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Chapter 7B

Simulation Algorithms in Gaussian Plume Modeling

Robert J. Yamartino

Integrals Unlimited, Portland, Maine (*USA*)
rjy@maine.rr.com

Abstract: This chapter focuses on the development of various Gaussian modeling techniques with an emphasis on the relevant mathematical and numerical details. Beginning with the diffusion equation in one-dimension, we show how one solution of this differential equation for pollutant mixing ratio involves the Gaussian function. The three-dimensional Gaussian plume solution is then constructed via consideration of the advection terms and the use of the separation of variables technique. Influences of the ground and other "reflecting" barriers is then added via the method of images and alternative mathematical formulations of this summation of images is considered, both from theoretical and numerical accuracy viewpoints. The issue of air density varying with height is then discussed as it complicates the solution expressed in terms of mass concentration (e.g., g/m^3) versus the more-fundamental mixing ratio (e.g., ppm) formulation. Having an impact on computed results in the 5-15% range, this density complication is presently nearly-universally overlooked. Focus then shifts to extending the point source formulation to various integrated forms that accommodate line and area sources, and including wind shear. Removal processes, particularly dry deposition, are then treated in some detail.

Key Words: Gaussian methods, atmospheric dispersion modeling.

1 Introduction

As introduced in Volume 1, Chapter 7A by Venkatram and Thé (2003), the Gaussian plume expression, given by their Eq.(1), serves as the starting point for much of the air pollution modeling that has taken place during the past half-century. First applied to the atmospheric diffusion problem for a steady-state source by Sutton (1932, 1953), this equation states that a time-independent, mass concentration distribution, $C(x,y,z)$, of:

$$C(x,y,z) = \frac{Q}{2\pi \cdot U \cdot \sigma_y(x) \cdot \sigma_z(x)} \cdot \exp\left[-\frac{(z - z_S)^2}{2\sigma_z(x)^2} - \frac{y^2}{2\sigma_y(x)^2} \right] \tag{1}$$

results when a steady source of strength *Q* (mass/time) positioned at coordinates ($0,\ 0,\ z_S$) emits into a uniform flow *U*(m/s) moving in the +*x* horizontal direction. This emitted material is free to spread out (or diffuse) in the two perpendicular directions *y* (horizontally transverse to the flow direction) and *z* (vertically), with the "dispersion coefficients", σ_y and σ_z, representing the standard deviation widths (m) of the distribution in the *y* and *z* directions, respectively.

Given the dimensions of the above expressions, one thing to note is that a *Q* expressed in g/s will give rise to a mass per unit volume (mass/volume) concentration *C* having units of g/m^3; thus, clarifying use of the terminology mass concentration. This terminology is worth clarifying because the word "concentration" is alternatively employed to indicate a mass concentration *C* or a mixing ratio concentration φ, frequently quoted in non-dimensional units of parts per million (ppm) or parts per billion (ppb), with the further qualification that these fractional mixing ratio "concentrations" represent fractional compositions on a mass basis, rather than a volumetric basis. These two pollutant measures, mass concentration *C* and mass mixing ratio φ, are related by the simple expression $C = \varphi \cdot \rho$, where ρ(g/m^3) is the local density of air. However, this simple relation gives rise to one of the many problems that often lie hidden and unresolved within the framework of the Gaussian plume formulation, and even within other air pollution modeling frameworks, such as numerical Eulerian models.

This chapter will examine various issues and simplifications intrinsic to the derivation of the Gaussian plume formulation and will point out various measures that are, or have been, suggested to correct these simplifications. The chapter will then proceed to consider numerous mathematical extensions of the simple plume formalism to account for real-world complexities, such as barriers to plume mixing, pollutants emitted from area and line sources, deposition of plume material to surfaces, wind directional shear, and concentration fluctuations. Emphasis will be placed on mathematical and algorithmic details rather than on considering the features and merits of specific Gaussian models that currently continue to be applied.

2 Theoretical Background

2.1 Diffusion and Advection

2.1.1 Diffusion in One-Dimension

Sir Isaac Newton is often credited with introducing the notion of gradient transfer of heat by noting that heat will move from hotter to cooler environments. This notion of "down-gradient" transfer accounts for the minus sign one sees in the heat conduction proportionality relation $q \propto -dT/dx$. Apparently, clarification of the units of the needed proportionality constant k, to yield the modern flux relation, $q = -k \cdot dT/dx$, was introduced many decades later in 1822 by the French mathematician, Joseph Fourier. Nevertheless, this notion of down-gradient transport is intrinsic to the second law of thermodynamics (variously attributed to Carnot, Clausius, or Lord Kelvin), which states that: in any physical process the entropy (or disorder) of an isolated system never decreases. This second law really forces the time arrow to have a single (forward) direction and explains why pollutant concentrations, fortunately for all of us, always move in the direction of greater, rather than lesser, dilution. We now know that counter-gradient transport can occur and can be important in convective mixing, but that is beyond the focus of this chapter.

The flux-gradient relation for heat was extended to diffusive mass transfer flux, F_d, by Adolf Fick in 1855 and was originally expressed as:

$$F = - K \cdot (dC/dx) \tag{2a}$$

where the diffusivity K, having units of m^2/s, gives rise to the flux, F_d, having units of $g/m^2/s$. As Fick's paper dealt with salt concentration diffusion in water, it was not concerned with density issues, but one would reformulate this to include density as:

$$F = -K \cdot \rho \cdot \frac{\partial \phi}{\partial x} \tag{2b}$$

This flux-gradient relation, known as Fick's First Law, serves as the basis of the time-dependent diffusion equation, also known as Fick's Second Law, which is expressed in flux-conservative form (and updated to include density) in one-dimension for the mixing ratio as:

$$\frac{d(\rho \cdot \phi)}{dt} = +\frac{\partial}{\partial x} \cdot K(x) \cdot \rho \cdot \frac{\partial \phi}{\partial x} \tag{3a}$$

where t is, of course, time. It is important to note that it is the mixing ratio which diffuses, and <u>not</u> the mass concentration per se. Thus, in an environment where the domain is bounded, maximum entropy or disorder is achieved when the mixing ratio is the same everwhere, such that any gradients in φ vanish. Also, the

ρ in Eq.(3a) may be a function of both x and t, though temporal changes in density usually occur on much longer time scales and do not involve diffusive processes. Equation (3a) may also be expressed as a diffusion equation for mass concentration as:

$$\frac{dC}{dt} = + \frac{\partial}{\partial x} \cdot K(x) \cdot \rho \cdot \frac{\partial (C/\rho)}{\partial x}. \tag{3b}$$

In the case of a space-time uniform density field, Eqs.(3a) and (3b) are identical; however, differences emerge when the air density, $\rho(x)$, becomes a function of x or more significantly, a function of z in the comparable 1D equation for vertical diffusion.

One of the simplest, non-trivial solutions of Eq.(3a) is given for the y direction and spatially uniform K as:

$$\phi(y,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp\left[-\frac{y^2}{2 \cdot \sigma^2} \right] \tag{4a}$$

$$\text{where } \sigma^2 \equiv \sigma_0^2 + 2 \cdot K_y \cdot (x/U) \tag{4b}$$

where σ_0 is an arbitrary constant, and the diffusivity has been given the subscript **y** to differentiate it from the appropriate diffusivities in other dimensions. It should be noted that Eq.(4a) satisfies the differential Eq.(3a) <u>only</u> if $\frac{d\sigma^2}{dx} = \frac{2 \cdot K}{U}$, which is realized for the constant K, appropriate for Brownian or molecular diffusion, by σ being constrained by Eq.(4b). However, the added unit normalization condition, expressed below through the constraint that the integral on y over all values from -∞ to +∞ yields one, or

$$\int_{-\infty}^{+\infty} dy \cdot \phi(y,\sigma) = 1. \tag{5}$$

This is valid for any definition of σ and is ensured by the factor $\sqrt{2\pi}$ in the denominator of Eq.(4a).

Assuming an Eq.(4a) solution to apply for both **y** and **z** dimensions, abandoning the constraint on σ provided by Eq.(4b), and blindly swaping C for φ enables one to come close to attaining the Gaussian plume of Eq.(1), except for the absence of the factor Q/U.

2.1.2 The Advection Term and Building the 3D Plume Solution

In order to understand the origin of the *Q/U* factor, one must expand Eqs.(3a) and (3b) to include the advective flux term, $F_a = U \cdot \rho \cdot \varphi = U \cdot C$, and write:

$$\frac{\partial(\rho \cdot \phi)}{\partial t} = -\frac{\partial}{\partial x} \cdot (U \cdot \rho \cdot \phi) + \frac{\partial}{\partial x} \cdot K(x) \cdot \rho \cdot \frac{\partial \phi}{\partial x} + (S - D) \tag{6a}$$

or

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \cdot [-U \cdot C + K(x) \cdot \rho \cdot \frac{\partial (C/\rho)}{\partial x}] + S - D \tag{6b}$$

where source, *S*, and depletion, *D*, terms have been added for completion and would have volumetric units of g/m^3/s.

Now in the steady-state limit, defined as existing when $dC/dt = 0$, and neglecting losses *D* and along-wind or *x* diffusion by setting *K* to zero, Eq.(6b) can be easily integrated in *x* to yield $C = C_0 + (\int dx \cdot S) / U$, where C_0 is an arbitrary integration constant or, more physically, a background concentration. Now just to minimize sleight of hand trickery, it must be pointed out that as the concentration *C* and source term *S* are both by definition volumetric, or 3D, entities, reconciling their 3D nature with the 1D nature of the equation demands that one integrate over *y* and *z* dimensions as well to encompass the entire source. Further postulating the source distribution *S* as the 3D delta function, $Q \cdot \delta^3(\underline{x}) = Q \cdot \delta(x) \cdot \delta(y) \cdot \delta(z-z_S)$, for a true point source located at $(0,0,z_S)$, and recalling that the normalization condition of Eq.(5) just yields unity for the *y* and *z* integrations over *C*, one obtains the result:

$$\overline{\overline{C}} = \frac{Q}{U} \quad \text{or} \quad \overline{\overline{\phi}} = \frac{(Q/\rho_0)}{U} \tag{7}$$

where ρ_0 is the presently-assumed-constant air density and the double overbar denotes integration over *y* and *z* dimensions. The fact that Eq.(7) becomes infinite as $U \to 0$ is simply a consequence of ignoring alongwind diffusion (i.e., setting $K(x)$ to zero in Eq.(6)) and should not be viewed as something that happens in nature. Nevertheless, the history of Gaussian plume modeling is so littered with concern over this infinity, that regulatory modelers are urged to use a minimal *U* of about 1 m/s to avoid serious overestimation. This subject of alongwind diffusion will be re-visited in detail in Chapter 8a.

Combining the result of Eq.(7) plus the Eq.(4) functional forms for the y and z dimensions, one "constructs" the 3D Gaussian plume solution for the mixing ratio, φ, due to a source located at $(0,0,z_S)$ as:

$$\phi(x,y,z) = \frac{(Q/\rho_0)}{U} \cdot P(y,\sigma_y) \cdot P(z - z_S, \sigma_z) \tag{8a}$$

where x distance and time are inextricably linked via the relation $x \equiv U \cdot t$,

$$P(y,\sigma_y) = \frac{1}{\sqrt{2\pi}\sigma_y} \cdot \exp\left[-\frac{y^2}{2\cdot{\sigma_y}^2}\right],\ P(z-z_S,\sigma_z) = \frac{1}{\sqrt{2\pi}\sigma_z} \cdot \exp\left[-\frac{(z-z_S)^2}{2\cdot{\sigma_z}^2}\right] \quad (8b)$$

and where:

$$\sigma_y^{\,2} \equiv \sigma_{y0}^{\,2} + 2 \cdot K_y \cdot t \quad \text{and} \quad \sigma_z^{\,2} \equiv \sigma_{z0}^{\,2} + 2 \cdot K_z \cdot t \quad (8c)$$

are the appropriate dispersion coefficients for the constant diffusivities associated with molecular/Brownian diffusion.

As indicated in the discussion of Eq.(4), other expressions for σ_y and σ_z are possible, provided that they satisfy the relation:

$$\frac{d\,\sigma^2}{dx} = \frac{2\cdot K(x)}{U} \ \text{ or } \ \frac{d\,\sigma^2}{dt} = 2\cdot K(t)\,. \quad (8d)$$

However, downwind-distance or transport-time dependent diffusivities have traditionally created discomfort among modelers, due to the questionable causal mechanism. Nevertheless, more modern understanding of turbulent spectra and the multiple turbulent length scales contributing to plume growth suggests that diffusivities proportional to the current plume size, that is, $K(x) = V_T \cdot \sigma$, where the proportionality constant, V_T, has the dimensions of a turbulence velocity, may not be unreasonable. In this case, appropriate solution dispersion coefficients would take the forms:

$$\sigma_y \equiv \sigma_{y0} + V_{Ty} \cdot t \quad \text{and} \quad \sigma_z \equiv \sigma_{z0} + V_{Tz} \cdot t \quad (8e)$$

or equivalently,

$$\sigma_y \equiv \sigma_{y0} + (V_{Ty}/U) \cdot x \quad \text{and} \quad \sigma_z \equiv \sigma_{z0} + (V_{Tz}/U) \cdot x. \quad (8f)$$

Note that here the terms add linearly, rather than in quadrature as in Eq.(8c). This is because the appropriate "addition rule", derived based on pseudo-transport times, can be shown to involve the reciprocal of the growth exponent, p, in x^p. Thus, sigmas that grow as $x^{1/2}$ or $t^{1/2}$ will have a $1/p = 2$, or quadrature addition rule, while those linear in x (i.e., p=1) will have a $1/p = 1$, or linear addition rule A yet wider range of dispersion coefficient forms, such as those involving various powers of x or t, or even more complex algebraic forms, have been used over the decades of Gaussian modeling, with their prime justification being that they provide viable predictions relative to tracer experiments or other measurements. Though many of these empirical dispersion coefficient forms lack a clear link to the diffusivity formulation of the advection-diffusion equation, their utility and retained characteristic of mass conservation (i.e., with respect to integrations over *y* and *z*) have been sufficient to justify their use in applied modeling.

It is important to note that Eq.(8a) is appropriate for the mixing ratio, φ; however, it is more frequently applied in its concentration form:

$$C(x,y,z) = \frac{Q}{U} \cdot P(y,\sigma_y) \cdot P(z - z_S, \sigma_z) \tag{9}$$

even though this expression can lead to underestimation of ground level concentrations for air density falling off with height, as will be discussed in a following subsection.

It is also worth noting that Eqs.(8a) and (9) do not contain the added "reflection" terms associated with the presence of the ground or inversion lids. These factors will be discussed later.

The only other seeming mystery involved in this construction of the 3D solution arises if one questions why a product solution or dimensionally-factorized form was chosen. This product factorization arises from the full 3D form of the advection-diffusion equation and the multi-dimensional solution methodology known as "separation of variables".

Finally, it should be noted that the form of Eq.(9) is also often simply conjectured or derived on intuitive grounds. That is, consider the mass of emissions, $Q \cdot \Delta t$, emitted during a time increment, Δt, and filling a box of along-wind length $U \cdot \Delta t$. Let this pollutant also uniformly fill-out the box's transverse dimensions of L_y and L_z to yield a concentration, $C = (Q \cdot \Delta t) / [(U \cdot \Delta t) \cdot L_y \cdot L_z]$, where the expression in brackets is recognized as simply the volume of the box. Noting that the Δt terms cancel, the resulting "box-normalized" concentration, $C = Q / [U \cdot L_y \cdot L_z]$, can be converted to Eq.(8g), by replacing the box normalizations of $1/L_y$ and $1/L_z$ with the Gaussian normalization forms given by Eq.(8b). This simple approach recognizes the key elements of mass conservation and flow uniformity, as well as the neglect of any along-wind diffusion stretching of the box's length. Furthermore, this box normalization highlights the fact that for 1D flow, that is the flow vector $(U,0,0)$, there is no distinction between the average wind speed and the vector mean wind speed, and this average wind speed is simply the arithmetic mean wind, $U = \langle u_i \rangle$, where $\langle\rangle$ denotes the averaging operation, and not some more exotic average, such as the "harmonic mean", $U = \langle 1/u_i \rangle^{-1}$.

Box models and the box normalization principle continue to play a large role in pollutant dispersion modeling and will re-appear later in this chapter.

2.1.3 Advection-Diffusion in Three-Dimensions

For completeness, the 3D expressions of the advection-diffusion equation are:

$$\frac{\partial(\rho\cdot\phi)}{\partial t} = -\underline{\nabla}\bullet(\underline{V}\cdot\rho\cdot\phi) + \underline{\nabla}\bullet(\underline{\underline{K}}\cdot\rho\cdot\underline{\nabla}\phi) + (S-D) \tag{10a}$$

and

$$\frac{\partial C}{\partial t} = \underline{\nabla}\bullet[-(\underline{V}\cdot C) + (\underline{\underline{K}}\cdot\rho\cdot\underline{\nabla}(C/\rho)] + (S-D) \tag{10b}$$

where scalar variables, C, φ, ρ, S and D, vector wind field $\underline{V}$**,** and tensor (or 2D matrix) diffusivity $\underline{\underline{K}}$ may all be 3D functions of x, y, and z. In these 3D forms, the ∇ symbol represents the vector 3D gradient operation, whereas the • symbol denotes the vector dot product operation. At various points in this chapter and in the subsequent chapter on puff modeling, it may be convenient to revisit these 3D equations.

Returning again to the solutions provided by Eq.(8), we note that these results only represent a solution of the 3D advection-diffusion equation in the simplified case of $\underline{V} = (U, 0, 0)$, with U uniform in space and time, and the sparse diffusivity matrix of $\underline{\underline{K}} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & K_{yy} & 0 \\ 0 & 0 & K_{zz} \end{bmatrix}$, containing only the "diagonal" diffusivity elements, K_{yy} and K_{zz} (or in their compressed notation form, K_y and K_z).

2.2 Normalization, Reflections, and Their Summation

Equation (5) showed that the normalization of the Gaussian form, $\varphi(y,t)$, given by Eq.(4a), or its Eq.(8) equivalent, $P(y,\sigma_y)$, when integrated over all y-space from $-\infty$ to $+\infty$ yields unity. This normalization is valid for any functional form of the σ, such as σ provided that σ is not itself a function of y. However, this normalization becomes problematic in the z-direction, where any $z < 0$ implies that one is considering material "below ground", where it cannot possibly be.

Again, considering the Eq.(8) Gaussian z distribution function as:

$$P(z-z_S,\sigma_z) = \frac{1}{\sqrt{2\pi}\cdot\sigma_z}\cdot\exp\left[-\frac{(z-z_S)^2}{2\cdot\sigma_z^{\ 2}}\right] \tag{11}$$

where $\sigma_z = \sigma_z(t)$, one notes that its integral from $z=z_1$ to $z=z_2$ is just:

$$N(z_S,z_1,z_2) \equiv \int_{Z_1}^{Z_2} dz\cdot P(z-z_S,\sigma_z) = \frac{1}{2}\cdot\left[erf(\frac{z_2-z_S}{\sqrt{2}\sigma_z})] - erf(\frac{z_1-z_S}{\sqrt{2}\sigma_z})\right] \tag{12}$$

where *erf* is the symbolic notation for the "error function", and it is defined by its integral expression. While the *erf* is often referred to as a "tabulated function", it is no more so than the more familiar sine and cosine functions. Like the sine function, the erf is an odd function, such that $erf(-x) = -erf(x)$, so $erf(0) = 0$. For small x, $erf(x) \approx 2\cdot x /(\pi)^{1/2}$, whereas for $x \to +\infty$, $erf(x) \to +1$. Also, there is a "complementary error function", $erfc(x)$, defined such that $erfc(x) = 1 - erf(x)$.

One may evaluate the plume mass residing "above ground" by considering the integration limits of $z_1 = 0$ and $z_2 = \infty$. The result is just $N(z_S) \equiv N(z_S,0,\infty)$ or

$$N(z_S) = \frac{1}{2}\left[1 - erf(\frac{-z_S}{\sqrt{2}\sigma_z})\right] = \frac{1}{2}\left[1 + erf(\frac{z_S}{\sqrt{2}\sigma_z})\right]. \qquad (13a)$$

This result says that $N(z_S) < 1$ for all finite source heights z_S, which falls short of the goal of accounting for 100% of the emitted mass. Now, imagine a source of identical strength located "below ground" at a depth of $z = z_S$. Immediately, one notes that this "image source" will lead to an above ground mass, $N(-z_S)$ of

$$N(-z_S) = \frac{1}{2}\left[1 - erf(\frac{+z_S}{\sqrt{2}\sigma_z})\right] \qquad (13b)$$

and that the sum of Eqs.(13a) and (13b) yields the desired result of:

$$N(z_S) + N(-z_S) = \tfrac{1}{2} \cdot (1 + 1) = 1. \qquad (13c)$$

That is, the *erf* terms cancel and 100% of the mass now resides above ground in the domain defined by the limits of $z_1 = 0$ and $z_2 = \infty$.

In addition to this desirable mass accounting property, the distribution function associated with this below-ground "image source" is such that its magnitude at $z = 0$ is just equal to the magnitude of the original above-ground source, and it tapers off above-ground in the same manner as the original above-ground source tapers off below-ground. That is, the below-ground "image source" gives rise to a mass distribution above ground of $P(z+z_S, \sigma_z)$ that appears to "reflect" material upwards that attempts to diffuse across the $z = 0$ boundary.

This "ground reflection" term is given as:

$$P(z + z_S, \sigma_z) = \frac{1}{\sqrt{2\pi}\cdot\sigma_z}\cdot\exp\left[-\frac{(z + z_S)^2}{2\cdot\sigma_z^{\,2}}\right]. \qquad (14)$$

This is the only other term that need be considered if the ground represents the only possibility for reflecting plume mass. In this case, the original Eq.(8a) solution for the mixing ratio, φ, due to a source located at $(0,0,z_S)$ now becomes:

$$\phi(x,y,z) = \frac{(Q/\rho_0)}{U} \cdot P(y,\sigma_y) \cdot [P(z - z_S, \sigma_z) + P(z + z_S, \sigma_z)]. \qquad (15)$$

This is consistent with the analogue to mirror images, in that if one stands in front of a single mirror, there will only be a single reflection that appears to be at a depth "behind" the mirror equal to our distance from the front of the mirror.

Just as with mirrors, the situation becomes more complicated, and infinitely so, if a second parallel mirror is placed behind us. One observes an infinite series of reflections (Pasquill, 1974; 1976) receding ever further into the distance.

An elevated thermal inversion at height $z = h$ positioned above the source at $z = z_S$ constitutes such an equivalent "second parallel mirror" impediment to vertical diffusion, and in this case, the single terms given by Eqs.(11) and (14) are replaced by two infinite series (i.e., one series for the direct term involving z-z_S, and one for the reflection term involving $z+z_S$) of distribution functions to yield:

$$\phi(x,y,z) = \frac{(Q/\rho_0)}{U} \cdot P(y,\sigma_y) \cdot [P(z - z_S, \sigma_z, h) + P(z + z_S, \sigma_z, h)] \qquad (16)$$

where

$$P(z \pm z_S, \sigma_z, h) = \frac{1}{\sqrt{2\pi} \cdot \sigma_z} \cdot \sum_{j=-\infty}^{j=+\infty} \exp\left[-\frac{(z \pm z_S + 2jh)^2}{2 \cdot \sigma_z{}^2} \right]. \qquad (17a)$$

It turns out that these series can be re-expressed in terms of the Jacobi theta function of the third kind as:

$$P(z \pm z_S, \sigma_z, h) = \frac{1}{\sqrt{2\pi} \cdot \sigma_z} \cdot \exp\left[-\frac{(z \pm z_S)^2}{2 \cdot \sigma_z{}^2} \right] \cdot \theta_3\left[\frac{i \cdot (z \pm z_S) \cdot h}{\sigma_z{}^2}, \alpha\right] \qquad (17b)$$

where $i \equiv (-1)^{½}$ and $\alpha \equiv exp(-2 \cdot h^2/\sigma_z{}^2)$. However, this re-expression of the infinite series might be of little more than academic interest except for another transformation, discovered in 1893 by Landsberg, which enables one to write:

$$P(z \pm z_S, \sigma_z, h) = \frac{1}{2 \cdot h} \cdot \theta_3\left[\frac{\pi \cdot (z \pm z_S)}{2 \cdot h}, \beta\right] \qquad (17c)$$

where $\beta \equiv exp[-(\pi \cdot \sigma_z)^2 / (2 \cdot h^2)]$. Expanding Eq.(17c) for small β, or large σ_z/h, then enables one to approximate the rightmost bracketed term in Eq.(16) to yield the final mixing ratio result:

$$\phi(x,y,z) \cong \frac{(Q/\rho_0)}{U \cdot h} \cdot P(y,\sigma_y) \cdot (1-\beta^2) \cdot [1 + \beta^2 + 2\beta \cdot \cos(\frac{\pi \cdot \mathrm{z}}{\mathrm{h}}) \cdot \cos(\frac{\pi \cdot \mathrm{z_S}}{\mathrm{h}})] \qquad (18a)$$

or to yet higher accuracy via the expression:

$$\phi(x,y,z) \cong \frac{(Q/\rho_0)}{U \cdot h} \cdot P(y,\sigma_y) \cdot (1-\beta^2) \cdot (1-\beta^4) \cdot \frac{1}{2} \cdot \left\{ \begin{array}{l} [1+\beta^2+2\beta \cdot \gamma_-] \cdot [1+\beta^6+2\beta^3 \cdot \gamma_-] + \\ [1+\beta^2+2\beta \cdot \gamma_+] \cdot [1+\beta^6+2\beta^3 \cdot \gamma_+] \end{array} \right\} \tag{18b}$$

where $\gamma_\pm \equiv cos[\pi \cdot (z \pm z_S) / h)]$. It is clear from Eqs.(18a) and (18b) that the mixing ratio distribution becomes uniform in z as $\beta \rightarrow 0$.

Figure 1 shows the worst case percentage error experienced (i.e., generally achieved with receptor and source separated by the layer depth, h) using the various techniques considered, and one is struck by how rapidly this error varies with σ_z/h. The "Sum 6" and "Sum 10" curves refer to using Eq.(16), with the sums in Eq.(17a) ranging from j = -1 to j = +1 for 6 terms and from j = -2 to j = +2 for 10 terms; whereas the "Uniform Mix" assumption is just $\varphi \propto 1/h$, or equivalently Eq.(17c) with β = 0 to yield θ_3 = 1. The "Jacobi 1" and "Jacobi 2" term curves refer to refining the uniform mixing assumption via use of Eqs.(18a) and (18b), respectively.

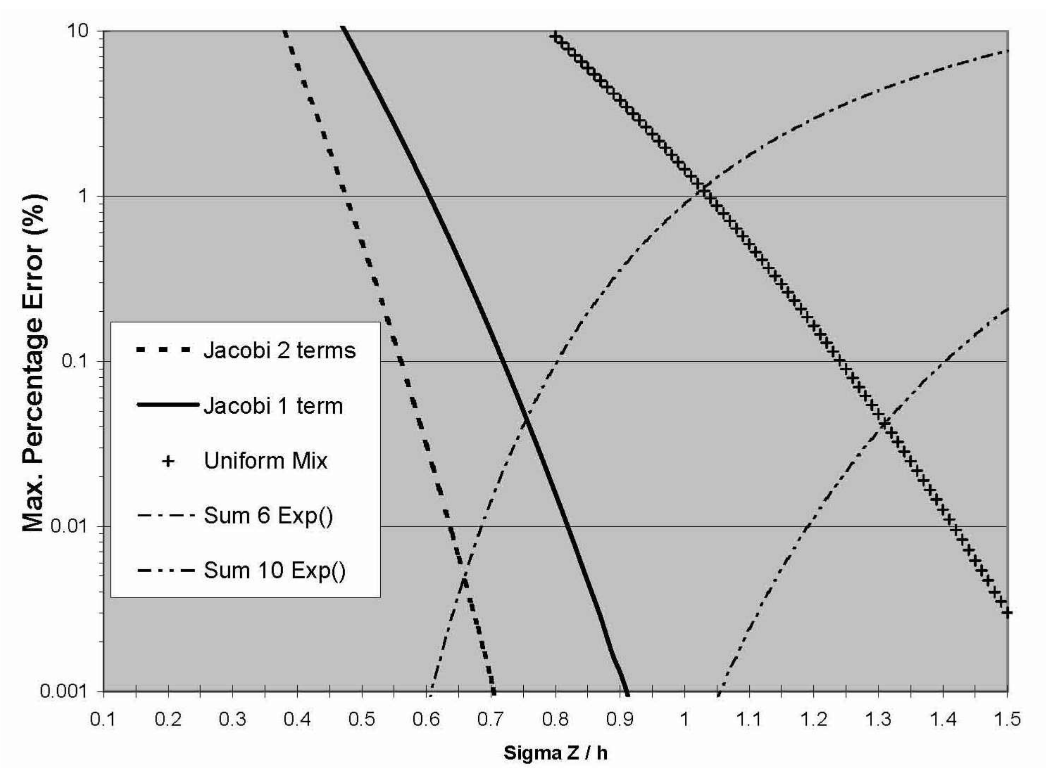

Figure 1. Maximum Computational Errors for Various Gaussian Plume Methods.

Various curve crossover points in Figure 1 provide strategies for building computational algorithms that guarantee a desired maximum error. For example, if one could tolerate errors as large as 1.12%, one could choose the "Sum 6" method for $\sigma_z/h \leq 1.03$ and then switch over to the uniform mixing calculation for $\sigma_z/h > 1.03$. Alternatively, one could incur the higher computational cost of the "Sum 10" method, transition to the uniform mixing calculation for $\sigma_z/h > 1.31$, and never suffer errors exceeding 0.042%. Neither of these two strategies employ the Jacobi theta function expansions of Eq.(18). However, using the simpler, 1-term Jacobi expansion of Eq.(18a) for the limited interval of $0.76 \leq \sigma_z/h \leq 1.30$ in-between the "Sum 6" and uniform mixing calculations yields maximum computation errors below 0.05%. Similarly, using the 2-term Jacobi expansion of Eq.(18b) for the somewhat larger interval of $0.66 \leq \sigma_z/h \leq 1.47$ in-between the "Sum 6" and uniform mixing calculations yields maximum computation errors below 0.005%. These algorithmic crossover points and maximum errors differ somewhat from those originally recommended by Yamartino (1977), as those earlier calculations were found to contain a programming bug that discarded some of the contributing "Sum 6" terms.

2.3 Ground Level Concentrations and the Air Density Issue

Accepting the limitations that are already-stated, one can feel relatively comfortable about using Eq.(15) (i.e., for $h = \infty$) or Eqs.(16) through (18) (i.e., for vertical mixing limited by a lid at $z=h$) to compute mixing ratios aloft and at ground level. However, transitioning from these expressions for the mixing ratio field φ to the original and widely-used Gaussian plume formula [e.g., Eq.(1) or Eq.(9)] for mass-based concentrations means that one must accept that air density remains constant throughout space. Yet, we clearly know that air density varies considerably throughout the depth of a mixed layer – especially if that mixed layer is several kilometers deep. To grasp the problem at hand, imagine that the atmosphere is divided into two vertically stacked boxes of equal depth. Furthermore, suppose that the pollutant is completely diffused vertically, giving rise to a mixing ratio $\varphi = 1.0$ everywhere. Now suppose that the density in the upper box is 0.85, but the density in the lower box has a higher value of 1.15. This means that the vertically-averaged density throughout this two-box atmosphere is $<\rho>_z = 1.0$, as is the vertically-averaged concentration, that is, $<C>_z =1.0$. However, as discussed previously, the actual concentration in the individual boxes is computed as $C = \rho \cdot \varphi$, so that the concentration in the upper box is $C_u = 0.85$ and in the lower box is $C_l = 1.15$. Nevertheless, the 2D version (i.e., well-mixed vertically) of the Eq.(1) Gaussian plume equation would yield $C_l = 1.0$. Is a 15% difference worth worrying about given the known uncertainties in the key mixing depth determination? Perhaps not, but it is surprising that this issue and its correction has been ignored for so long.

A more detailed look at this problem begins by invoking the hydrostatic assumption for an isothermal atmosphere, such that the density falloff with height is given as $\rho(z) = \rho_0 \cdot exp(-z/L)$, where L is the "scale height" of the atmosphere, known to be about 8 km. The exact solution for mixing ratio from K-theory may then be written as:

$$\phi(x,y,z)=\frac{A\cdot Q}{[U\cdot\rho(z_S)]}\cdot P(y,\sigma_y)\cdot\begin{Bmatrix}P[z-\delta-z_S,\sigma_z,h]+\\ P[z-\delta+z_S,\sigma_z,h]\end{Bmatrix} \tag{19a}$$

where A is a normalization constant with $A \approx 1$ very near the source, and where the "receptor shift distance", δ, is given as:

$$\delta\equiv\frac{K_{zz}\cdot \mathrm{x}}{\mathrm{U}\cdot L}=\frac{\sigma_z^2}{2\cdot L} \tag{19b}$$

and with choice of the + sign in the vertical term corresponding to the mirror image density function , $\rho(z) = \rho_0 \cdot exp(+z/L)$. This "receptor shift distance", δ, accommodates the variable density with no other alteration to the "method of images" summation. The expression for concentration may then be written as:

$$C(x,y,z)=\frac{A\cdot Q\cdot\exp[-(z-z_S)/L)}{U}\cdot P(y,\sigma_y)\cdot\begin{Bmatrix}P[z-\delta-z_S,\sigma_z,h]+\\ P[z-\delta+z_S,\sigma_z,h]\end{Bmatrix} \tag{19c}$$

where the normalization "constant", A, is obtained by integrating C over all y, the positive z domain of $(0,+h)$, and requiring a final integrated result of Q/U.

This normalization integration is best performed by completing the square in z, and this leads to the more convenient crosswind-integrated form:

$$\overline{C}(x,z)=\frac{A\cdot Q}{U}\cdot\sum_{j=-\infty}^{+\infty}\exp\left(\frac{2\cdot j\cdot h}{L}\right)\cdot\begin{Bmatrix}\exp\left[\frac{-1}{2}\cdot(z+\delta-z_S+2\cdot j\cdot h)^2/\sigma_z{}^2\right] \quad + \\ \exp\left(\frac{2\cdot z_S}{L}\right)\cdot\exp\left[\frac{-1}{2}\cdot(z+\delta+z_S+2\cdot j\cdot h)^2/\sigma_z{}^2\right]\end{Bmatrix}. \tag{19d}$$

While for arbitrary h, the resulting integration in z yields a not-so-convenient infinite series of error function differences, the case of the unbounded atmosphere (i.e., $h \to\infty$) involves only the $j = 0$ term, and performing this integration yields the exact result:

$$A^{-1}=\frac{1}{2}\cdot\left\{erfc\left(\frac{\delta-z_S}{\sqrt{2}\cdot\sigma_z}\right)+\exp\left(\frac{+2\cdot z_S}{L}\right)\cdot erfc\left(\frac{\delta+z_S}{\sqrt{2}\cdot\sigma_z}\right)\right\} \tag{20a}$$

which for small arguments for the *erfc*(…) expands to yield a form consistent to lowest order in σ_z/L with the approximation:

$$A^{-1}\approx\exp\left(\frac{+z_S}{L}\right)\cdot\left[1-\frac{\sigma_z}{\sqrt{2\cdot\pi}\cdot L}\right]. \tag{20b}$$

In the far field where $\sigma_z \geq h$, we revert back to Eq.(19c) and use the series expansion of the Jacobi theta function[1]. Integrating in z from 0 to h yields:

$$A^{-1} \approx \exp\left(\frac{+z_S}{L}\right) \cdot \left\{ \frac{L}{h} \cdot \left[1 - \exp\left(\frac{-h}{L}\right)\right] + \frac{2}{\pi} \cdot \sum_{k=1}^{+\infty} \beta^{k^2} \cdot \cos\left(\frac{k \cdot \pi \cdot z_S}{h}\right) \bullet \left[1 - (-1)^k \cdot \exp\left(\frac{-h}{L}\right)\right] \cdot \left[\frac{\sin(b_k) + a_k \cdot \cos(b_k)}{k \cdot (1 + a_k^2)}\right] \right\} \quad (20c)$$

where, as before, $\beta \equiv exp[-(\pi \cdot \sigma_z)^2 / (2 \cdot h^2)]$, $a_k \equiv h/(k \cdot \pi \cdot L)$, $b_k \equiv k \cdot \pi \cdot \delta / h$, and δ is given by Eq.(19b). Now Eq.(20c) hardly represents a convenient normalization "constant", but noting that in the truly well-mixed regime, where $\beta \rightarrow 0$, one may expand the first term in Eq.(20c) to obtain:

$$A^{-1} \approx \exp\left(\frac{+z_S}{L}\right) \cdot \left[1 - \frac{h}{2 \cdot L}\right]. \quad (20d)$$

Thus, one may construct a continuous normalization "constant" by combining Eq.(20b) for small σ_z with Eq.(20d), or, better yet, the first term of Eq.(20c), for larger σ_z. This final, somewhat-optimized systhesis for A (i.e., not A^{-1}) is:

$$A \approx \exp\left(\frac{-z_S}{L}\right) / \left\{ W + (1 - W) \cdot \frac{L}{h} \cdot \left[1 - \exp\left(\frac{-h}{L}\right)\right] \right\}$$

where (20e)

$$W \approx \left[1 - \frac{3.16 \cdot \sigma_z}{L}\right] \text{ for } \sigma_z / L \leq 1/3.16 \text{, and } W \equiv 0 \text{ for larger } \sigma_z .$$

---

[1] Justifying this conclusion requires using the series expansion for the Jacobi theta function of the third kind and summing the two θ_3 terms to yield:

$$P(z, \sigma_z) = \frac{\exp[-(z - z_S)/L)}{2 \cdot h} \cdot \left\{ 2 + 2 \sum_{k=1}^{\infty} \beta^{k^2} \cdot \left[\cos\left(\frac{k \cdot \pi \cdot (z - \delta - z_S)}{h}\right) + \cos\left(\frac{k \cdot \pi \cdot (z - \delta + z_S)}{h}\right) \right] \right\}$$

In integrating over z from 0 to h, all terms in the k sum vanish for $L = \infty$ (and hence $\delta = 0$); however, for finite L, and trigonometric expansion to isolate the z term, the integral over $\sin(k \cdot \pi \cdot z/h)$ for odd k values survives, as seen in the resulting Eq.(20c).

Also, noting that the $exp(z_S/L)$ terms cancel when A from Eq.(20e) is inserted into Eq.(19c), one finds that the far-field effect of a realistic density profile on concentrations is effectively to multiply them by an overall factor, F, of:

$$F \approx \exp\left(\frac{-z}{L}\right) \cdot \left[1 + \frac{h}{2 \cdot L}\right] \tag{20f}$$

which is exactly the magnitude of effect envisioned at the outset. That is, for well-mixed conditions, a convective mixing height of $h \approx 2.4$ km, and an atmospheric scale height, L, of 8 km, ground-level mass concentrations should be increased by 15%, with smaller effects seen for shallower mixing heights. As decades of regulatory modeling rests upon the presumed validity of the simpler Eq.(1) (i.e., with $F \equiv 1$ presumed), the sub-sections which follow will not further consider inclusion of this atmospheric density refinement.

3 Extending the Plume Formulation Beyond Point Sources

Returning to Eq.(1) as the basic Gaussian plume equation arising from a point source, one naturally is led to ask how this result can be extended to sources having various and more complex distributions in space, such as lines and areas (e.g., see Turner, 1970), or in space and time, such as moving point sources.

3.1 Line Source Models

The straight-line source is a natural choice if one wishes to estimate impacts from roadway segments. In Volume 1, Chapter 7A by Venkatram and Thé (2003), the equation for line source impacts under perpendicular wind flow conditions (i.e., where the wind direction defines the $+x$ direction and the straight roadway defines the y axis), is presented for the infinite length line. This is accomplished by summing the concentration increments, dC, arising from infinitesimal sources of length dy and source strength $q \cdot dy$, where q is the line's emission density having units of mass/length/time. The total line's direct impact is then computed as the integral over these infinitesimal point elements as:

$$C(x, y, z) = \int dC = \frac{q}{U} \cdot P(z - z_S, \sigma_z) \cdot \int_{y_1}^{y_2} dy \cdot P(y, \sigma_y) \tag{21a}$$

where the integration limits, y_1 and y_2, represent the endpoints of the line, and $P(z - z_S, \sigma_z)$ and $P(y, \sigma_y)$ are as in Eqs.(8b), except that σ_y and σ_z are typically taken as functions of x rather than travel time t, and are written:

$$P(y,\sigma_y) = \frac{1}{\sqrt{2\pi}\sigma_y} \cdot \exp\left[-\frac{y^2}{2 \cdot \sigma_y^{\ 2}}\right], \ P(z - z_S, \sigma_z) = \frac{1}{\sqrt{2\pi}\sigma_z} \cdot \exp\left[-\frac{(z - z_S)^2}{2 \cdot \sigma_z^{\ 2}}\right]. \tag{21b}$$

Just as with the normalization integral of Eq.(12), one is able to express the result of the integration in Eq.(21a) as:

$$N(y_1,y_2) \equiv \int_{y1}^{y2} dy \cdot P(y,\sigma_y) = \frac{1}{2}\left[erf(\frac{y_2}{\sqrt{2}\sigma_y})] - erf(\frac{y_1}{\sqrt{2}\sigma_y}) \right] \tag{21c}$$

where *erf* is again the symbolic notation for the "error function", as previously discussed in Section 2.2. Note that for an infinite line, $y_1 \rightarrow -\infty$ and $y_2 \rightarrow +\infty$, so that $N(y_1,y_2) \rightarrow 1$.

Thus, for the typical line source at $z_S = 0$, where the effect of adding in the ground reflection term is simply a factor of 2, the final result for the concentration due to perpendicular flow across an infinite, ground-level line is:

$$C(x) = \frac{2 \cdot q}{\sqrt{2\pi} \cdot \sigma_z \cdot U} \cdot \exp\left[\frac{-z^2}{2 \cdot \sigma_z^2} \right] \quad . \tag{21d}$$

3.1.1 Arbitrary Wind Angle Solutions

The great simplicity associated with the perpendicular wind is that the downwind distance, *x*, does not vary as one integrates along the line. Hence, the values of the dispersion coefficients, σ_y and σ_z, remain constant along the line source and the integrations can be performed as shown in Eq.(21). If instead the wind crosses the roadway at an angle θ away from perpendicular, the problem becomes far more difficult, as the σ_y and σ_z values vary with y position along the line and the integrals cannot be performed analytically for arbitrarily varying functions, $\sigma_y(x')$ and $\sigma_z(x')$, where x' is now the downwind distance as depicted in Figure 2 below. For the receptor located a perpendicular distance $x = x_R$ from the roadway, this receptor is now located a distance x'_R, directly downwind of a point declared to be $l = 0$ along the roadway. Thus, at other points l along the line, the downwind distance, x', and crosswind distance, y', will be given as:

$$\begin{aligned} x' &= x'_R + l \cdot sin(\theta) = x_R / cos(\theta) + l \cdot sin(\theta) \\ y' &= l \cdot cos(\theta) \quad . \end{aligned} \tag{22}$$

These definitions make the dependence of x' and y' explicit as l varies during the integration along the line. As the dispersion coefficients, $\sigma_y(x')$ and $\sigma_z(x')$, are often defined as piecewise, power-law functions, or some other awkward functional form, we know that general attempts to evaluate the concentration as:

$$C(x,y,z) = \int dC = \frac{q}{U} \cdot \int_{\ell_1}^{\ell_2} d\ell \cdot P(z - z_S, \sigma_z) \cdot P(y', \sigma_y) \tag{23a}$$

where l_1 and l_2 are the end points of the integration, are likely to require numerical evaluation. Note that as "downwind" portions of the line's emissions cannot contribute, the lower (or leftmost) limit l_1 must be greater than (or equal to) the point seen shown in the drawing as l_0, where

$$l_0 = -x'_R / sin(\theta) = -x_R / [cos(\theta) \cdot sin(\theta)] \quad . \qquad (23b)$$

As mentioned, solution of Eq.(23a) must generally be performed numerically; however, it can be evaluated analytically if one makes the reasonable assumption that the key contribution to the integral comes primarily from the portion of the line nearly directly upwind of the receptor. In this case, one may linearize the dispersion coefficient dependence on downwind distance and write:

$$\begin{aligned} \sigma_z(x') &= \sigma_z(x_R'+x_0) + i_z \cdot (x' - x_R') \\ \sigma_y(x') &= \sigma_y(x_R') + i_y \cdot (x' - x_R') \end{aligned} \qquad (24a)$$

where the pseudo-distance, x_0, has also been added to allow for initial mixing, $\sigma_{z0} \equiv \sigma_z(x_0)$, at the line source due to various effects (e.g., vehicle induced mixing of exhaust). As $\sigma_y(x')$ dependence generally plays a minor role in line source integrations, disappearing, in fact, for the long crosswind line, we make an additional assumption that:

$$\sigma_y(x') = (i_y / i_z) \cdot \sigma_z(x') \qquad (24b)$$

for all x'. This has the relatively minor impact of forcing the equality condition,

$$\sigma_y(x_R') = (i_y / i_z) \cdot \sigma_z(x_R'+x_0) \qquad (24c)$$

on the value of $\sigma_y(x_R')$ at the upwind point of maximum impact. This then allows the Eq.(24a) expressions for the dispersion coefficients to be rewritten simply as:

$$\begin{aligned} \sigma_z(x') &= i_z \cdot [a' + l \cdot sin(\theta)] \\ \sigma_y(x') &= i_y \cdot [a' + l \cdot sin(\theta)] \end{aligned} \qquad (24d)$$

where $a' \equiv \sigma_z(x_R'+x_0) / i_z$.

This then permits the integral expression of Eq.(23a) to be expressed as:

$$C(x, y, z) = \frac{q}{2 \cdot \pi \cdot U \cdot i_y \cdot i_z} \cdot I_0 \qquad (24e)$$

where

$$I_0 \equiv \int_{\ell_1}^{\ell_2} d\ell \cdot \exp\left\{-\frac{1}{2}\cdot\frac{[(b^2+(\ell\cdot\cos\theta)^2]}{i_y^2\cdot(a'+\ell\cdot\sin\theta)^2}\right\}/(a'+\ell\cdot\sin\theta)^2$$

has dimensions of (m^{-1}) and

$$b \equiv (i_y / i_z)\cdot(z - z_S) \tag{24f}$$

represents the appropriately scaled z-coordinate for the direct plume term. In most cases, the source and receptor will be located near enough to ground level that b can be set to zero and the overall expression for C in Eq.(24e) can be multiplied by two to account for the ground reflection, but for now we will carry the b term and consider only the direct plume impact.

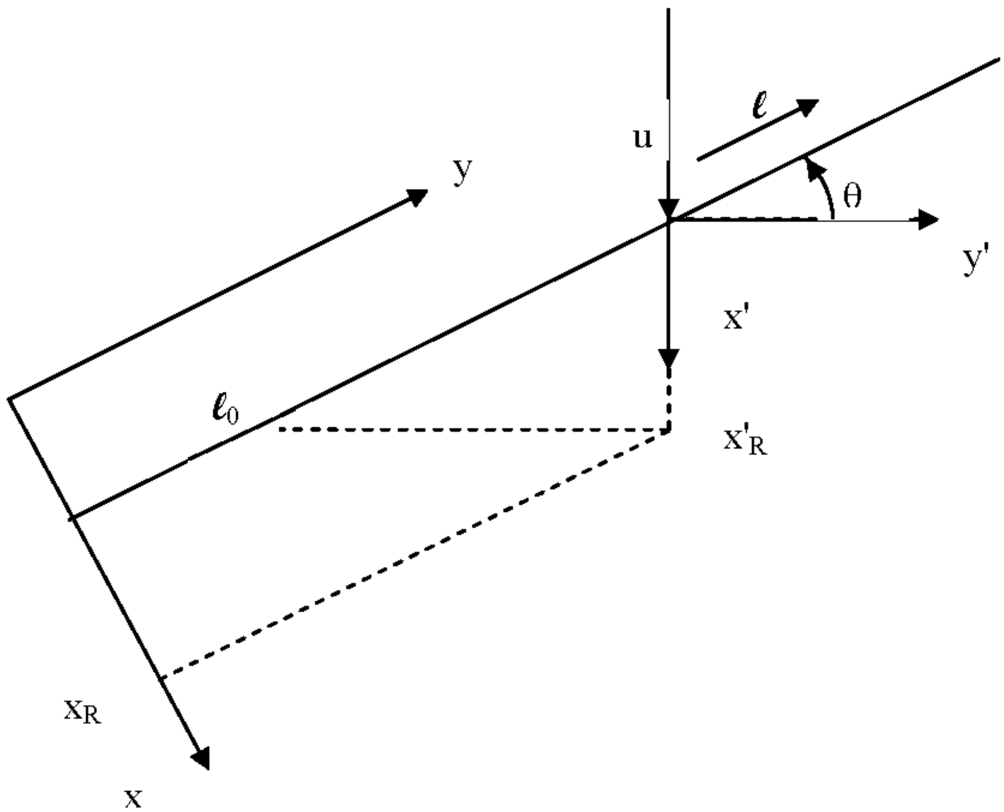

Figure 2. Roadway Coordinate System (x, y) rotated by the Angle θ relative to the Downwind-Crosswind System (x', y'). The receptor is located a perpendicular distance x_R from the roadway and a distance x'_R directly downwind of the line.

The variable substitution, $p \equiv [a' + l \cdot sin(\theta)]^{-1}$, such that $l = (p^{-1} - a') / sin(\theta)$, transforms I_0 in Eq.(24e) to:

$$I_0 \equiv \frac{-1}{\sin\theta} \cdot \int_{p_1}^{p_2} dp \cdot \exp\left\{-\frac{[1 - 2\cdot a'\cdot p + b'^2 \cdot p^2]}{2\cdot i_y^2 \cdot \tan^2\theta}\right\} \tag{24g}$$

with

$$b'^2 \equiv b^2 \cdot tan^2(\theta) + a'^2 \tag{24h}$$

and integration limits, p_1 and p_2, corresponding to limits l_1 and l_2, respectively.

The subsequent change of variables from p to s via $s \equiv b'\cdot p - a'/b'$ transforms the numerator within the exponential from the expression within the brackets […] to $[s^2 - (a'/b')^2 + 1]$; thus, "completing the square" and yielding the I_0 solution:

$$I_0 = \frac{i_y \cdot \exp\left\{-\dfrac{b^2}{2\cdot i_y^2 \cdot b'^2}\right\}}{b'\cdot\cos\theta} \cdot \frac{\sqrt{2\cdot\pi}}{2} \cdot \left\{erf\left[\frac{s_1}{\sqrt{2}\cdot i_y \cdot \tan\theta}\right] - erf\left[\frac{s_2}{\sqrt{2}\cdot i_y \cdot \tan\theta}\right]\right\} \tag{24i}$$

and hence, the solution for the time-averaged concentration at (x,y,z) is:

$$C(x,y,z) = \frac{q\cdot\exp\left\{-\dfrac{b^2}{2\cdot i_y^2\cdot b'^2}\right\}}{\sqrt{2\cdot\pi}\cdot U\cdot b'\cdot i_z \cdot \cos\theta} \bullet \frac{1}{2}\cdot\left\{erf\left[\frac{s_1}{\sqrt{2}\cdot i_y\cdot\tan\theta}\right] - erf\left[\frac{s_2}{\sqrt{2}\cdot i_y\cdot\tan\theta}\right]\right\} \tag{25a}$$

where

$$s_1 = b'\cdot[a' + l_1\cdot sin(\theta)]^{-1} - a'/b' \quad \text{and} \quad s_2 = b'\cdot[a' + l_2\cdot sin(\theta)]^{-1} - a'/b' \tag{25b}$$

The final result given by Eq.(25) [i.e., with symbols a', b, and b' defined in Eqs.(24d, f, and h)] is not very intuitively appealing, but it becomes more recognizable when one considers the limit of small θ. In this case, $b' \rightarrow a' = \sigma_z(x_R'+x_0) / i_z$, $s_1 / [i_y \cdot tan(\theta)] \rightarrow - l_1\cdot cos(\theta) / \sigma_y(x_R')$, and $s_2 / [i_y \cdot tan(\theta)] \rightarrow - l_2\cdot cos(\theta) / \sigma_y(x_R')$, yielding the more familiar solution:

$$C(x,y,z) = \frac{q\cdot\exp\left\{-\dfrac{(z-z_S)^2}{2\cdot\sigma_z^2(x_R'+x_0)}\right\}}{\sqrt{2\cdot\pi}\cdot U\cdot\sigma_z(x_R'+x_0)\cdot\cos\theta}\cdot\frac{1}{2}\cdot\left\{erf\left[\frac{-\ell_1\cdot\cos\theta}{\sqrt{2}\cdot\sigma_y(x_R')}\right] - erf\left[\frac{-\ell_2\cdot\cos\theta}{\sqrt{2}\cdot\sigma_y(x_R')}\right]\right\} \tag{26}$$

where $\sigma_y(x_R')$ is dictated by Eq.(24c). For a very long line, $l_1 \rightarrow -\infty$, $l_2 \rightarrow +\infty$, and the odd property of the *erf* yields the condition that the expression ½ ·{…} → +1. Furthermore, recalling that Eq.(21d) is for a ground level line (i.e., z_S = 0) and includes the ground reflection term as a multiplicative factor of two, leads one to the conclusion that Eqs.(21d) and (26) are identical except for the fact that the line source strength, q, in Eq.(21d) is replaced with $q/cos(\theta)$ in Eq.(26). This means that as the wind shifts from the perpendicular wind flow situation (i.e., $\theta = 0$), one dominant effect is that the foreshortened line is effectively "seen" by the receptor as being unrotated, but having an increased line-source emission density, $q/cos(\theta)$. However, this effect is countered by the facts that: (i) the "error function" terms roll off at large angles, and (ii) the centerline, upwind distance, $x'_R = x_R / cos(\theta)$, is also increasing. For typical, urban dispersion (i.e., neutral stability), the near-field vertical growth of a plume is quite linear with downwind distance, and for the case of no initial mixing (i.e., x_0 =0) in the vertical, one has simply: $\sigma_z(x_R'+x_0) = i_z \cdot x'_R = i_z \cdot x_R / cos(\theta)$. Thus, the two factors of $cos(\theta)$ cancel exactly and one is left with little wind angle dependence in the concentrations estimated by Eq.(26). Of course, Eq.(26) was developed assuming small θ; however, a numerical study of Eq.(25) under comparable conditions, shown in Figure 3 below, displays modest angular dependence in $C(\theta)/C(0)$ for angles less than about 40 to 50 degrees, with almost none of this arising from the *erf* terms. This rather weak angular dependence was first described by Calder (1973) as part of his numerical integration studies of line source impacts.

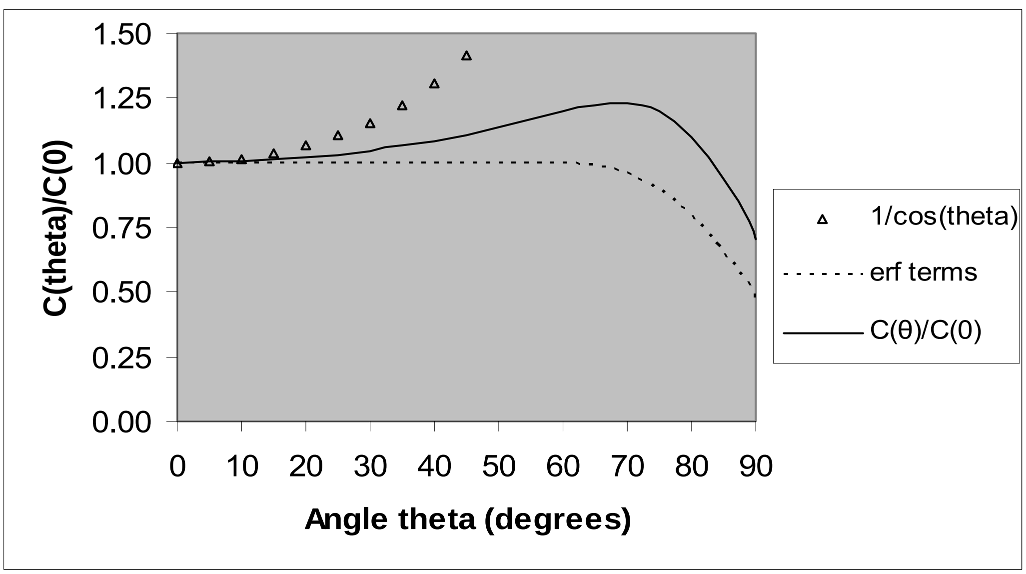

Figure 3. Angular dependence of Eq.(25). The dotted line shows only the sum of error function terms, whereas the solid line depicts the full ratio C(θ)/C(0). Parameter values assumed include: $\sigma_Z(x_0) = 1m$; $x_R = 10m$; and $i_Z = i_Y = 0.2$.

Another way to view Figure 2 is to imagine that the x'_R is held fixed and the line source itself is rotated by θ. For line sources that are short relative to the value of the appropriate Y-diffusion coefficient, that is, $L \equiv l_2 - l_1 << \sigma_y(x_R')$, the *erf*( ) terms in Eq.(26) can be expanded using the small argument approximation, $erf(x) \approx 2 \cdot x / \pi^{1/2}$.

Inserting $l_2 = L/2 = - l_1$ into Eq.(26) and expanding yields the result:

$$C(x,y,z) = \frac{q \cdot \exp\left\{ -\frac{(z-z_S)^2}{2\cdot\sigma_z^2(x_R'+x_0)} \right\}}{\sqrt{2 \cdot \pi} \cdot U \cdot \sigma_z(x_R'+x_0)\cdot \cos\theta} \bullet \frac{1}{2}\cdot\frac{2}{\sqrt{\pi}}\left\{ \left[\frac{-(-L/2)\cdot\cos\theta}{\sqrt{2}\cdot\sigma_y(x_R')} \right] - \left[\frac{-(L/2)\cdot\cos\theta}{\sqrt{2}\cdot\sigma_y(x_R')} \right] \right\} = \frac{q\cdot L\cdot \exp\left\{ -\frac{(z-z_S)^2}{2\cdot\sigma_z^2(x_R'+x_0)} \right\}}{2\cdot\pi\cdot U\cdot\sigma_z(x_R'+x_0)\cdot\sigma_y(x_R')} \tag{27}$$

which is recognized as the Y-centerline value of a point source concentration (i.e., ignoring reflections). This is a reasonable result, because if a line source is small enough, it should be equivalent to a point source of strength $q{\cdot}L$ and the line's orientation angle, θ, should vanish from consideration.

3.1.2 Extension to Lines of Finite Width

Most line sources of interest, such as highways, have a finite width, W, that may be significant relative to the distance, x_R, of the receptor from the centerline of the roadway or lane. For the case of perpendicular wind flow, finite roadway width may be accomodated in Eq.(25) or Eq.(26) through the use of a multiplicative integral-averaging correction factor, F_W, defined such that:

$$F_W \equiv \frac{\sigma_z(x_R'')}{W}\cdot\int_{X1}^{X2}\frac{dx}{\sigma_z(x)} \tag{28}$$

where $x_1 = x''_R - W/2$, $x_2 = x''_R + W/2$, $x_2 - x_1 = W$, and the distance, x''_R, includes all pseudo-distance effects as well (i.e., $x''_R = x'_R + x_0$). Equation (28) has the simple solution:

$$F_W \equiv \frac{\sigma_z(x_R'')}{i_z\cdot W}\cdot \ln\left[\frac{\sigma_z(x_R''+W/2)}{\sigma_z(x_R''-W/2)}\right]. \tag{29a}$$

Now at first glance, Eq. (29a) seems to blow-up as $W \rightarrow 0$, but if one multiplies both numerator and denominator inside the log with $1/\sigma_z(x_R'')$ and linearizes the expansion of $\sigma_z(x_R'' \pm W/2\ ) / \sigma_z(x_R'') \approx 1 \pm \varepsilon$, where $\varepsilon \equiv ½ \cdot i_z \cdot W / \sigma_z(x_R'')$, then Eq.(29a) becomes:

$$F_W \approx \frac{1}{2 \cdot \varepsilon} \cdot \ln\left[\frac{1+\varepsilon}{1-\varepsilon}\right]. \tag{29b}$$

Equation (29b) only serves to bring the apparent problem into a clearer focus, which in turn demands expansion of the natural log as: $ln(1 \pm \varepsilon) \approx 1 \pm \varepsilon - \varepsilon^2/2 \pm \varepsilon^3/3$. Provided all terms up to ε^3 are retained, one arrives at the final result of:

$$F_W \approx 1 + \frac{\varepsilon^2}{3} = 1 + \frac{1}{12} \cdot \left[\frac{i_z \cdot W}{\sigma_z(x_R'')}\right]^2 \tag{29c}$$

where this result is strictly valid only for $|\varepsilon| < 1$ or $|\ i_z \cdot W / \sigma_z(x_R'')\ | < 2$. Equation (29c) is primarily useful for showing that F_W does not have problems as the roadway width, W, shrinks to zero, but it should not be used for values of ε beyond about ½. Instead, the more robust equation [i.e., Eq.(29a) or Eq.(29b)] should be used. Taking a rather wide roadway width of W = 20 m, and a vertical turbulent intensity of i_z = 0.5 over the turbulent roadway environment, a roadside receptor might experience a near-field plume as shallow as say $\sigma_z(x_R''-W/2) \approx$ 1m, However, given the assumed level of turbulence suggests that $\sigma_z(x_R''+W/2) \approx$ 11m and $\sigma_z(x_R'') \approx$ 6m, thus, yielding a value of $\varepsilon \equiv 0.833$. Using these values, both Eqs.(29a) and (29b) yield F_W = 1.44, whereas Eq.(29c) yields the smaller value of F_W = 1.23 as the expansion of $ln(1 \pm \varepsilon)$ converges rather slowly for these larger values of ε.

Additionally, one notes that the Eq.(29a) [or Eq.(29b)] correction factor for Eq.(25) or Eq.(26) might also be approximately extended to arbitrary angles, by replacing W with $W/cos(\theta)$.

Finally, one may think that, with the ever-increasing speed of computers, one might just leave all these line source issues to numerical integration. In fact, the AERMOD regulatory model does just this and does not presently include explicit formulae for line sources. One consequence of this is that individuals running long-term simulations (e.g., one-year) for airports and/or highway systems containing many line elements continue to complain of long run times.

3.1.3 The Moving Point Source Solution

The source strength, q, considered in the subsections above, including Eqs.(21) through (27), represented a steady-state source having a linear emission density of q (mass/length/time). Typically, q might be given in units of g/m/s. Suppose instead, that the source consists of small point sources traveling along the line, such as depicted in Figure 2, at speed V_0. If there are N (#/s) sources passing a fixed point each second, then the separation between sources is just $\Delta l = V_0 / N$. In addition, if each of these sources emits pollutant at a rate, E (g/s), then the emission density is just:

$$q = E / \Delta l \; = N \cdot E / V_0 \tag{30a}$$

and all the equations developed above [i.e., Eqs.(21) through (27)] are still valid.

Suppose instead that there is just one source traveling along this same line over the interval of the concentration averaging period, τ, with starting and ending times chosen such that the source's concentration impact at a given receptor is fully realized between these start/end times. In this case, one could compute an N of $N = 1 / \tau$, so that the emission density, q, to be used in the case of a single point source traverse, would be:

$$q = E / (V_0 \cdot \tau) \,. \tag{30b}$$

While it seems odd to have the concentration averaging time appear in expressions for the average concentration, such will be the case when only a single source passes by during the duration of the concentration-averaging period.

The above discussion may appear obvious to many, but now consider the case where the single source of strength E moves along the line l as some function of time. For example, for a constant velocity source, $l(t)$ is given as:

$$l(t) = l_0 + \; V_0 \cdot t \tag{31a}$$

so that then

$$dl = \; V_0 \cdot dt. \tag{31b}$$

The integration yielding the average concentration, as given by Eq.(24e), could just as well have been written as:

$$C(x, y, z) = \frac{E}{2 \cdot \pi \cdot U \cdot i_y \cdot i_z} \cdot \frac{I_C}{\tau} \tag{32a}$$

where

$$I_C \equiv \int_{t_1}^{t_2} dt \cdot \exp\left\{ -\frac{1}{2} \cdot \frac{[(b^2 + (\ell(t) \cdot \cos\theta)^2]}{i_y^2 \cdot (a' + \ell(t) \cdot \sin\theta)^2} \right\} / (a' + \ell(t) \cdot \sin\theta)^2 \tag{32b}$$

has units of (s/m^{-2}), and the time-integration, end-point limits, t_1 and t_2, are given simply as: $t_1 = [l_1 - l_0] / V_0$ and $t_2 = [l_2 - l_0] / V_0$.

Performing the integration in time t now requires replacing all the appearances of $l(t)$ in Eq.(32b) with the explicit function of t given in Eq.(31). By now everyone is demanding that this madness be stopped and the change be made back to the more convenient integration variable dl. Substituting dt with dl / V_0 and resetting the integration limits to l_1 and l_2 , one notes that the integral, I_C , for a constant speed source returns to the solution form I_0 of Eq.(24e), except for the appearance of a factor of $(1/V_0)$ inside of I_C. Of course, this constant factor can be taken outside the integral, so $I_C = I_0 / V_0$, thus permitting the average concentration to again be expressed as:

$$C(x, y, z) = \frac{E /(\tau \cdot V_0)}{2 \cdot \pi \cdot U \cdot i_y \cdot i_z} \cdot I_0 \tag{33}$$

where a final form for I_0 is given by Eq.(24i). Again, this solution is identical to simply substituting the q in Eqs.(25) through (27) with $E/(V_0 \cdot \tau)$, as discussed previously. The motivation for these seemingly trivial changes of variables will become clear in the next subsection.

3.1.4 The Accelerating Point Source Solution

Let us now consider a source of strength E (g/s) that is accelerating at some constant acceleration rate, $A(\mathrm{m}^2/\mathrm{s})$, along the line depicted in Figure 2, with $A > 0$ corresponding to positive acceleration toward the right of the figure.

Lest one thinks that this is merely a problem of academic interest, I note that a present-day automobile's emission rate is very high during "hard" accelerations (i.e., as the catalytic reactor is intentionally bypassed), and jet aircraft emit most of their ground-level NO_x during their high-thrust, rapid-acceleration takeoff mode.

For these accelerating source cases, we redefine the relationship between $l(t)$ and time to be:

$$l(t) = V_0 \cdot t + ½ \cdot A \cdot t^2 \tag{34a}$$

where V_0, rather than uniform along the line as before, is now defined as the velocity at point $l = t = 0$ corresponding to the line element directly upwind. Now, when one changes from integration variable dt to dl, it must be noted that:

$$dl = (V_0 + A \cdot t) \cdot dt = (V_0^2 + 2 \cdot A \cdot l)^{½} \cdot dt \;\text{ or }\; dt = (dl / V_0) \cdot (1 + 2 \cdot A \cdot l / V_0^2)^{-½} \tag{34b}$$

so the accelerating source integral, I_A , with units $(\mathrm{s/m^{-2}})$ becomes:

$$I_A \equiv \frac{1}{V_0} \cdot \int_{\ell_1}^{\ell_2} d\ell \cdot \exp\left\{ -\frac{1}{2} \cdot \frac{[(b^2 + (\ell \cdot \cos\theta)^2]}{i_y^2 \cdot (a' + \ell \cdot \sin\theta)^2} \right\} \frac{(1 + 2 \cdot A \cdot \ell / V_0^2)^{-1/2}}{(a' + \ell \cdot \sin\theta)^2} \tag{35a}$$

where, as before, $a' \equiv \sigma_z(x_R' + x_0) / i_z$.

Following the same transformations from *l* to p to s that accompanied Eqs.(24) and (25), one finds that the relations between *l* and *s* are just:

$$\ell = \frac{b' - a' \cdot (s + a'/b')}{(s + a'/b') \cdot \sin\theta} \quad \text{and} \quad s = \frac{b'}{(a' + \ell \cdot \sin\theta)} - \frac{a'}{b'} \tag{35b}$$

where, as before, $b \equiv (i_y / i_z) \cdot (z - z_S)$ and $b'^2 \equiv b^2 \cdot tan^2(\theta) + a'^2$, and this leads to the substitution:

$$(1 + 2 \cdot A \cdot \ell / V_0^2)^{-1/2} = \frac{1}{\gamma^{1/2}} \cdot \left[\frac{(s + a'/b')}{(s + \delta/\gamma)}\right]^{1/2} \tag{35c}$$

with

$$\gamma = 1 - \left[\frac{2 \cdot A \cdot a'}{V_0^2 \cdot \sin(\theta)}\right] \text{ and } \delta = \frac{a'}{b'} + \left[\frac{2 \cdot A \cdot b'}{V_0^2 \cdot \sin(\theta)}\right] \cdot \left[1 - \left(\frac{a'}{b'}\right)^2\right] \;. \tag{35d}$$

Then, reversing the limits of integration, the final integral expression in *s* is:

$$I_A = \frac{\exp\left\{-\frac{b^2}{2 \cdot i_y^2 \cdot b'^2}\right\}}{V_0 \cdot b' \cdot \sin\theta} \cdot \int_{s_2}^{s_1} ds \cdot \exp\left[\frac{-s^2}{2 \cdot i_y^2 \cdot \tan^2\theta}\right] \cdot \frac{1}{\gamma^{1/2}} \cdot \left[\frac{(s + a'/b')}{(s + \delta/\gamma)}\right]^{1/2} . \tag{35e}$$

While it does not appear that this integral is solvable analytically, the fact that most of the contribution to the integral occurs near $l \approx 0$, or $s_p \approx b'/a' - a'/b'$, suggests detailed consideration of the factor, *F*, defined as:

$$F \equiv \frac{1}{\gamma^{1/2}} \cdot \left[\frac{(s + a'/b')}{(s + \delta/\gamma)}\right]^{1/2} = \left[\frac{1 + (a'/b') \cdot A' \cdot (s - s_p)}{1 + (a'/b') \cdot (1 - A') \cdot (s - s_p)}\right]^{1/2} \tag{36a}$$

where

$$A' \equiv \frac{2 \cdot A \cdot a'}{V_0^2 \cdot \sin(\theta)} \text{ is a dimensionless acceleration factor.} \tag{36b}$$

One may expand *F* around small values of $(s - s_p)$ to obtain:

$$F \approx 1 + \frac{1}{2} \cdot (a'/b') \cdot A' \cdot (s - s_p) \equiv F_C + F_S \cdot s \tag{36c}$$

where

$$F_C = 1 - \frac{1}{2}\cdot(a'/b')\cdot A'\cdot s_p = 1 - \frac{A'}{2}\cdot\left(1-(\frac{a'}{b'})^2\right)$$
$$= 1 - \frac{A\cdot a'}{V_0^2\cdot\cos^2(\theta)}\cdot\frac{b^2\cdot\sin(\theta)}{b^2\cdot\sin(\theta)+a'^2} \tag{36d}$$

and

$$F_S\cdot s = +\frac{1}{2}\cdot(a'/b')\cdot A'\cdot s = \frac{A\cdot a'^2}{b'\cdot V_0^2\cdot\sin(\theta)}\cdot s\,. \tag{36e}$$

Noting that F_C is independent of s and the linear s dependence in $F_S \cdot s$ leads to an integral that can be transformed to the integral of a simple exponential, one may write the solution as:

$$I_A = F_C\cdot I_C + F_S\cdot\frac{\exp\left\{-\frac{b^2}{2\cdot i_y^2\cdot b'^2}\right\}}{V_0\cdot b'\cdot\sin\theta}\cdot i_y^2\cdot\tan^2\theta\cdot\left\{\exp\left[\frac{-s_2{}^2}{2\cdot i_y^2\cdot\tan^2\theta}\right]-\exp\left[\frac{-s_1{}^2}{2\cdot i_y^2\cdot\tan^2\theta}\right]\right\} \tag{36f}$$

with the concentration given as:

$$C(x,y,z) = \frac{E/\tau}{2\cdot\pi\cdot U\cdot i_y\cdot i_z}\cdot I_A\,. \tag{37}$$

Referring back to the Eqs.(36d) and (36e) definitions of F_C and F_S, recalling that $I_C = I_0 / V_0$, and examining Eq.(36f), one notes that if $A = 0$, one immediately recovers the Eq.(33) solution for the constant velocity source. Also, one can see that if the wind flow is perpendicular to the line (i.e., $\theta = 0$), I_A reverts to I_C, which simply means that one is insensitive to acceleration or deceleration under such perpendicular flows, and only the velocity at the upwind point on the line is important. This implies that the lower speed, higher emission density, left-of-centerline (i.e., for $A > 0$) portion of the line's contribution is exactly offset by the higher speed, lower emission density, right-of-centerline contribution to the receptor concentration.

The Eq.(37) solution for the concentration due to an accelerating sources is appropriate for a wide variety of conditions. However, in some instances (e.g., when the upwind point does not lie on the physical line or when $V_0 = 0$), an alternative formulation of I_A must be considered, starting with a simple redefinition of the Eq.(34a) relationship between $l(t)$ and time t.

3.2 Area Source Models

Area sources are a natural extension of the line source problem. The direct concentration (i.e., not counting reflection terms) from a steady-state area source of emission strength, q_A (g/m^2/s), can be written as:

$$C(x,y,z) = \frac{q_A}{U} \cdot \int_{x_1}^{x_2} dx \cdot P(z - z_S, \sigma_z) \cdot \int_{y_1}^{y_2} dy \cdot P(y, \sigma_y) \tag{38}$$

where x and y are the along-wind and cross-wind coordinates, respectively, and the integration may be performed over an arbitrarily shaped area for which one is able to define the cross-wind limits, y_1 and y_2, as a function of increasing x.

Now as the y integration is purely a crosswind integration, σ_y remains constant, and Eq.(21c) may be invoked and Eq.(38) reduced to the single integration:

$$C(x,y,z) = \frac{q_A}{U} \cdot \int_{x_1}^{x_2} dx \cdot P(z - z_S, \sigma_z) \cdot \frac{1}{2} \cdot \left[erf\,(\frac{y_2}{\sqrt{2}\sigma_y})] - erf\,(\frac{y_1}{\sqrt{2}\sigma_y}) \right]. \tag{39}$$

However, as both $\sigma_y(x)$ and $\sigma_z(x)$ are functions of x, evaluation of the Eq.(39) integration in x is generally accomplished via an efficient numerical integration method (e.g., Romberg).

If one invokes the "narrow plume hypothesis" of Gifford (1959), or alternatively considers a very wide area source, such that the *erf*( ) terms saturate to 1 and -1, respectively, one is able to consider the simpler integral:

$$C(x,y,z) = \frac{q_A}{\sqrt{2\pi} \cdot U} \cdot \int_{x_1}^{x_2} \frac{dx}{\sigma_z(x)} \cdot \exp\left[-\frac{(z - z_S)^2}{2 \cdot \sigma_z^2(x)} \right]. \tag{40}$$

To solve this integral, one must choose an explicit form for $\sigma_z(x)$. Assuming the typical power-law form:

$$\sigma_z(x) = a \cdot (x + x_0)^b \tag{41a}$$

where x_0 is the pseudo-distance implicitly determined from the initial mixing, σ_{z0}, as $\sigma_z(x_0) = \sigma_{z0}$, one may transform to the variable s defined as:

$$s = \frac{(z - z_S)^2}{2 \cdot \sigma_z^2(x)}. \tag{41b}$$

After some algebra, one finds that:

$$\frac{dx}{\sigma_z(x)} = \frac{-ds}{2\cdot s}\cdot\left[\frac{d\sigma_z(x)}{dx}\right]^{-1} = \frac{-ds}{2\cdot s}\cdot\left(\frac{1}{b\cdot a^{1/b}}\right)\cdot\left[\frac{(z-z_S)^2}{2\cdot s}\right]^{(1-b)/(2\cdot b)}$$

or

$$\frac{dx}{\sigma_z(x)} = -\alpha\cdot ds\cdot s^{-1+\frac{b-1}{2\cdot b}} \tag{41c}$$

where

$$\alpha \equiv \left(\frac{1}{2\cdot b\cdot a^{1/b}}\right)\cdot\left[\frac{(z-z_S)^2}{2}\right]^{(1-b)/(2\cdot b)} \text{ is a dimensionless constant.} \tag{41d}$$

This change of variables permits Eq.(40) to be rewritten as:

$$C(x,y,z) = \frac{q_A\cdot\alpha}{\sqrt{2\pi}\cdot U}\cdot\int_{s_2}^{s_1} ds\cdot s^{-1+\frac{b-1}{2\cdot b}}\cdot\exp(-s) \tag{42a}$$

where $s_1 = \dfrac{(z-z_S)^2}{2\cdot\sigma_z^{\,2}(x_1+x_0)}$ and $s_2 = \dfrac{(z-z_S)^2}{2\cdot\sigma_z^{\,2}(x_2+x_0)}$, and the solution of Eq.(42a) can be written in terms of the incomplete Gamma function (Abramowitz and Stegun, 1972) as:

$$C(x,y,z) = \frac{q_A\cdot\alpha}{\sqrt{2\pi}\cdot U}\cdot\left[\Gamma\left(\frac{b-1}{2\cdot b},s_2\right)-\Gamma\left(\frac{b-1}{2\cdot b},s_1\right)\right]. \tag{42b}$$

While this solution may be useful, its form does not facilitate an easy grasp of the overall behavior of the solution. To achieve this understanding, it is preferable to consider the simplified case of a surface source and receptor (i.e., $z = z_S = 0$) and also add in the effect of the ground reflection. In this case, and assuming the same Eq.(41b) form for $\sigma_z(x)$, Eq.(40) reduces to the simpler expression:

$$C(x,y,z) = \frac{q_A}{\sqrt{2\pi}\cdot U\cdot a}\cdot\int_{x_1}^{x_2} dx\cdot(x+x_0)^{-b} = \frac{q_A\cdot[(x_2+x_0)^{1-b}-(x_1+x_0)^{1-b}]}{\sqrt{2\pi}\cdot U\cdot a\cdot(1-b)} \tag{43a}$$

for $b \neq 1$, and for $b = 1$ yields:

$$C(x,y,z) = \frac{q_A\cdot\log[(x_2+x_0)/(x_1+x_0)]}{\sqrt{2\pi}\cdot U\cdot a}\ . \tag{43b}$$

A disturbing aspect of Eq.(43) is that for $b \leq 1$, an infinite source (i.e., $x_2 \rightarrow \infty$) will cause infinite concentrations; however, infinite extent sources will also be a problem for $b > 1$, as the presence of the reflecting lid will eventually cancel out the seeming benefit of having $b > 1$. Studies performed for various real and idealized cities have shown (Hanna et al., 1982) that urban concentrations can range from about $50 \cdot q_A / U$ for unstable conditions to as much as $1000 \cdot q_A / U$ under stable atmospheric conditions.

3.3 Incorporation of Wind Shear

Of course there are many types of wind shears, $\partial u_i / \partial x_j$, where u_i might represent any of the three wind components and x_j any of the three spatial dimensions; however, in Gaussian plume modeling, the dominant shear that is generally ignored is due to the turning of the wind with height. To first order, one may represent such turning with height by injecting a plume transverse velocity, $v(z)$, of the form $v(z) = (\partial v/\partial z) \cdot (z\text{-}z_S)$, where $\partial v/\partial z$ is taken to be a constant in space. Walcek (2004, 2007) has recently obtained an analytic solution to the steady-state diffusion equation appropriate for this problem. The differential equation for the steady-state plume which Walcek solves is:

$$u \cdot \frac{\partial C}{\partial x} + v \cdot \frac{\partial C}{\partial y} = K_h \cdot \frac{\partial^2 C}{\partial y^2} + K_z \cdot \frac{\partial^2 C}{\partial z^2} \tag{44}$$

and the solution he obtains for a source at $x = y = 0$ can be written as:

$$C(x,y,z) = \frac{Q}{2\pi \cdot u \cdot \sigma_y \cdot \sigma_z \cdot f} \cdot \exp\left[-\frac{1}{2}\left\{\frac{y^2}{f^2 \cdot \sigma_y^2} + \frac{(z-z_S)^2 \cdot (1+s^2/3)}{f^2 \cdot \sigma_z^2} - \frac{(z-z_S) \cdot y \cdot s}{f^2 \cdot \sigma_y \cdot \sigma_z}\right\}\right] \tag{45a}$$

where

$$f^2 \equiv 1 + s^2/12 \;\text{ and }\; s \equiv \frac{\partial v}{\partial z} \cdot \frac{x}{u} \cdot \frac{\sigma_z}{\sigma_y} = \frac{\partial v}{\partial z} \cdot \frac{x}{u} \cdot \sqrt{\frac{K_z}{K_h}} \;\; \underline{\text{or}} \;\; s \equiv \frac{\partial \theta}{\partial z} \cdot x \cdot \frac{\sigma_z}{\sigma_y}. \tag{45b}$$

The latter, alternative definition of s is expressed in terms of a constant rate of turning of the wind direction, $\partial\theta/\partial z$, with height, z.

This generalization to include plume transverse wind shear is a particularly important and timely development, especially as data on wind shears are now rather widely available.

4 Removal Processes in Gaussian Plume Modeling

Processes which can deplete the mass within a pollutant plume include: radioactive decay, chemical reactions, dry deposition and wet removal. The goal of this section will be to present adjustment factors and altered plume formulations to take these various depletion mechanisms into account.

Radioactive decay is accommodated quite simply by multiplying the source strength, Q, by the exponential factor $F = exp(-t/\tau)$, where t, the travel time is given as, $t \equiv x/U$, and τ represents the relevant decay time scale. Such an approach is also appropriate for removal by first-order chemical reactions, such as irreversible destruction by sunlight or other transformation pathways not dependendent on the concentration of another trace gas depleted by the reaction. Higher-order chemical reactions involving the reaction of two trace species with one another to produce one or more different species generally requires numerical grid approaches, which are beyond the scope of this section.

4.1 Wet Removal

The removal of tropospheric pollutants by cloud systems is accomplished primarily through rainout or washout. Rainout generally refers to in-cloud scavenging of gases or aerosols, whereas washout (or sweepout) generally refers to below cloud processes. Within-cloud processes can often involve vertical transport and mixing of the pollutant, especially in convective systems, making a detailed treatment difficult within the realm of Gaussian plume modeling; however, below cloud scavenging, and particularly irreversible scavenging, is a Poisson process that also leads to exponential depletion of the plume mass below the cloud. In this case, the factor k in the exponential factor, $F = exp(-k \cdot t)$, is referred to as the scavenging coefficient. Computation of this scavenging coefficient is beyond the scope of this chapter, but it can entail detailed information on the spectrum of particle sizes and raindrop sizes for particulate plumes or, for gases, consideration of the Henry's law solubility constant and, of course, the rainfall rate. Some attempts are also made to deal with a fractional cloud/rain coverage fraction, f, by replacing the simple exponential, $exp(-k \cdot t)$, with a factor $F = \{1 - f \cdot [1 - exp(-k \cdot t)]\}$, which prevents the plume mass being depleted to zero by halting it at $F = 1 - f$.

4.2 Dry Deposition Removal

Removal of pollutants at the surface through dry deposition is generally modeled via the use of a deposition velocity, first formulated by more than fifty years ago by Chamberlain (1953). This approach states that the deposited pollutant flux, F_d, can be computed as:

$$F_d = v_d \cdot C_0 \tag{46}$$

where v_d is the deposition velocity and C_0 is the pollutant concentration at a reference height, typically not far above the surface. The actual value of the deposition velocity depends on the reference height used, as well as many surface-, species-, and meteorology-dependent variables that will not be discussed further here. However, once v_d is determined, the amount of plume mass, *dM*, removed per unit time in a distance interval *dx* is given as simply:

$$dM \;=\; dx \cdot v_d \cdot \overline{C}(x, z_{ref}) \;=\; dx \cdot v_d \cdot \int_{-\infty}^{+\infty} dy \cdot C(x, y, z_{ref}) \tag{47a}$$

where $\overline{C}(x, z_{ref})$ is the crosswind-integrated concentration at reference height z_{ref}. Substituting the Gaussian plume expression into Eq.(47a) then yields the following differential expression for *dM*:

$$dM = dx \cdot v_d \cdot \frac{Q}{U} \cdot D(z_{ref}, z_S, \sigma_z, h) \tag{47b}$$

where $D(z_{ref}, z_S, \sigma_z, h)$ signifies the desired vertical distribution function, such as:

$$D(z_{ref}, z_S, \sigma_z, h) = P(z_{ref} - z_S, \sigma_z, h) + P(z_{ref} + z_S, \sigma_z, h) \tag{47c}$$

where the couplings, such as $P(z_{ref} \pm z_S, \sigma_z, h)$, are the vertical couplings defined in Eq.(17) at height $z = z_{ref}$ for a plume at source height z_S, reflected by both the ground and inversion lid at height *h*.

The precise manner in which *dM* is removed from the pollutant plume gives rise to two, quite different plume depletion approaches.

4.2.1 Source Depletion

If one makes the simplifying assumption that information about the amount of pollutant mass, *dM*, removed at the surface is instantly communicated throughout the entire depth of the plume, then the removed amount might effectively be thought of as being removed from the source strength itself, that is, $dM = dQ$. This enables one to rewrite Eq.(47b) to yield the simple differential equation for $Q(x)$ as:

$$\frac{dQ}{Q(x)} = dx \cdot \frac{v_d}{U} \cdot D(z_{ref}, z_S, \sigma_z(x), h)\,. \tag{48}$$

This has the simple formal solution:

$$\frac{Q(x)}{Q} = \exp\left[-\frac{v_d}{U} \cdot \int_{x0}^{x+x0} dx' \cdot D(z_{ref}, z_S, \sigma_z(x'), h) \right] \tag{49}$$

where x_0 is the pseudo-distance accounting for initial mixing, and Q is the initial or unmodified source strength $Q(0)$. The integral in Eq.(49) is often evaluated numerically and with the reference height, z_{ref}, set to zero; however, this choice of z_{ref} does not really simplify the problem, as the integral is over the x' dependence contained within the dispersion coefficient, $\sigma_z(x')$. A typical term in the D sum over couplings is expressed as:

$$P(Z,\sigma_z(x')) = \frac{1}{\sqrt{2\pi}\cdot\sigma_z(x')}\cdot\exp\left[-\frac{Z^2}{2\cdot\sigma_z^2(x')}\right] \tag{50a}$$

where

$$\sigma_z(x') = a\cdot(x')^b \tag{50b}$$

and Z represents one of the infinity of terms, $Z_{\pm,j} = z_{ref} \pm z_S + 2\cdot j\cdot h$, with j ranging from $-\infty$ to $+\infty$ [i.e., see Eq.(17a)]. Substituting Eq.(50a) into Eq.(49), and making use of the basic definition of the incomplete Gamma function, $\Gamma(a,x)$, yields:

$$\Gamma(\alpha,x) \equiv \int_x^{\infty} dt\cdot\exp(-t)\cdot t^{\alpha-1} \tag{50c}$$

which ultimately leads to the solution:

$$\frac{Q(x)}{Q} = F(Z_{\pm,j}) = \exp\{-\beta\cdot[\Gamma(p,t_2)-\Gamma(p,t_1)]\} \tag{51a}$$

where $$\beta = \frac{v_d}{2\cdot U\cdot\sqrt{\pi}\cdot b\cdot Z_{\pm,j}}\cdot\left(\frac{Z_{\pm,j}}{\sqrt{2}\cdot a}\right)^{1/b},\quad p = \frac{b-1}{2\cdot b}, \tag{51b}$$

$$t_2 = \frac{{Z_{\pm,j}}^2}{2\cdot\sigma_z^2(x+x_0)}\text{, and } t_1 = \frac{{Z_{\pm,j}}^2}{2\cdot\sigma_z^2(x_0)}.$$

As a has units of $(\text{m})^{1-b}$, one notes that β is dimensionless. Also, the computation of the sum over coupling coefficients becomes equivalent to a product over exponentials (i.e., given that the summation ($\sum$) and integration ($\int$) operators are interchangeable). Thus, a final form for the solution is:

$$\frac{Q(x)}{Q(0)} = \prod_{j=-\infty}^{j=+\infty} F(Z_{-,j})\cdot F(Z_{+,j}) \;\approx\; F(Z_{-,0})\cdot F(Z_{+,0})\cdots \tag{51c}$$

where the product expansion generally converges quite rapidly; however, as with the sum over reflections (Section 2.2), nearly-well-mixed plumes require more terms. Actual computations of the $F(Z)$ terms in Eq.(51c) are aided by the series expansion,

$$\Gamma(p,t_2)-\Gamma(p,t_1)=\sum_{n=0}^{\infty}(-1)^n\cdot\left[\frac{t_1^{n+p}-t_2^{n+p}}{(p+n)\cdot n!}\right] \tag{51d}$$

and recursion relations, such as:

$$\Gamma(p,t)=\frac{1}{p}\left[\Gamma(1+p,t)-t^p\cdot e^{-t}\right]. \tag{51e}$$

Equation (51e) can be particularly useful, as the range $⅓ < b < 1$ leads to $-1 < p < 0$. Note also that for the special case of $p = 0$, which arises for exponent $b = 1$, L'Hospital's rule gives the $n = 0$ term in Eq.(51d) as $ln(t_1) - ln(t_2)$.

For downwind distances beyond the point $x = x_m$, where the plume can be considered well-mixed, the x' integration in Eq.(49) can be broken up into two pieces. The first piece, from x_0 to $x_m + x_0$, would be computed as indicated in Eq.(51a), and the part beyond $x' = x_m$ would contribute the multiplicative factor:

$$F(x-x_m)=\exp\left[-\frac{v_d}{U}\cdot\frac{(x-x_m)}{h}\right]=\exp(-t_m/\tau) \tag{52}$$

where $t_m = (x-x_m)/U$ is the transport time while well-mixed, and $\tau = h/v_d$ is the depletion time scale for a pollutant, well-mixed within a layer of depth h and having a deposition velocity v_d. The Eq.(52) form of source depletion is widely used in simple models of long-range transport.

Equations (51) and (52) served as the primary approach for dealing with dry deposition removal for nearly two decades in some regulatory models, such as the German regulatory model, AUSTAL-86 (Fath and Luehring, 1986). However, a major problem with this source depletion methodology is that it assumes that the loss of material at the surface is instantly communicated throughout the entire plume, and this can create a significant problem, particularly under stable conditions where the material loss at the surface lowers the surface concentration substantially (and hence subsequent deposition), as the vertical mixing rate is not rapid enough to replenish depleted surface concentrations with plume material from aloft. Thus, surface depletion generally:

- depletes the plume mass too quickly;
- overpredicts the deposited mass flux, $F = v_d \cdot C$; and
- overpredicts near-surface concentrations.

A "poor-man's way" of coping with this problem is to decrease the value of v_d by increasing the atmospheric resistance term (i.e., as deposition velocities are generally computed as the reciprocal of a sum of resistances, one of which is the atmospheric resistance term). This approach can eliminate the overdepletion of plume mass and lead to improved flux estimates; however, it cannot correct the profile of concentrations near the surface.

4.2.2 Surface Depletion

The surface depletion model was introduced by Horst (1977) to eliminate the problems associated with source depletion. In his approach, the concentration is defined as the concentration due to the unabsorbed plume minus the sum of concentration "deficits" due to all upwind surface depletions. These deficits, or "anti-matter" plumes, emitted from the surface are assumed to disperse the same as normal plume material; thus, yielding the integral equation:

$$\overline{C}(x,z) = \frac{Q}{U}\cdot D(z,z_S,\sigma_z(x),h) - \frac{v_d}{U}\cdot \int_{x0}^{x+x0} dx'\cdot \overline{C}(x',z_{ref})\cdot D(z,0,\sigma_z(x-x'),h) \quad (53)$$

where $\overline{C}(x,z_{ref})$ is the crosswind-integrated concentration at reference height z_{ref}, where deposition and "re-emission" as concentration deficits is assumed to occur.

As Eq.(53) involves the unknown, crosswind-integrated concentration inside an integral as well as on the left-hand side, it is referred to as a Volterra integral equation of the second kind. Additionally, the fact that the integral involves a convolution (i.e., containing both a function of x' and one of x-x') that defies splitting into a product of x and x' terms complicates converting the problem to a simple differential equation. Equation (53) is generally solved using interative numerical methods that can render the process excessively time-consuming for many dispersion modeling applications; however, Laplace transforms also provide a convenient way (Yamartino, 1981) to solve Eq.(53) because of several convenient properties. For example, with respect to convolution integrals, one finds that:

$$\text{£}\cdot\int_0^x dx'\cdot f(x)\cdot g(x-x') = \text{£ f(x)}\cdot\text{£ g(x)} = \text{F(s)}\cdot\text{G(s)} \quad (54a)$$

and with respect to integrals:

$$\text{£}\cdot\int_0^x dx'\cdot f(x) = \text{F(s)/s}. \quad (54b)$$

£ is the Laplace transform operator defined such that:

$$\text{£ f(x)} \equiv \text{F(s)} \equiv \text{£} \cdot \int_0^\infty dx \cdot \exp(-s \cdot x) \cdot f(x) \tag{54c}$$

and £ $^{-1}$ is the inverse Laplace transform operator defined as:

$$\text{f(x)} \equiv \text{£}^{-1}\text{F(s)} \equiv \frac{1}{(2 \cdot \pi \cdot \text{i})} \cdot \int_{a-i\infty}^{a+i\infty} ds \cdot \exp(s \cdot x) \cdot F(s) \tag{54d}$$

where "*a*" is chosen so the complex integration is performed to the right of all singularities. While evaluating inverse Laplace transforms can take one into the intricacies of contour integration, it is useful to know that Laplace transforms and their inverses exist for many common functions and are tabulated in various math reference works and can now be found on the Web as well.

Taking the Laplace transform of Eq.(53) at $z = z_{ref}$ yields:

$$\text{£}\overline{C}(x, z_{ref}) = \frac{Q}{U} \cdot \text{£}D(z_{ref}, z_S, \sigma_z, h) - r \cdot \text{£}\overline{C}(x, z_{ref}) \cdot \text{£}D(z_{ref}, 0, \sigma_z, h) \tag{55a}$$

where $r \equiv \frac{v_d}{U}$. Rearranging terms algebraically yields:

$$\text{£}\overline{C}(x, z_{ref}) = \frac{Q}{U} \cdot \left\{ 1 - \frac{r \cdot \text{£}D(z_{ref}, 0, \sigma_z, h)}{[1 + r \cdot \text{£}D(z_{ref}, 0, \sigma_z, h)]} \right\} \cdot \text{£}D(z_{ref}, z_S, \sigma_z, h) \tag{55b}$$

and taking the inverse transform yields the integral equation solution:

$$\overline{C}(x, z_{ref}) = \frac{Q}{U} \cdot \left\{ D(z, z_S, \sigma_z, h) - \int_{x0}^{x+x0} dx' \cdot D^*(z_{ref}, 0, \sigma_z(x), h) \cdot D(z, z_S, \sigma_z(x - x'), h) \right\} \tag{55c}$$

where D^* is now defined via the relation:

$$\text{£D}^*(z_{ref}, 0, h, x) = \frac{r \cdot \text{£}D(z_{ref}, 0, \sigma_z, h)}{\{1 + r \cdot \text{£}D(z_{ref}, 0, \sigma_z, h)\}} \tag{55d}$$

or via the integral equation:

$$D^*(z_{ref}, 0, h, x) = r \cdot \left\{ D(z_{ref}, 0, \sigma_z(x), h) - \int_{x0}^{x+x0} dx' \cdot D^*(z_{ref}, 0, \sigma_z(x'), h) \cdot D(z, 0, \sigma_z(x - x'), h) \right\}. \tag{55e}$$

One might question what has been accomplished in trading the integral equation, Eq.(53), evaluated at $z = z_{ref}$ to give the near-surface concentration, for the convolution solution of Eq.(55c) plus the subsidiary integral equation for D^*, Eq.(55e). The advantage is that convolution integrals may be evaluated quickly (i.e., without the iterative means needed for integral equations), and the one remaining integral equation, Eq.(55e), need only be evaluated once each modeling hour for the specific stability class and mixing height, h, as D^* is not a function of source height, z_S.

As another example of this approach, consider what happens when Eq.(53) is integrated over all appropriate z (i.e., from z = 0 to z = h). In this case, Eq.(53) becomes:

$$\frac{Q(x)}{U} \equiv \int_0^h dz \cdot \overline{C}(x,z) = \frac{Q}{U} - \frac{v_d}{U} \cdot \int_{x0}^{x+x0} dx' \cdot \overline{C}(x', z_{ref}) \ . \tag{56}$$

Invoking the Eq.(54b) property that $£\int_0^x dx' \cdot \overline{C}(x', z_{ref}) = \frac{1}{s} \cdot £\overline{C}(x, z_{ref})$, and utilizing Eq.(55b) for $£\overline{C}(x, z_{ref})$, one obtains the solution:

$$\frac{Q(x)}{Q} = 1 - r \cdot \left\{ \int_{x0}^{x+x0} dx' \cdot D^{**}(z_{ref}, 0, \sigma_z(x), h) \cdot D(z_{ref}, z_S, \sigma_z(x-x'), h) \right\} \tag{57a}$$

where D^{**} is now defined via the relation:

$$£D^{**}(z_{ref}, 0, \sigma_z, h) = \frac{(1/s)}{\{1 + r \cdot £D(z_{ref}, 0, \sigma_z, h)\}} \tag{57b}$$

or via the integral equation:

$$D^{**}(z_{ref}, 0, h, x) = 1 - r \cdot \int_{x0}^{x+x0} dx' \cdot D^{**}(z_{ref}, 0, \sigma_z(x'), h) \cdot D(z_{ref}, 0, \sigma_z(x-x'), h) \ . \tag{57c}$$

What is again important here is that: (i) Eq.(57c) need only be solved once for each modeling hour involving a unique stability class and mixing height, and (ii) the convolution in Eq.(57a) for the remaining plume mass is as easy to solve as the source depletion equation, Eq.(49), and yet yields a result free of the objectionable assumption of instantaneous vertical re-mixing of the deposited mass deficit throughout the entire plume.

Despite the elegance of the surface depletion methodology and the extent to which its solution procedure can be simplified via the use of Laplace transforms, it is a methodology that has gone largely unused in regulatory dispersion models.

4.2.3 Surface-Corrected Source Depletion

Possibly recognizing the modeling community resistance to dealing with integral equations, Horst (1983) developed a modified methodology to incorporate a corrected plume profile into the source depletion methodology. This resulted in a hybrid approach which corrected for the major shortcoming of source depletion, but required invoking results from K-theory. This approach was incorporated into the ISC-2 and ISC-3 models, which served as the primary, U.S. EPA Guideline model for short-range applications for many years.

In this hybrid approach, Eq.(49) now becomes:

$$\frac{Q(x)}{Q} = \exp\left[-\frac{v_d}{U} \cdot \int_{x0}^{x+x0} dx' \cdot D(z_{ref}, z_S, \sigma_z(x'), h) \cdot P(x', z_{ref})\right] \tag{58a}$$

where $D(\ldots)$ is the dispersion function unmodified by deposition and $P(x, z_{ref})$ is the correction factor to the profile arising from the deposition. The crosswind-integrated concentration at downwind points becomes:

$$\overline{C}(x,z) = \frac{Q(x)}{U} \cdot D(z, z_S, \sigma_z(x), h) \cdot P(x,z) \tag{58b}$$

where mass conservation requires that the non-dimensional $P(x, z)$ be normalized such that:

$$\int_0^h dz \cdot D(z, z_S, \sigma_z(x), h) \cdot P(x,z) \equiv 1 \approx \int_0^h dz \cdot D(z, 0, \sigma_z(x), h) \cdot P(x,z)\,. \tag{58c}$$

Horst argues that this approximation of a ground level source height is reasonable for downwind distances where dry deposition is significant as $\sigma_z > z_S$ at these distances, and thus, the actual source height assumed becomes unimportant. This normalization integral is important, as it is ultimately utilized to determine $P(x,z_{ref})$.

Further assuming that concentration variations close to the surface, in the constant flux layer, are due solely to this profile correction factor P, and not to variations in $D(\ldots)$, 1D K-theory tells us that:

$$P(x,z) = P(x, z_{ref}) \cdot [1 + v_d \cdot R(z, z_{ref})] \tag{58d}$$

where the atmospheric resistance between z_{ref} and z are given from K-theory as:

$$R(z, z_{ref}) \equiv \int_{z_{ref}}^{z} \frac{dz'}{K(z')} = \frac{1}{U} \int_{z_{ref}}^{z} \frac{dz'}{\sigma_z(x) \cdot [d\sigma_z(x)/dx]} \quad . \tag{58e}$$

Note that the Eq.(58e) expression in terms of plume sigmas relies on the point-source, K-theory relation, $\sigma_z^2(x) = 2 \cdot K \cdot (x/U)$, for the second moment, and is attributable is to Briggs' formulas for σ_z (Gifford, 1976). Nevertheless, this form for the resistance is peculiar in that $\sigma_z(x)$ is usually not an explicit function of z; however, it can be seen to be an implicit function of z through the first moment relation, $z' = \bar{z} = \sqrt{2/\pi} \cdot \sigma_z$. Thus, before the integral on the right side of Eq.(58e) is evaluated, one must first replace all terms in x with its equivalent in terms of σ_z, and then replace σ_z with the first-moment relation in z'. As a check, one should note that the simple, stable dispersion expression, $\sigma_z = \sqrt{2K/U} \cdot \sqrt{x}$, results in the resistance, $R(z, z_{ref}) = (z - z_{ref}) / K$. The ISC3 User's Guide (EPA, 1995) presents results for these resistance integrals, $R(z, z_d)$, and the resulting profile functions, $P(x, z_{ref})$, for the unstable through stable dispersion functions used within ISC3. A typical result for the depletion factor, $P(x, z_{ref})$, and the profile correction factor, $[1 + v_d \cdot R(z, z_{ref})]$, is given in Figure 4.

It should also be noted that Eq.(58d) represents a simplification applicable to the case of negligible gravitational settling velocity, v_g. The more general expression is:

$$P(x,z) = P(x, z_{ref}) \cdot \left\{ 1 + \frac{v_d - v_g}{v_g} \cdot \left[1 - \exp[-v_g \cdot R(z, z_{ref})] \right] \right\}. \tag{58f}$$

However, inserting this expression into the normalization integral [i.e., the right hand side of Eq.(58c)] essentially guarantees that a numerical integration must be performed, whereas the normalization integration associated with the simpler Eq.(58d) can often be performed analytically.

Horst has shown that use of the methodology prescribed by Eqs.(58a) through (58e) leads to suspended mass, $Q(x)/Q$, and surface concentration estimates that are generally within a few percent of the reference surface depletion values, and thus, far more accurate than source depletion approximated values, particularly for the stable dispersion cases.

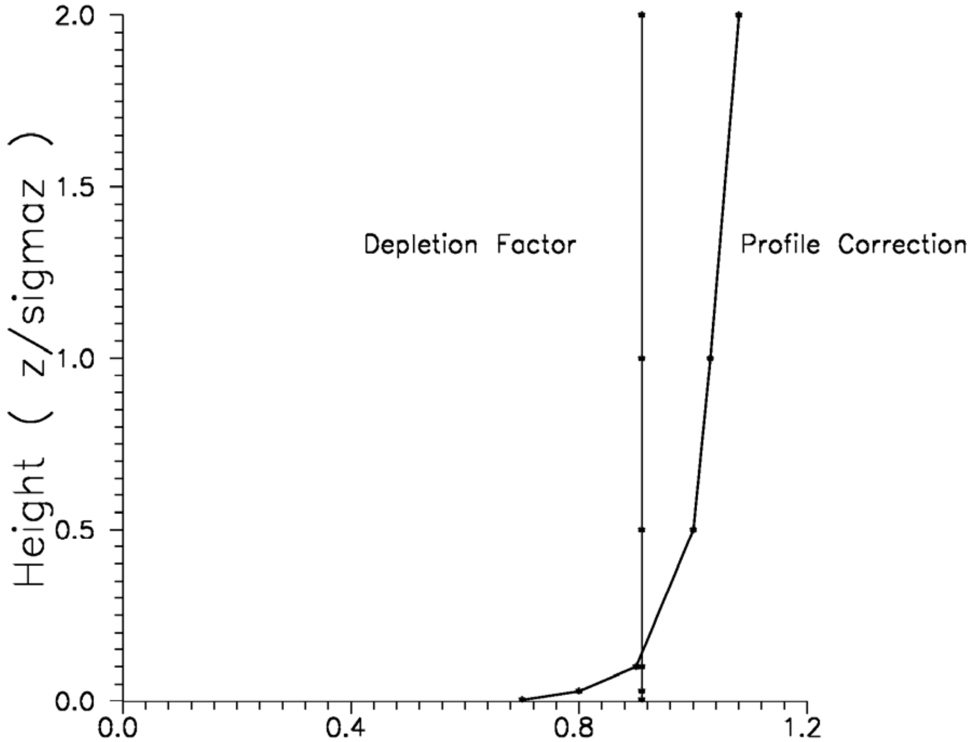

Figure 4. A typical for the Depletion factor, $P(x, z_{ref})$, and the associated Profile Correction factor, $[1 + v_d \cdot R(z, z_{ref})]$. Source: Fig. 1-7, U.S. EPA (1995).

4.2.4 Gravitational Settling and the Tilted Plume

Particles that are bigger than several microns are known to undergo dry deposition enhanced by their gravitational settling velocity, v_g. The terminal velocity of a particle of given physical (or Stokes) diameter, d_p, and density, ρ, is determined from the balance of gravitational and viscous drag forces to be:

$$v_g = \frac{g \cdot (\rho - \rho_A) \cdot d_p^2 \cdot C_S}{18 \cdot \mu} \tag{59}$$

where g is the gravitational acceleration, ρ_A is the ambient (air) density, C_S is the Cunningham slip factor (which is approximately 1.0 for particles larger than one micron), and μ is the viscosity of air. While this gravitational velocity is only about 0.03 cm/s for a unit density particle (i.e., ρ = 1 g/cc) of diameter 3µ, it increases with the square of particle diameter, such that a 10µ particle would settle at about 0.3 cm/s, and a more typical density 10µ particle might settle at about 1.0 cm/s. These velocities seem quite small relative to turbulent velocity scales, yet their persistent effect makes them hard to ignore when modeling the transport of particulate plumes over travel times of an hour or more.

Perhaps the simplest "fix" to plume modeling that one might imagine is correcting the effective source height z_S for such gravitational sinking via the "tilted" plume. That is, computing a corrected source height z_S' defined as:

$$z_S' = z_S - v_g \cdot t \tag{60}$$

where t is the downwind travel time, $t = x/U$. This simple idea works well until the effective source height reaches the ground and then effectively has the primary plume digging into the ground, and worse, has the ground reflection term simulating a plume climbing up from the ground at upward velocity, v_g . The simplest solution to this problem is to simply freeze the plume centerline at ground level once it reaches the ground, which is the solution that has been incorporated into many dispersion models. However, this approach erroneously suggests that gravity stops acting on these particles once the plume centerline reaches ground level. In the ISC-3 model, this subsequent settling has been incorporated as a correction to the plume's vertical dispersion coefficient. For example, if the plume's uncorrected plume spread is given as $\sigma_z(x)$ and $z_S' = 0$, then the mean plume centerline height $<z>$ of this plume is just $(2/\pi)^{1/2} \cdot \sigma_z(x)$, so one can compute the gravitationally corrected dispersion rate as:

$$\sigma_z'(x) = \sigma_z(x) - (\pi/2)^{1/2} \cdot v_g \cdot (t - t_T) \tag{61}$$

subject to the additional constraint that $\sigma_z'(x)$ remains positive.

4.2.5 Deposition in K-Theory

K-theory continues to be used in numerical grid models. Exploiting the linkage between K-theory solutions and plume models dates back to the early days of modeling by Csanady (1955) and Smith (1962). While the substitution

$$\sigma_z^2(x) = 2 \cdot K \cdot (x/U) \tag{62a}$$

is strictly valid only for stable conditions, Rao (1981) has exploited the K-theory solution for depositing particles and developed a solution for the crosswind-integrated concentration as:

$$C(x,z) = \frac{Q}{\sqrt{2\pi} \cdot U \cdot \sigma_z} \cdot \exp\left[-\frac{v_g \cdot (z - z_S) \cdot x}{U \cdot \sigma_z^2} - \frac{v_g^2 \cdot x^2}{2 \cdot U^2 \cdot \sigma_z^2} \right] \bullet \left\{ \exp\left[-\frac{(z - z_S)^2}{2 \cdot \sigma_z^2} \right] + \exp\left[-\frac{(z + z_S)^2}{2 \cdot \sigma_z^2} \right] \cdot \left[1 - 2 \cdot \sqrt{2\pi} \cdot \frac{V \cdot x}{U \cdot \sigma_z} \cdot \exp(\xi^2) \cdot erfc(\xi) \right] \right\} \tag{62b}$$

where

$$V = v_d - v_g/2 \tag{62c}$$

and

$$\xi = \frac{(z + z_S)}{\sqrt{2} \cdot \sigma_z} + \sqrt{2} \cdot \frac{V \cdot x}{U \cdot \sigma_z} \quad . \tag{62d}$$

For non-settling particles (i.e., $v_g = 0$ and $V = v_d$), Eq.(62) depletes only the image source, as one might intuitively expect from the notion that deposition is equivalent to imperfect reflection of matter from the surface, as was suggested quite early by Csanady (1955) and later by Overcamp (1976). While Eq.(62b) does not conserve mass for the general case where σ_z does not obey Eq.(62a), Rao forces the proper analytic normalization by integrating Eq.(62b) over z. Horst (1984) shows that Rao's solution is always intermediate in accuracy between the source depletion and surface depletion solutions. That is, it is superior to source depletion, but not as accurate as Horst's surface-corrected source depletion and the reference surface depletion solution.

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