nonlinear system of Eqs. (22) through (25). The accuracy of the estimates of characteristics of maximum concentrations from multiple point sources via Eqs. (1) through (36) reflects the ability of Eqs. (37) through (58) to describe the atmospheric diffusion process (e.g., Hanna 1982). However, it is obvious that a regulatory dispersion model must have simple input requirements, such as wind speed, wind direction, stability class, ambient temperature, stack locations, stack heights, emission rates, plume rise buoyancy fluxes, etc. While Gaussian plume models, for the most part, have been supplanted by more sophisticated dispersion models, a place for the models based on the Gaussian diffusion equation still exists in many cases. Despite the fundamental criticisms of the Gaussian plume dispersion formula, this model, because of its simplicity, is a straightforward and widely used approach for obtaining quick, but reliable, preliminary estimates of the mean ground-level concentrations of nondepositing and nonreactive air pollutants, resulting from an elevated point source diffusing over flat terrain (e.g., see Peterson 1985). For these reasons, many U.S. Environmental Protection Agency regulatory models use the Gaussian plume formula as a basis for short-distance calculations (e.g., Hanna et al. 1982).

TABLE 4. A step-by-step screening model approach.

Variable	Search range	Step size	Final value	Numerical scheme
Run 1				
U (m s^{-1})	1.0–21.0	2.0	3.0	
A (rad)	0–6.28	0.628	5.024	
K (stability)	1–4	1	2	
X (km)	0–10.0	2.0	2.0	
AA (rad)	0–6.28	0.628	1.884	
C_{MAX} (mg m^{-3})			0.680460	
Run 2				
U (m s^{-1})	1.0–5.0	1.0	2.0	
A (rad)	4.396–5.652	0.157	4.867	
K (stability)	1–3	1	1	
X (km)	0–4.0	1.0	1.0	
AA (rad)	1.256–2.512	0.157	1.727	
C_{MAX} (mg m^{-3})			1.087353	
Run 3				
U (m s^{-1})	1.0–3.0	0.5	1.5	
A (rad)	4.710–5.024	0.0628	4.7728	
K (stability)	1–2	1	1	
X (km)	0–2.0	0.2	1.0	
AA (rad)	1.570–1.884	0.0628	1.6328	
C_{MAX} (mg m^{-3})			1.149082	
Run 4				
U (m s^{-1})	1.0–2.0	0.2	1.6	
A (rad)	4.710–4.8356	0.0314	4.8042	
K (stability)	1	—	1	
X (km)	0.8–1.2	0.05	1.0	
AA (rad)	1.570–1.6956	0.0314	1.6642	
C_{MAX} (mg m^{-3})			1.149106	
Run 5				
U (m s^{-1})	1.4–1.8	0.1	1.6	1.546178
A (rad)	4.7728–4.8356	0.0157	4.7728	4.577571
K (stability)	1	—	1	1
X (km)	0.95–1.05	0.01	0.98	0.988060
AA (rad)	1.6328–1.6956	0.0157	1.6485	1.466954
C_{cr} (mg m^{-3})			1.149288	1.152624

The Gaussian equation is an easy and fast method for the simulation of atmospheric dispersion phenomena that, however, cannot properly simulate complex nonhomogeneous conditions in a three-dimensional domain (e.g., Tirabassi et al. 1986). For example, the Gaussian diffusion equation is not applicable near the surface as recognized by Gifford (1968), Pasquill and Smith (1983), and others. In addition, the vertical concentra-

TABLE 5. A screening model approach with smaller step sizes.

Variable	Search range	Step size	Computer time
Run 6			
U (m s^{-1})	1.0–2.0	0.1	
A (rad)	0–6.28	0.0314	
K (stability)	1		
X (km)	0.5–1.05	0.01	
AA (rad)	0–6.28	0.0314	
C_{cr} (mg m^{-3})			7h, 12 min, 4 s

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tion profile of air pollutants has been shown by observations to follow the general exponential form rather than the Gaussian distribution (e.g., Huang 1979; Zoumakis 1995). Thus, it has been suggested that the K theory or the Lagrangian similarity theory is better than the Gaussian model for diffusion estimates from a point source near (or at) the ground (e.g., Pasquill and Smith 1983; Huang 1979).

Different analytical solutions for the atmospheric diffusion equation were obtained for an elevated point source, under different simplifying assumptions, by a number of authors. For example, by introducing power law approximations for wind profile and vertical eddy diffusivity, Yeh and Huang (1975) developed analytical solutions of the steady-state advection and diffusion equation. As suggested by several authors (e.g., see Tirabassi et al. 1986), this analytical non-Gaussian model is preferable to the steady-state Gaussian three-dimensional model because it better represents the vertical stratification of the atmosphere and, especially, the wind shear. Therefore, by the incorporation of a more appropriate analytical expression (C_i) for the concentration field (e.g., a generalized non-Gaussian diffusion formula) into the set of equations (1)–(61), it may be possible to represent properly the effects of wind direction, wind speed, and atmospheric stability category on the maximum ground-level concentrations. It is obvious then that different analytical expressions for the concentration field require minor modifications of the resultant equations discussed above [such as Eqs. (42) through (50)]. Consequently, by using an alternative analytical dispersion formula (C_i) for the concentration field, it may be possible to improve the search procedure to determine the characteristics of maximum concentrations from multiple point sources. For progress, it is reasonable to suppose that a physically realistic analytical solution of the atmospheric diffusion equation has, for multiple point sources, the general representation

$$C \equiv C(X, \text{AA}, U, A, \xi_1, \xi_2, \ldots, \xi_m), \qquad (62)$$

where the additional diffusion parameters $\xi_1, \xi_2, \xi_3, \ldots, \xi_m$ in Eq. (62) are generally dependent (in a complex manner) on the atmospheric stability (e.g., the Monin–Obukhov stability length L) and the surface roughness length (z_0). For example, the diffusion parameters $\xi_1 \equiv p_w$ and $\xi_2 \equiv p_d$ (i.e., the wind speed p_w and eddy diffusivity p_d profile power-law exponents) in the non-Gaussian dispersion model proposed by Huang (1979) can be expressed as universal functions depending on L and z_0. The special case in which $\xi_i \equiv \xi_i(L, z_0)$ for $i = 1, 2, \ldots, m$ (with $z_0 \equiv$ constant) yields the following equation:

$$\frac{\partial C}{\partial L} = \sum_{i=1}^{n} \left(\frac{\partial C_i}{\partial L} \right) = 0, \qquad (63)$$

which must be incorporated into the set of the nonlinear equations (22)–(25).

Since the diffusion parameters ξ_i (for $i = 1, 2, \ldots, m$) are, in general, not independent variables, it is reasonable to consider the function (62) subject to some constraint conditions of a general form,

$$\mu_i (X, \text{AA}, U, A, \xi_1, \xi_2, \ldots, \xi_m) = 0, \qquad (64)$$

for $i = 1, 2, \ldots, k$. A method for obtaining a relative maximum of the function (62) subject to the constraint conditions (64) consists of the formation of the auxiliary function

$$\Omega \equiv C + \sum_{i=1}^{k} \lambda_i \mu_i \qquad (65)$$

subject to the (necessary) conditions

$$\frac{\partial \Omega}{\partial \delta_j} = 0, \qquad (66)$$

where $\delta_j \equiv X, \text{AA}, U, A, \xi_1, \xi_2, \ldots, \xi_m$. The parameters $\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_k$, which are independent of δ_j, are the Lagrangian multipliers. Then the critical receptor location and atmospheric conditions of wind direction, wind speed, and stability, which produce the critical ground-level concentration, can be calculated by solving the following system of nonlinear equations:

$$\frac{\partial \Omega}{\partial \delta_j} = \frac{\partial C}{\partial \delta_j} + \sum_{i=1}^{k} \lambda_i \left(\frac{\partial \mu_i}{\partial \delta_j} \right) = 0. \qquad (67)$$

5. Conclusions

Now there is a basis for developing a methodology for estimating the characteristics of maximum ground-level concentrations in air quality modeling over short distances for multiple point sources.

A simple numerical scheme suitable for execution on a small personal computer was used to perform an exhaustive search for the worst-case meteorology and receptor. Also, the proposed iteration algorithm was applied to investigate the combination of location **DIST**, wind vector **WIND**, and atmospheric stability category that produces the highest possible ground-level concentration, the so-called critical concentration. The sufficient conditions, under which the quasi-Newton numerical method used in this study converges, are also discussed. The model is simple to use, as it depends on routinely available data (such as wind speed, wind direction, stability class, ambient temperature, stack locations, stack heights, emission rates, and plume rise buoyancy fluxes).

Since the purpose of this study is to demonstrate a search approach rather than a model development, the simple Gaussian plume model for chemically inert pollutants was used for all calculations. However, the performance of the proposed search procedure may be further improved by the incorporation of a more appro-

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priate analytical expression (C_i) for the concentration field (e.g., a generalized non-Gaussian diffusion formula) into the set of equations (1)–(61) because it may be possible to represent properly the effects of wind direction, wind speed, and atmospheric stability category on the maximum ground-level concentrations.

In summary, the present method is adapted from Wu (1982). An important difference, however, is that the proposed methodology uses a quickly converging and computationally efficient quasi-Newton numerical scheme, giving the exact solution vector for the worst-case meteorology and the worst receptor location in short-term dispersion modeling for multiple point sources. A comparison of the method presented herein with the screening model approach indicates that the numerical model gives a more accurate estimate of the maximum concentration. On the other hand, results from the screening model approach may be delayed because of the time required to select the successive step sizes for the meteorological and receptor location variables and perform the calculations.

In conclusion, because of the numerical simplicity of the methodology adopted here, this search algorithm should become useful for regulatory applications. It may be used in applications in design of stacks, air quality management, and air pollution episode control planning.

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