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The Mathematics of Atmospheric Dispersion Modeling*

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Abstract. The Gaussian plume model is a standard approach for studying the transport of airborne contaminants due to turbulent diffusion and advection by the wind. This paper reviews the assumptions underlying the model, its derivation from the advection-diffusion equation, and the key properties of the plume solution. The results are then applied to solving an inverse problem in which emission source rates are determined from a given set of ground-level contaminant measurements. This source identification problem can be formulated as an overdetermined linear system of equations that is most easily solved using the method of least squares. Various generalizations of this problem are discussed, and we illustrate our results with an application to the study of zinc emissions from a smelting operation.

Key words. advection-diffusion equation, atmospheric dispersion, contaminant transport, Gaussian plume solution, inverse problem, linear least squares

AMS subject classifications. 76R, 65M06, 65F20, 86A10

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1. Introduction.

Atmospheric dispersion modeling refers to the mathematical description of contaminant transport in the atmosphere. The term *dispersion* in this context is used to describe the combination of diffusion (due to turbulent eddy motion) and advection (due to the wind) that occurs within the air near the Earth's surface. The concentration of a contaminant released into the air may therefore be described by the advection-diffusion equation, which is a second-order partial differential equation (PDE) of parabolic type.

This problem is an excellent example of interdisciplinary mathematics that has direct application to problems with industrial relevance. In addition to forming the basis for an extensive and active body of current research in atmospheric dispersion modeling, this material is also ideal for inclusion in an upper-year undergraduate or graduate course in mathematical modeling or scientific computing. The results discussed here may be used to illustrate basic techniques from PDEs (Green's functions, Laplace transforms, asymptotics, special functions), constrained optimization (linear least squares), numerical analysis, and inverse problems. The suggested prerequisites are an introductory course in PDEs that covers basic solution techniques such as separation of variables and Laplace transforms, as well as some prior computing experience. With reference to the material in section 4 and a few of the more advanced exercises, the reader would benefit from some experience with linear algebra and more

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advanced knowledge of PDEs. We employ the software package MATLAB for the numerical simulations in this paper, and have posted the relevant codes on the website http://www.math.sfu.ca/∼stockie/atmos. On this site we also provide supplemental notes that give detailed derivations of numerous results appearing in the main text, solutions to selected exercises, and MATLAB code.

Since the pioneering work of Roberts [32] and Sutton [39], analytical and approximate solutions for the atmospheric dispersion problem have been derived under a wide range of simplifying assumptions, as well as various boundary conditions and parameter dependencies. These analytical solutions are especially useful to engineers and environmental scientists who study pollutant transport, since they allow parameter sensitivity and source estimation studies to be performed. The simplest of these exact solutions is called the *Gaussian plume*, corresponding to a continuous point source that emits contaminants into a unidirectional wind blowing in a domain of infinite extent. This Gaussian plume solution, along with numerous variants, has been incorporated into industry-standard software packages that are used for monitoring and regulatory purposes. Gaussian plume models have been applied extensively in the study of emissions from large industrial operations as well as a variety of other applications including ash release from volcanic eruptions [41]; seed, pollen, and insect dispersal [19, 23, 47]; and odor propagation from livestock facilities [37]. The same approach (with slight modifications) may also be used to describe the flow of gas or liquid in porous soils and rocks, with applications to oil reservoirs, groundwater, and pollutant transport in aquifers, etc. [12, 13]. There has been a great deal of recent interest in applications relating to nuclear and biological contaminant release [18, 43], for which the importance of analytical approaches is nicely summed up in a review article by Settles: *"plume dispersion modeling is central to homeland security"* [34].

Our aim in this paper is to guide the reader through the entire mathematical modeling process, from the original conception of the model to the interpretation of results in the context of an actual industrial application. We begin by deriving the Gaussian plume solution to the advection-diffusion equation, investigating its mathematical properties, and drawing conclusions regarding the usefulness and limitations of the Gaussian plume approach. The model is illustrated using a simplified version of a real industrial emissions scenario in which airborne contaminants are released from a smelting operation such as that pictured in Figure 1.1. We then move onto the study of the associated inverse problem in which our objective is to estimate the unknown contaminant emission rate(s) given a series of ground-level concentration measurements. This inverse problem is formulated as an overdetermined linear system of equations, and the resulting solution is obtained using a constrained linear least squares algorithm. We discuss the conditioning and well-posedness of the inverse problem, and relate these aspects back to the original source identification problem and their significance in regulatory applications.

Throughout the discussion of the plume model and associated inverse problem, we provide details of various derivations that, although elementary, are not easily found in the literature or textbooks on the subject. We also emphasize that our focus here is on *simple* analytical solutions to the atmospheric dispersion problem and that simplicity, understandability in physical terms, and acceptance by practitioners are sometimes much more important in a regulatory environment than complex solutions that may require use of more advanced mathematical or numerical techniques. Consequently, we hope that this material will be a useful reference not only for applied and industrial mathematicians, but also for environmental engineers and other practitioners who use Gaussian plume and related models in their everyday work.

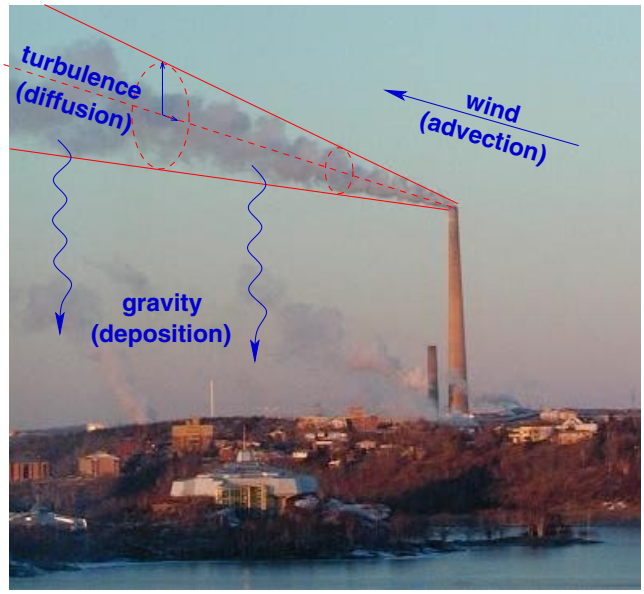


Fig. 1.1 *A photograph of emissions from the Inco Superstack (in Sudbury, ON, Canada) that illustrates the three main contributions to atmospheric contaminant transport: advection from the wind; diffusion from turbulent eddy motion; and deposition owing to gravitational settling.*

2. Governing Equations. A readable introduction to atmospheric dispersion modeling is available on Wikipedia [45], while a more in-depth treatment including details about analytical solutions can be found in the books by Arya [1] or Seinfeld and Pandis [33]. We will restrict our attention at the outset to the transport of a single contaminant whose mass concentration (or density) at location $\vec{x} = (x, y, z) \in \mathbb{R}^3$ [m] and time $t \geqslant 0$ [s] can be described by a smooth function $C(\vec{x}, t)$ [kg/m^3]. The law of conservation of mass for C may be expressed in differential form as

$$\frac{\partial C}{\partial t} + \nabla \cdot \vec{J} = S, \tag{2.1}$$

where $S(\vec{x}, t)$ [kg/m^3 s] is a source or sink term and the vector function $\vec{J}(\vec{x}, t)$ represents the *mass flux* [kg/m^2 s] of contaminant owing to the combined effects of diffusion and advection. The diffusive contribution to the flux arises from turbulent eddy motion in the atmosphere, for which a full description can be found in texts such as [1, 33]. The main result is that atmospheric diffusion may be assumed to follow Fick's law, which states that the diffusive flux is proportional to the concentration gradient or $\vec{J}_{D} = -\mathbf{K}\nabla C$. The negative sign ensures that the contaminant flows from regions of high concentration to regions of low concentration, and the diffusion coefficient $\mathbf{K}(\vec{x}) = \mathrm{diag}(K_x, K_y, K_z)$ [m^2/s] is a diagonal matrix whose entries are the turbulent eddy diffusivities that in general are functions of position. The second contribution to the flux is due to simple linear advection by the wind, which can be expressed as $\vec{J}_{A} = C\vec{u}$, where $\vec{u}$ [m/s] is the wind velocity. By adding these two contributions together, we obtain the total flux $\vec{J} = \vec{J}_{D} + \vec{J}_{A} = C\vec{u} - \mathbf{K}\nabla C$, which after substitution into the equation of conservation of mass (2.1) yields the three-dimensional

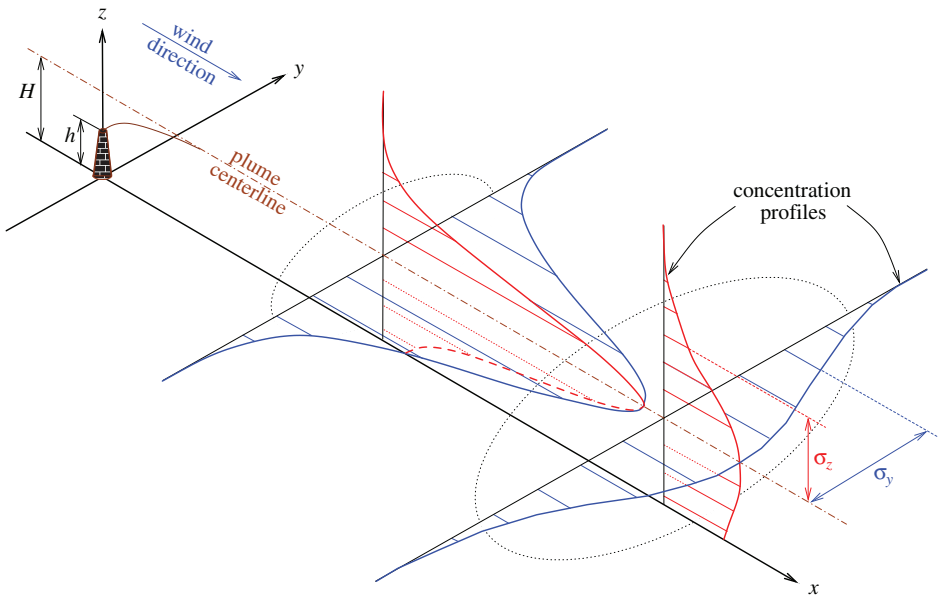


Fig. 2.1 *A contaminant plume emitted from a continuous point source, with wind direction aligned with the x-axis. Profiles of concentration are given at two downwind locations (vertical in red, horizontal in blue) and the Gaussian shape of the plume cross-sections are shown relative to the plume centerline.*

advection-diffusion equation

$$\frac{\partial C}{\partial t} + \nabla \cdot (C\vec{u}) = \nabla \cdot (\mathbf{K}\nabla C) + S. \tag{2.2}$$

We next make a number of simplifying assumptions that will permit us to derive a closed-form analytical solution:

A1. The contaminant is emitted at a constant rate Q [kg/s] from a single point source $\vec{x} = (0, 0, H)$ located at height H above the ground surface, as depicted in Figure 2.1. Then the source term may be written as

$$S(\vec{x}) = Q\,\delta(x)\,\delta(y)\,\delta(z - H), \tag{2.3}$$

where $\delta(\cdot)$ is the Dirac delta function. Note that the units of the delta function are $[\mathrm{m}^{-1}]$. For the stack-like configuration pictured in Figure 2.1 the height is actually an *effective height* $H = h + \delta h$, which is the sum of the actual stack height h and the *plume rise* δh that arises from buoyant effects.

A2. The wind velocity is constant and aligned with the positive x-axis so that $\vec{u} = (u, 0, 0)$ for some constant $u \geqslant 0$. We relax this assumption later on in section 4.3 to allow a uniform time-varying wind field $\vec{u} = \vec{u}(t)$, with $|\vec{u}| \geqslant 0$.

A3. The solution is steady state, which is reasonable if the wind velocity and all other parameters are independent of time and the time scale of interest is long enough.

A4. The eddy diffusivities are functions of the downwind distance x only, and diffusion is isotropic so that $K_x(x) = K_y(x) = K_z(x) =: K(x)$.

A5. The wind velocity is sufficiently large that diffusion in the x-direction is much smaller than advection; then the term $K_x \partial_x^2 C$ can be neglected.

A6. Variations in topography are negligible so that the ground surface can be taken as the plane $z = 0$.

A7. The contaminant does not penetrate the ground.

Making use of assumptions A1–A6, (2.2) reduces to

$$u\,\frac{\partial C}{\partial x} = K\frac{\partial^2 C}{\partial y^2} + K\frac{\partial^2 C}{\partial z^2} + Q\,\delta(x)\,\delta(y)\,\delta(z-H), \tag{2.4a}$$

and we are only concerned with the solution for values of $x, z \in [0,\infty)$ and $y \in (-\infty,\infty)$. In order to obtain a well-posed problem, we must supplement the PDE with an appropriate set of boundary conditions, namely,

$$C(0,y,z) = 0, \quad C(\infty,y,z) = 0, \quad C(x,\pm\infty,z) = 0, \quad C(x,y,\infty) = 0. \tag{2.4b}$$

The first condition is a consequence of the unidirectional wind and the assumption that there are no contaminant sources for $x < 0$. The remaining conditions at infinity are consistent with the requirement that the total mass of contaminant must remain finite. According to assumption A7, the vertical flux at the ground must vanish, which leads to the final boundary condition

$$K\,\frac{\partial C}{\partial z}(x,y,0) = 0. \tag{2.4c}$$

When taken together, (2.4a)–(2.4c) represent a well-posed problem for the steady-state contaminant concentration $C(x,y,z)$.

An equivalent formulation of this problem can be found by eliminating the source term from the PDE and instead introducing a delta function term into the boundary condition [10]:

$$u\,\frac{\partial C}{\partial x} = K\frac{\partial^2 C}{\partial y^2} + K\frac{\partial^2 C}{\partial z^2}, \tag{2.5a}$$

$$C(0,y,z) = \frac{Q}{u}\,\delta(y)\delta(z-H), \tag{2.5b}$$

$$C(\infty,y,z) = 0, \quad C(x,\pm\infty,z) = 0, \quad C(x,y,\infty) = 0, \tag{2.5c}$$

$$K\,\frac{\partial C}{\partial z}(x,y,0) = 0. \tag{2.5d}$$

The equivalence between problems (2.4) and (2.5) for $x > 0$ is presented as a theorem in [38, p. 59]. It is this second form of the governing equations that will be used in deriving the analytical solution in the next section.

Exercise 1. Prove Stakgold's theorem [38, p. 59]. Show that (2.5) is consistent with the alternate formulation in (2.4) by integrating the PDE (2.4a) over the interval $x \in [-d,d]$, letting $d \to 0^+$, and then imposing $C \equiv 0$ for $x < 0$. Explain why the boundary conditions for the two problems are consistent.

Exercise 2. Investigate assumption A5 by considering the steady three-dimensional advection-diffusion problem in the same form as (2.5), except that the term $\partial_x^2 C$ is retained and K is held constant. Nondimensionalize the PDE and initial/boundary conditions using the change of variables $\widetilde{x} = (K/uH^2)\,x$, $\widetilde{y} = y/H$, $\widetilde{z} = z/H$, and $\widetilde{C} = (uH^2/Q)\,C$ (a similar rescaling of variables is used in other studies such as [25] and [31]). Compare the relative sizes of terms in the equation for typical values of the parameters given in Table 3.1, and consequently show that neglecting the diffusion term in the x-direction is a reasonable approximation. Hint: You will need to make use of the delta function scaling property $\delta(\alpha x) = \delta(x)/\alpha$.

3. Derivation of the Gaussian Plume. Most books and articles aimed at practitioners present the Gaussian plume solution as a *fait accompli* and avoid both working through the details of the derivation and discussing the underlying assumptions (for example, [15, Chaps. 3 and 7] and [33]). The atmospheric dispersion problem is derived in a few more mathematical treatises such as Tayler [40, Chap. 4], but even then a number of important details are omitted. Our main aim in this section is therefore to lead the reader through the derivation in enough detail that the problem can be generalized to other more complicated situations.

The eddy diffusion coefficients in the atmospheric boundary layer are strong functions of downwind distance, not to mention that they vary with weather conditions and time from release, and consequently they are difficult to determine in practice. It is therefore common practice to replace x with the new independent variable

$$r = \frac{1}{u}\int_0^x K(\xi)\,d\xi, \tag{3.1}$$

which has units of [m^2]. We will see later on that r is a constant multiple of the variance of the concentration distribution, which is introduced later in section 3.3 (and denoted by σ). This change of variables eliminates the K coefficients in (2.5a), leading to the following constant coefficient problem for $c(r, y, z) := C(x, y, z)$:

$$\frac{\partial c}{\partial r} = \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}. \tag{3.2}$$

The boundary conditions for c are identical to those for C from (2.5b)–(2.5d), except that x is replaced with r.

We next apply the method of separation of variables to (3.2), assuming that the dependence of the solution on y and z can be separated according to[1]

$$c(r, y, z) = \frac{Q}{u}\,a(r, y)\cdot b(r, z). \tag{3.3}$$

We then obtain two reduced dimension problems that have the form of two-dimensional diffusion equations:

$$\frac{\partial a}{\partial r} = \frac{\partial^2 a}{\partial y^2} \quad \text{for } 0 \leqslant r < \infty \text{ and } -\infty < y < \infty, \tag{3.4a}$$

$$a(0, y) = \delta(y), \quad a(\infty, y) = 0, \quad a(r, \pm\infty) = 0, \tag{3.4b}$$

and

$$\frac{\partial b}{\partial r} = \frac{\partial^2 b}{\partial z^2} \quad \text{for } 0 \leqslant r < \infty \text{ and } 0 < z < \infty, \tag{3.5a}$$

$$b(0, z) = \delta(z - H), \quad b(\infty, z) = 0, \quad b(r, \infty) = 0, \quad \frac{\partial b}{\partial z}(r, 0) = 0. \tag{3.5b}$$

In both problems, the variable r can be viewed as a *time-like variable* and so the boundary conditions at $r = 0$ (which contain the delta functions) act as initial conditions for the respective diffusion equations.

Exercise 3. Derive (3.4) and (3.5) from (2.5), using the change of variables in (3.1) and assuming a separable solution of the form (3.3).

[1] This is a slight modification of the "usual" separation of variables approach where one would normally assume a fully separable solution of the form $c(r, y, z) = R(r)Y(y)Z(z)$.

3.1. Solution using Laplace Transforms. There are many methods that can be used for solving problems (3.4) and (3.5). We choose here to use Laplace transforms because this approach is most easily extended to deal with more general boundary conditions, as we will see later in section 3.6.

We begin with the problem for $a(r, y)$ in (3.4) and take the Laplace transform of the PDE in r to get

$$\rho\hat{a} - a(0, y) = \frac{\partial^2 \hat{a}}{\partial y^2},$$

where $\hat{a}(\rho, y) := \mathscr{L}_r\{a(r, y)\} = \int_0^\infty e^{-\rho r}\, a(r, y)\, dr$ and ρ is the transform variable. Applying the source boundary condition (3.4b), we obtain the following ordinary differential equation (ODE) for $\hat{a}$:

$$\frac{\partial^2 \hat{a}}{\partial y^2} - \rho\hat{a} = -\delta(y).$$

Next, take the Laplace transform in y,

$$\eta^2\hat{\hat{a}} - \eta\hat{a}(\rho, 0) - \frac{\partial \hat{a}}{\partial y}(\rho, 0) - \rho\hat{\hat{a}} = -1,$$

where $\hat{\hat{a}}(\rho, \eta) := \mathscr{L}_y\{\hat{a}(\rho, y)\} = \int_0^\infty e^{-\eta y}\, \hat{a}(\rho, y)\, dy$ and η is the transform variable. For the moment, we restrict ourselves to values of $0 \leqslant y < \infty$, but we will see shortly that symmetry permits the solution to be extended over the entire range $-\infty < y < \infty$. This last equation can be solved to obtain

$$\hat{\hat{a}}(\rho, \eta) = \frac{\eta c_1 + c_2}{\eta^2 - \rho},$$

where we have defined $c_1 = \hat{a}(\rho, 0)$ and $c_2 = \partial_y \hat{a}(\rho, 0) - 1$. We then apply the inverse transform in η to get

$$\begin{aligned}\hat{a}(\rho, y) &= c_1 \cosh(\sqrt{\rho} y) - \frac{c_2}{\sqrt{\rho}} \sinh(\sqrt{\rho} y) \\ &= \frac{c_1}{2}\left(e^{\sqrt{\rho} y} + e^{-\sqrt{\rho} y}\right) - \frac{c_2}{2\sqrt{\rho}}\left(e^{\sqrt{\rho} y} - e^{-\sqrt{\rho} y}\right).\end{aligned}$$

In order that $\hat{a} \to 0$ as $y \to \infty$, it is necessary that $c_1 = c_2/\sqrt{\rho}$, after which the above formula for $\hat{a}$ reduces to

$$\hat{a}(\rho, y) = \frac{c_2}{\sqrt{\rho}}\, e^{-\sqrt{\rho} y}.$$

Assuming for the moment that c_2 is independent of ρ, we may apply the inverse transform in ρ to get $a(r, y) = (c_2/\sqrt{\pi r}) \exp(-y^2/4r)$. By employing the delta function identity $\delta(y) = \lim_{r \to 0} \exp(-y^2/4r)/\sqrt{4\pi r}$, we find that $c_2 = \frac{1}{2}$ is in fact a constant and that

$$a(r, y) = \frac{1}{\sqrt{4\pi r}}\, e^{-y^2/4r}. \tag{3.6}$$

We have so far restricted ourselves to $0 \leqslant y < \infty$ in order to apply the Laplace transforms. However, the original problem as stated in (3.4) clearly has even symmetry about $y = 0$, and since the solution (3.6) is also an even function, then it is possible to simply extend the domain of validity for $a(r, y)$ to $y \in (-\infty, \infty)$.

We now move on to the solution of (3.5) for $b(\rho, z)$ and apply the Laplace transform in r of the PDE to get

$$\frac{\partial^2 \hat{b}}{\partial z^2} - \rho \hat{b} = -\delta(z - H),$$

where $\hat{b}(\rho, z) := \mathscr{L}_r\{b(r, z)\}$. Taking the Laplace transform in z and defining $\hat{\hat{b}}(\rho, \zeta) := \mathscr{L}_z\{\hat{b}(\rho, z)\}$, we find that

$$\zeta^2 \hat{\hat{b}} - \zeta \hat{b}(\rho, 0) - \frac{\partial \hat{b}}{\partial z}(\rho, 0) - \rho \hat{\hat{b}} = -e^{-\zeta H}.$$

After applying the transformed Neumann boundary condition $\partial_z \hat{b}(\rho, 0) = 0$, we can solve for

$$\hat{\hat{b}}(\rho, \zeta) = \frac{\zeta \hat{b}(\rho, 0) - e^{-\zeta H}}{\zeta^2 - \rho}$$

and apply the inverse transform in ζ to obtain

$$\hat{b}(\rho, z) = \hat{b}(\rho, 0) \cosh(\sqrt{\rho} z) - \frac{1}{\sqrt{\rho}} \sinh(\sqrt{\rho}(z - H)).$$

We then impose the condition that $\hat{b} \to 0$ as $z \to \infty$, which means that $\hat{b}(\rho, 0) = \exp(-\sqrt{\rho} H)/\sqrt{\rho}$ and hence

$$\hat{b}(\rho, z) = \frac{1}{2\sqrt{\rho}} \left(e^{-\sqrt{\rho}(z-H)} + e^{-\sqrt{\rho}(z+H)} \right).$$

Finally, applying the inverse transform in ρ yields

$$b(r, z) = \frac{1}{\sqrt{4\pi r}} \left(e^{-(z-H)^2/4r} + e^{-(z+H)^2/4r} \right). \tag{3.7}$$

The contaminant concentration can now be determined by substituting (3.6) and (3.7) into (3.3):

$$c(r, y, z) = \frac{Q}{4\pi u r} \exp\left(-\frac{y^2}{4r}\right) \left[\exp\left(-\frac{(z-H)^2}{4r}\right) + \exp\left(-\frac{(z+H)^2}{4r}\right) \right]. \tag{3.8}$$

This equation is commonly referred to as the *Gaussian plume solution* for the advection-diffusion equation, owing to the fact that the exponential dependence on both y and z is similar to that of a Gaussian-type function. The exponential character of the solution in y and z is clearly depicted in the concentration profiles shown in Figure 2.1. We mention in conclusion that identical expressions for a and b can be found using other approaches based on infinite series and Fourier transforms [14], as well as similarity methods [26, p. 144], all of which are interesting illustrations in the use of alternative PDE solution techniques.

Exercise 4. Integrate (3.8) in y and so derive a simpler cross-wind averaged solution that depends on x and z only. This is a formula that is used commonly by practitioners for regulatory applications; see [1, 16], for example.

3.2. Alternate Derivation Using Green's Functions. The Gaussian plume solution (3.8) may also be derived using a Green's function approach, which we briefly outline next. More details on the derivation of Green's functions can be found in the classic PDE books by Carslaw and Jaeger [5, Chap. 14] and Crank [7].

To this end, the solution to the problem (3.4) can be written $a(r,y) = \int_{-\infty}^{\infty} \delta(\eta) G_a(r,y;0,\eta)\, d\eta$, where the Green's function or *fundamental solution* is

$$G_a(r,y;\rho,\eta) = \frac{1}{\sqrt{4\pi(r-\rho)}} \exp\left(-\frac{(y-\eta)^2}{4(r-\rho)}\right).$$

The solution for $b(r,z)$ is slightly more complicated because of the Neumann boundary condition, which suggests extending the problem on the half-interval $z \geqslant 0$ to the entire real line and then applying the method of images. The Green's function for this modified problem is

$$G_b(r,z;\rho,\zeta) = \frac{1}{\sqrt{4\pi(r-\rho)}} \left[\exp\left(-\frac{(z-\zeta)^2}{4(r-\rho)}\right) + \exp\left(-\frac{(z+\zeta)^2}{4(r-\rho)}\right)\right],$$

in terms of which the solution may be written as $b(r,z) = \int_{-\infty}^{\infty} \delta(\zeta - H)\, G_b(r,z;0,\zeta)\, d\zeta$. A straightforward evaluation of the two integrals for $a(r,y)$ and $b(r,z)$ yields expressions that are identical to the ones obtained using Laplace transforms in the previous section.

The interested reader is encouraged to delve more into the fascinating topic of Green's functions by referring to the book by Duffy [9], which contains a wealth of applications drawn from physical systems, including diffusion problems very similar to those ones studied here. Another biographical study of George Green by Cannell [4] provides a historical perspective that is sure to prove stimulating for students being introduced to Green's functions for the first time. Of particular interest are Cannell's Chapter 10 and Appendix VIb, which provide fascinating accounts of the influence that Green's work had on the work of many 19th and 20th century "giants" from the fields of mathematics and physics.

3.3. Plume Properties: Constant and Variable Diffusivity. In this section we discuss the specification of the eddy diffusion coefficient $K(x)$, which is extremely important in applications. It is important to remember that the Gaussian plume solution is only strictly valid when K is a constant; however, in order to reproduce observed contaminant distributions, practitioners have found that it is necessary to allow K to vary with the downwind distance x, and the precise form of $K(x)$ (and hence also $r(x)$) is determined by fitting with experimental observations.

It is standard practice in the atmospheric science literature to replace the variable r in (3.8) with the closely related expression

$$\sigma^2(x) = \frac{2}{u}\int_0^x K(\xi)\, d\xi = 2r, \tag{3.9}$$

where σ is commonly referred to as the *standard deviation* of the (Gaussian) concentration distribution. These σ coefficients are much easier to determine experimentally than the eddy diffusivities. A variety of functional forms have been proposed, with one of the most common being a simple power law $\sigma^2(x) = ax^b$ [33]. Experimental measurements have been used to estimate the coefficients a and b under a variety of atmospheric conditions, and typical values are shown in Table 3.1. This type of dependence of σ on downwind distance can be justified by noting that as one moves further from a source, the plume becomes broader and hence σ must increase (refer to Figure 2.1).

It is interesting to point out a common inconsistency in the way that the Gaussian plume model is applied both in the literature and in many regulatory applications.

Table 3.1 *Parameter values used in the Gaussian plume model, based on the zinc smelter studied in* [24].

Parameter	Symbol	Value	Units
Wind speed	u	5	m/s
Stack height	H_s	$[15, 35, 15, 15]$	m
Emission rate	Q_s	$[1.1, 2.5, 0.16, 0.16] \times 10^{-3}$	kg/s
Diffusion parameter	a	0.33	m^{2-b}
Diffusion parameter	b	0.86	–
Settling velocity	w_{set}	2.7×10^{-3}	m/s
Deposition velocity	w_{dep}	5×10^{-3}	m/s
Viscosity of air	μ	1.8×10^{-5}	kg/m s
Gravitational acceleration	g	9.8	$\mathrm{m/s}^2$
Particle density	ρ	3500	$\mathrm{kg/m}^3$
Particle radius	R	2.5×10^{-6}	m

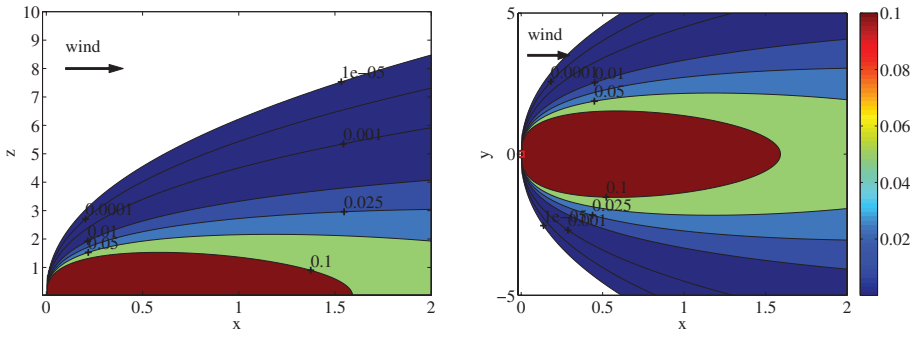
According to the definition of σ, the eddy diffusivity can be written in the form $K(x) = \frac{1}{2}\, u\partial_x\sigma^2$. If we consider the special case when K is constant, then $\sigma^2 = 2Kx/u$, which means that $\sigma \propto x^{1/2}$. Even when the experimentally measured values of standard deviation follow a power law relationship, they typically do not correspond to an exponent $b = \frac{1}{2}$; in fact, experiments suggest that $b > 0.70$ under most conditions. Nevertheless, it is common practice to determine the eddy diffusivity by way of the formula $K(x) = u\sigma^2/2x$, where $\sigma^2(x)$ is given by a power law or other experimentally determined fit. This inconsistency is discussed in more detail by Llewelyn [22] and will come into play in section 3.6, where incorporating the effects of settling and deposition of contaminant particles yields a solution that requires specifying both σ^2 and K.

For the sake of simplicity, we assume in the remainder of this section that K is constant so that (3.1) can be integrated to obtain $r = Kx/u$. In order to understand the typical behavior of the plume solution (3.8), we then consider two cases where the source is either located on the ground ($H = 0$) or else slightly elevated above ground level ($H = 2$). Values of the remaining physical parameters are taken to be $Q = 1$, $u = 1$, and $K = 1$, and the concentrations for the two source heights are displayed as contour plots in Figures 3.1 and 3.2, respectively. For both values of H, the left-hand contour plot demonstrates that the maximum value of concentration occurs at the same position $(0, 0, H)$ as the source, and that the contaminant is swept downwind from there into an elongated "plume" shape. The right-hand plot in each figure depicts the concentration in the plane $z = 0$ and shows that the peak ground-level concentration occurs at the origin when $H = 0$ (Figure 3.1) or else is shifted to a location further downwind when the source is elevated (Figure 3.2). This behavior is intuitively obvious from a physical standpoint, and is a qualitative validation of the plume solution.

A slightly simpler expression for the ground-level concentration can be obtained by setting $z = 0$ in the concentration solution, yielding

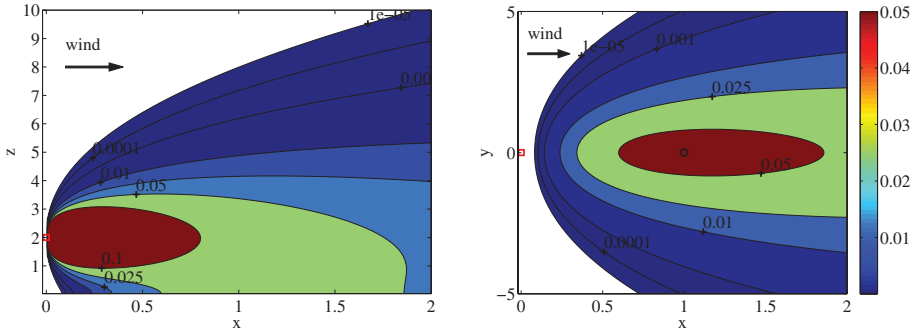
$$C(x, y, 0) = \frac{Q}{2\pi Kx} \exp\left(-\frac{u(y^2 + H^2)}{4Kx}\right). \tag{3.10}$$

We observe that when the source is elevated ($H > 0$), the concentration attains a maximum value of $C_{max} = 2Q/(\pi u H^2 e)$ at the downstream location $x_{max} = uH^2/(4K)$ along the plume centerline $y = 0$ (indicated by a black circle in Figure 3.2(b)).



(a) Vertical cross-section ($y = 0$) (b) Horizontal cross-section ($z = 0$)

Fig. 3.1 *Contour plots of concentration $C(x, y, z)$ for a source at ground level ($H = 0$): (left) in the vertical plane $y = 0$; (right) in the horizontal plane $z = 0$. The location of the contaminant source is indicated by a red square.*



(a) Vertical cross-section ($y = 0$) (b) Horizontal cross-section ($z = 0$)

Fig. 3.2 *Contour plots of concentration $C(x, y, z)$ for an elevated source ($H = 2$), but otherwise the same as Figure* 3.1*. The location of the peak ground-level concentration is marked on the right with a black circle.*

It is worthwhile noticing that in the limit of vanishing velocity,

$$\lim_{u \to 0^+} C(x, y, z) = \frac{Q}{2\pi K x}, \tag{3.11}$$

which seemingly contradicts a common perception in the literature that the Gaussian plume solution breaks down when $u = 0$ [2, 16, 35, 42]. The reason for this confusion is that the plume solution is most often written in terms of the variable r as in (3.8), and so can appear to have a singularity as $u \to 0$ if the dependence of r on velocity via $r = \frac{1}{u} \int_0^x K(\xi)\, d\xi$ is forgotten.

Nevertheless, it is essential to remember that the Gaussian plume solution only makes physical sense when the wind velocity is nonzero because of assumption A5, which neglects the diffusion term in the x-direction relative to the advection term. When $u = 0$, the advection term vanishes and the concentration is governed instead by the steady diffusion equation (or Poisson equation)

$$\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} = -\frac{Q}{K} \delta(x)\delta(y)\delta(z - H),$$

which has the following solution on the half-space $x > 0$:

$$C(x,y,z) = \frac{Q}{4\pi K}\left(\frac{1}{\sqrt{x^2+y^2+(z-H)^2}} + \frac{1}{\sqrt{x^2+y^2+(z+H)^2}}\right). \tag{3.12}$$

Notice that this result only holds when K is a constant, because $\partial_x(K\partial_x C) \neq K\partial_x^2 C$ if K depends on x. The steady-state profile (3.12) has asymptotic behavior $C \sim Q/(2\pi K x)$ as $x \to \infty$, which is identical to that for the zero-velocity limit (3.11) of the Gaussian plume solution.

A more common approach for dealing with very low or calm winds is to approximate the plume by a series of *Gaussian puffs*, which are solutions to the time-dependent advection-diffusion equation having a delta function source of the form $\delta(x)\delta(y)\delta(z-H)\delta(t)$. This puff solution is then integrated in time yielding an expression that can be used whether or not winds are calm. An example of the puff solution for an instantaneous release at $t = 0$ is given in section 3.5.6, and more details can be found in [22, 30].

3.4. Application: Emissions from Multiple Sources. We now apply the Gaussian plume solution to a simplified version of an actual emissions scenario studied in [24], where a zinc smelting operation has four major sources that release zinc particles into the atmosphere. The sources have locations $\vec{X}_s = (X_s, Y_s, H_s)$ and emission rate Q_s for $s = 1, \ldots, 4$, and are depicted in Figure 3.3 by the points labeled S1 to S4. The positive x-axis is aligned with the primary wind direction and the heights and emission rates for each source are listed in Table 3.1. The contribution from an individual source Ss to the contaminant concentration at any point (x, y, z) is then given by the Gaussian plume solution, which we denote by $C(x'_s, y'_s, z; Q_s, H_s)$. Here we have defined shifted coordinates

$$x' = x - X_s \qquad \text{and} \qquad y' = y - Y_s,$$

so that the source location corresponds to $x'_s = y'_s = 0$ for each s. The total concentration resulting from all four sources is simply given by the sum

$$C_T(x,y,z) = \sum_{s=1}^{4} C(x'_s, y'_s, z; Q_s, H_s).$$

In Figure 3.3, we present two concentration contour plots for the individual sources S1 and S2 and a third plot with S3 and S4 displayed together. The superposition of all four sources is shown separately in Figure 3.4. The largest ground-level concentration appears downwind from source S1, with weaker peaks occurring downwind of S2. It is interesting to note that even though S2 has by far the largest emission rate, it makes a smaller contribution to the ground-level concentration because it is at a much higher elevation. The weaker sources at S3 and S4 have a relatively small effect on the total concentration. These effects are consistent with physical intuition which suggests that increasing the height of a given source should decrease the ground-level deposition from that source, and vice versa. Furthermore, there should exist a "cross-over point" where the deposition from a high-Q source is exceeded by that of a low-Q/low-H source when the elevation of the first source exceeds some critical value; this and other similar effects are ideal topics for numerical experiments that can serve to develop intuition about contaminant emission problems.

The code that generates these plots is provided as three separate MATLAB files:

- `setparams.m`: assigns all values of the physical and numerical parameters;
- `gplume.m`: calculates the concentration using the Gaussian plume solution;

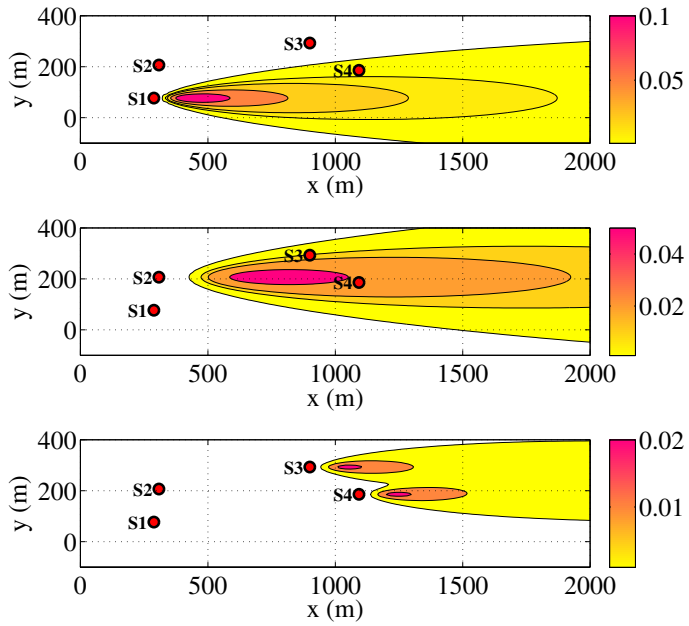


Fig. 3.3 *Ground-level concentration (in* $\mathrm{mg/m^3}$*) for the individual sources: S*1 *(top), S*2 *(middle), S*3*/S*4 *(bottom).*

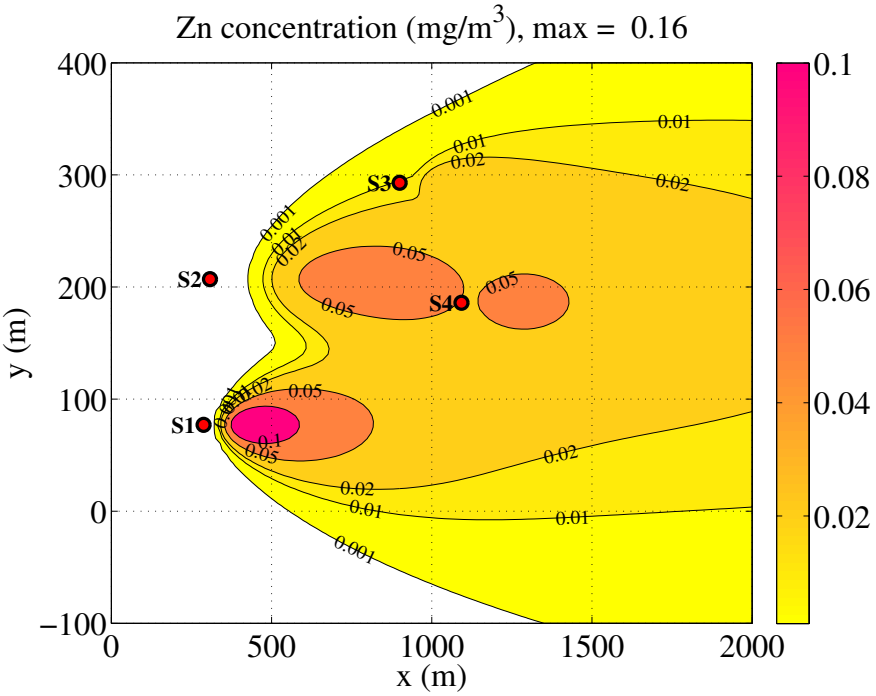


Fig. 3.4 *Total ground-level concentration (in* $\mathrm{mg/m^3}$*) for all four sources combined.*

- `forward.m`: main program that calculates and plots the concentration (calls `setparams` and `gplume`).

Exercise 5. Redo the forward calculation of Figures 3.3 and 3.4 by adding noise to the source emission rates of magnitude (a) ±10%; (b) ±20%. Compare the results and indicate the relative influence of noise on your computed concentrations.

3.5. A Menagerie of Plume Solutions. In this section we present a number of other Gaussian plume–type solutions that generalize the expression for concentration derived in section 3 by modifying either the boundary conditions, emission source type, or eddy diffusivities.

3.5.1. Anisotropic Eddy Diffusivities. When the eddy diffusion coefficients K_y and K_z are not equal, then it is helpful to define the following parameters: $r_{y,z}(x) = \frac{1}{u}\int_0^x K_{y,z}(\xi)\,d\xi$. Using these definitions and working through the same steps as before, we find that

(3.13)
$$C(x,y,z) = \frac{Q}{4\pi u\sqrt{r_y r_z}}\exp\left(-\frac{y^2}{4r_y}\right)\left[\exp\left(-\frac{(z-H)^2}{4r_z}\right)+\exp\left(-\frac{(z+H)^2}{4r_z}\right)\right],$$

which clearly reduces to (3.8) when $r_y = r_z$.

3.5.2. Perfectly Absorbing Ground. When the reflecting boundary condition (2.5d) is replaced by a perfectly absorbing condition at the ground, $c(r,y,0) = 0$, then a slight modification of the method of images for the derivation of $b(r,z)$ yields

$$c(r,y,z) = \frac{Q}{4\pi ur}\exp\left(-\frac{y^2}{4r}\right)\left[\exp\left(-\frac{(z-H)^2}{4r}\right)-\exp\left(-\frac{(z+H)^2}{4r}\right)\right]. \tag{3.14}$$

3.5.3. Inversion Layer. In the atmospheric boundary layer, the air temperature most often decreases with increasing altitude. However, there are situations where an *inversion* occurs, which corresponds to a layer in which the temperature increases with altitude and hence is stable and resistant to vertical mixing. These inversion layers act as reflecting boundaries and are notorious for trapping smog above cities such as Los Angeles and Mexico City [46]. If we replace the condition at infinity $c(r,y,\infty) = 0$ with a Neumann boundary condition $K\,\partial_z c(r,y,D) = 0$ corresponding to an inversion layer at height D above the ground, then the solution can be written as an infinite series of the form

$$c(r,y,z) = \frac{Q}{uD\sqrt{\pi r}}\exp\left(-\frac{y^2}{4r}\right)\left[\frac{1}{2}+\sum_{n=1}^{\infty}\cos\left(\frac{n\pi z}{D}\right)\cos\left(\frac{n\pi H}{D}\right)\exp\left(-\left(\frac{n\pi}{D}\right)^2 r\right)\right].$$

For a more detailed discussion of the solution of this problem, refer to [33] or [40, Ex. 4.1(b)].

3.5.4. Line Sources. A common application of atmospheric dispersion models is in the estimation of vehicle emissions from cars driving along busy highways, which can be approximated as continuous line sources. If a road is long and straight and runs perpendicular to the wind direction, then the road can be approximated by a linear source of infinite length along the y-axis, which corresponds to the boundary condition $c(0,y,z) = (Q_L/u)\delta(z)$. The quantity Q_L [kg/m s] is a constant emission rate per unit length of road, and must be distinguished from the emission rate parameter Q that

we have been using so far. The solution to the advection-diffusion equation with this new boundary condition is

$$c(r,y,z) = \frac{Q_{_L}}{2\pi u r}\exp\left(-\frac{z^2}{4r}\right)\int_{-\infty}^{\infty}\exp\left(-\frac{y^2}{4r}\right)\,dy = \frac{Q_{_L}}{\sqrt{\pi u}}\exp\left(-\frac{z^2}{4r}\right). \tag{3.15}$$

Notice that we have taken $H = 0$ here since roads are located at ground level.

A more realistic scenario than the road of infinite extent is a road of finite length L, which can be modeled using a boundary condition of the form $c(0,y,z) = (Q_{_L}/u)\delta(z)$ when $|y| \leqslant \frac{1}{2}L$, and $c(0,y,z) = 0$, otherwise. The solution to this problem takes the form [8]

$$c(r,y,z) = \frac{Q_{_L}}{2u\sqrt{\pi r}}\exp\left(-\frac{z^2}{4r}\right)\left[\operatorname{erf}\left(\frac{y+L/2}{2\sqrt{r}}\right) - \operatorname{erf}\left(\frac{y-L/2}{2\sqrt{r}}\right)\right], \tag{3.16}$$

where $\operatorname{erf}(x) = 2\pi^{-1/2}\int_0^x e^{-\xi^2}\,d\xi$ is the *error function*. A detailed discussion of line source emission modeling can be found in [28].

3.5.5. Height-Dependent Parameters. In many applications, the contaminant plume may extend a significant distance above the ground and it is therefore important to take into account the vertical structure of the atmosphere. The wind speed and diffusion coefficients are then taken to be functions of the vertical coordinate, with the most common form being the power laws [21]

$$u(z) = u_o z^{\alpha}, \qquad K_y(x,z) = k_y(x)z^{\beta}, \qquad \text{and} \qquad K_z(xf,z) = k_z(x)z^{\beta}. \tag{3.17}$$

By defining functions $r_{y,z} = \frac{1}{u_o}\int_0^x k_{y,z}(\xi)\,d\xi$ as in section 3.5.1, the following expression can be derived for concentration:

$$C(x,y,z) = \frac{Q}{2u_o\sqrt{\pi r_y}}\exp\left(-\frac{y^2}{4r_y}\right)\frac{(zH)^{(1-\beta)/2}}{\lambda r_z}\exp\left(-\frac{z^{\lambda}+H^{\lambda}}{\lambda^2 r_z}\right)I_{-\nu}\left(\frac{2(zH)^{\lambda/2}}{\lambda^2 r_z}\right), \tag{3.18}$$

where $\lambda = 2+\alpha-\beta$, $\nu = (1-\beta)/\lambda$, and $I_{-\nu}$ is the modified Bessel function of the first kind of order $-\nu$. It is possible to show (see Exercise 6) that (3.18) reduces to (3.13) in the case when $\alpha = \beta = 0$.

Exercise 6. Use the Bessel function identity $I_{-1/2}(x) = (2/\pi x)^{1/2}\cosh(x)$ to show that (3.18) reduces to (3.13) in the case when the wind velocity is constant and eddy diffusivities are functions of x only.

Exercise 7 (adapted from Tayler [40, pp. 197–198]). Consider a simplified version of the problem from section 3.5.5 obeying the reduced-dimensional PDE $u(z)\,\partial_x\bar{C} = \partial_z(K(z)\partial_z\bar{C})$ in terms of the cross-wind averaged concentration $\bar{C}(x,z) = \int_{-\infty}^{\infty} C(x,y,z)\,dy$. Assume that the height-dependent parameters have the simpler form $u(z) = z^{\alpha}$ and $K(z) = K_z(z) = z^{\beta}$ for α and β positive constants, and take the source height $H = 1$. Perform the change of variables $z = s^p$ and $\bar{C}(x,z) = s^{\nu}\,\mathcal{C}(x,s)$, and hence show that the Laplace transform $\hat{\mathcal{C}} = \mathscr{L}_x\{\mathcal{C}\}$ of the new dependent variable obeys

$$\frac{d^2\hat{\mathcal{C}}}{ds^2} + \frac{1}{s}\frac{d\hat{\mathcal{C}}}{ds} - \left(\xi p^2 + \frac{\nu^2}{s^2}\right)\hat{\mathcal{C}} = -p\delta(s-1),$$

where ξ is the transform variable, $\lambda = 2+\alpha-\beta$, $\nu = (1-\beta)/\lambda$, and $p = 2/\lambda$. Determine the solution in terms of Bessel functions with an imaginary argument, and

discuss the special case $\lambda = 0$. Finally, show that (3.18) is identical to your Bessel function solution when $u_o = k_z = 1$ and the concentration is averaged cross-wind (in the y-direction).

3.5.6. Gaussian Puff: Instantaneous and Time-Varying Sources. All situations considered so far assume that the source emits contaminant continuously in time and at a constant rate. There are many applications in which the emissions are either nearly instantaneous (occurring over a relatively short time interval), or are intermittent or time-varying. A common approach to dealing with such problems is to take the time-dependent advection-diffusion equation (including the time-derivative term on the left-hand side of (2.5a)) and consider an instantaneous puff of contaminant released at time $t = 0$. The source boundary condition is therefore replaced with

$$c(0, y, z, t) = \frac{Q_{_T}}{u}\,\delta(y)\delta(z - H)\delta(t), \tag{3.19}$$

where $Q_{_T}$ [kg] represents the total amount of contaminant emitted (note the difference between the physical units of Q and $Q_{_T}$). The solution can be derived using an approach similar to that we applied in section 3.1 to obtain [1, 22]

$$c(r, y, z, t) = \frac{Q_{_T}}{8(\pi r)^{3/2}}\,\exp\left(-\frac{(x-ut)^2+y^2}{4r}\right)\left[\exp\left(-\frac{(z-H)^2}{4r}\right)+\exp\left(-\frac{(z+H)^2}{4r}\right)\right], \tag{3.20}$$

which is typically referred to as the *Gaussian puff solution*. To deal with a time-varying source, one simply needs to evaluate an appropriate integral (or sum) of puff solutions in time.

Exercise 8. Show that the superposition of an infinite sequence of Gaussian puffs in time yields the same concentration profile as the Gaussian plume. In other words, integrate the puff formula (3.20) over the time interval $t \in [0, \infty)$ and compare with the plume solution (3.8).

3.5.7. Other Generalizations. Many other variations of the Gaussian plume solution have been derived for different emissions scenarios. For example, the line source solution can be integrated to obtain sources of strip, area, and volume type [6, 37]. Others have considered horizontal diffusion coefficients that depend on other variables such as wind speed [29]. Lin and Hildemann [20] provide an extensive summary of various plume-type solutions that are available in the literature.

Exercise 9 (adapted from [1, p. 218]). Emissions from burning agricultural waste may be treated as a line source of 200 m in length that emits organic matter into the air at a rate of 0.5 g/m s. The wind is steady and unidirectional and blows with a velocity of 2.5 m/s, directed perpendicular to the line source. Estimate the average ground-level concentrations of organic material at distances of 500 m and 5000 m downwind from the source and along the plume centerline. Assume that the dispersion coefficient takes the form $r(x) = ax^b$ with $a = 0.16$, $b = 0.70$, and that x is measured in m. Compare the solution for the line source with a simpler (but rougher) estimate based on replacing the line source with an equivalent point source of strength 100 g/s (which is simply the product of the strength of the line source and its length). Discuss your results.

3.6. Deposition and Settling: The Ermak Solution. In many practical situations, contaminant particles are more massive than air and so they tend to settle out

of the atmosphere at a well-defined rate known as the *settling velocity*, w_{set} [m/s]. For spherical particles of uniform size, the settling velocity can be approximated using Stokes' law, $w_{set} = 2\rho g R^2/(9\mu)$, where ρ is the particle density [kg/m^3], R is the particle radius [m], μ is the dynamic viscosity of air [kg/m s], and g is the gravitational acceleration [m/s^2]. To incorporate the effect of settling, we supplement the advection velocity with a vertical component, $\vec{u} = (u, 0, -w_{set})$, which means that the advection-diffusion equation (3.2) becomes

$$\frac{\partial c}{\partial r} - \frac{w_{set}}{K}\frac{\partial c}{\partial z} = \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}. \tag{3.21}$$

In addition to vertical settling within the atmosphere, observations suggest that taking a no-flux condition at the ground surface is not a reasonable approximation; instead, some portion of particles that reach the surface actually deposit on the ground and are absorbed. Experimental measurements suggest that the vertical flux of contaminant particles at the surface is proportional to the surface concentration and so may be written as

$$\left(K\frac{\partial c}{\partial z} + w_{set}c\right)\Big|_{z=0} = w_{dep}c|_{z=0}\,, \tag{3.22}$$

where w_{dep} [m/s] is the so-called *deposition velocity*.

The earliest analytical solution to the Gaussian plume equations with deposition was derived in [36]; however, Ermak [10] was the first to consider pollutant dispersion with both deposition and settling. Ermak applied Laplace transform methods to (3.21), (2.5d), and (3.22) and obtained the solution

$$\begin{aligned} c(r,y,z) = {} & \frac{Q}{4\pi u r}\exp\left(-\frac{y^2}{4r}\right)\,\exp\left(-\frac{w_{set}\,(z-H)}{2K} - \frac{w_{set}^2\,r}{4K^2}\right) \\ & \times\left[\exp\left(-\frac{(z-H)^2}{4r}\right) + \exp\left(-\frac{(z+H)^2}{4r}\right)\right. \\ & \left. - \frac{2w_o\sqrt{\pi r}}{K}\,\exp\left(\frac{w_o(z+H)}{K} + \frac{w_o^2\,r}{K^2}\right)\,\operatorname{erfc}\left(\frac{z+H}{2\sqrt{r}} + \frac{w_o\sqrt{r}}{K}\right)\right], \end{aligned} \tag{3.23}$$

where $w_o := w_{dep} - \frac{1}{2}w_{set}$ and $\operatorname{erfc}(x) = 1 - \operatorname{erf}(x)$ is the *complementary error function*. This is a generalization of the Gaussian plume solution which clearly reduces to (3.8) when $w_{set} = w_{dep} = 0$.

The most detailed derivation of the Ermak solution using transform methods can be found in [44, pp. 358–361] in the context of a general discussion of diffusion problems with radiation boundary conditions. The deposition-settling problem was also studied by Fisher and McQueen [11] for the case of constant diffusivity, and they derived a number of the corresponding properties that we discussed in section 3.3. Llewelyn [22] solved a time-dependent version of the atmospheric dispersion problem and showed that his solution reduces asymptotically to Ermak's at steady state. An alternative derivation using complex variable techniques was used by MacKay, McKee, and Mulholland [25] for the problem with deposition but no settling. Interestingly, similar solutions have been derived for other problems arising, for example, in diffusion of ligand molecules in a protein matrix [27].

Exercise 10. Find Ermak's paper in your library, and show that his formula for the contaminant concentration (Eq. (5) from [10]) is dimensionally inconsistent.

Hence, identify and correct two typographical errors in Ermak's paper. Show that the corrected formula is identical to our (3.23) by replacing his $\sigma_y^2 = \sigma_z^2 = 2r$ and relabeling other parameters appropriately.

Exercise 11. Derive the Ermak solution for (3.21), (3.22), (2.5b), and (2.5c) by looking for a separable solution of the form

$$c(r, y, z) = \frac{Q}{u}\, a(r, y)\, b(r, z)\, \exp\left[-\frac{w_{set}(z - H)}{2K} - \frac{w_{set}^2 r}{4K^2}\right].$$

This substitution replaces (3.3) and the extra exponential factor is specially chosen so as to eliminate the gravitational settling term in the PDE. The resulting initial-boundary value problem for a is identical, while that for b differs in that the Neumann boundary condition is replaced with the *radiation condition* $\partial_z b = w_o b/K$; hence, the only difference here is in the Laplace transform solution for b. Show that your solution is identical to (3.23). Hint: Some guidance on using Laplace transforms to solve the diffusion equation with a radiation boundary condition can be found in [5, sec. 14.2(II)].

Exercise 12. Generalize (3.23) to the case where the diffusivities $K_y(x)$ and $K_z(x)$ are not equal. This case is also considered by Ermak and an outline of his derivation can be found in the appendix of [10].

Exercise 13. Modify the MATLAB code from section 3.4 to calculate concentrations using Ermak's solution for the case $K_y(x) \neq K_z(x)$ that you derived in Exercise 12. Compute the ground-level concentration using values of w_{set} and w_{dep} in Table 3.1 and compare your results to those obtained with the standard plume solution in Figure 3.4 on a rectangle of dimension $[0, 100] \times [-50, 50]$. Compute the absolute and relative difference between the two solutions at each point on the ground (using a 100×100 equally spaced grid) and comment on where the largest discrepancies lie. Because the differences between the two solutions will be quite small owing to the relatively small values of the physical parameters w_{set} and w_{dep}, we suggest you repeat this calculation using values of w_{set} and w_{dep} 10 times larger and then observe how the solutions differ. Finally, modify the code so as to calculate the amount (in g) of zinc deposited at each of the receptors listed in the `setparams.m` file (with locations given by `recept.{x,y,z}`) over a time period of 30 days.

4. Inverse Problem: Source Identification. We are now ready to tackle the problem we originally set out to solve, namely, that of determining a contaminant source emission rate for a given a set of measurements on the ground. This is particularly important in certain practical pollutant dispersion scenarios where the emission rate cannot be measured directly at the source, but rather only indirectly at a distance from the source (see [24], for example). In other applications, such as biological contaminant releases [18, 43] or volcanic eruptions [41], the emission rate (or even location) may be unknown by its very nature. Pollutant emission applications are also typically complicated by a number of other factors such as

- *multiple sources:* in large industrial settings where many stacks are involved;
- *multiple receptor measurements:* at least as many as the number of sources. Furthermore, increasing the number of receptors also increases the solution accuracy by countering errors and uncertainties inherent in wind and deposition data;
- *time-varying wind velocities:* since atmospheric conditions are never constant outside of a laboratory setting.

In what follows, we will introduce these three complications one at a time.

4.1. Single Source, Multiple Receptors. We begin by first writing an expression for the vertical flux of contaminant at a given location $\vec{x} = (x, y, z)$ due to a source Q at location $\vec{X} = (X, Y, H)$. The deposition flux [kg/m^2 s] is simply the product of the local concentration and the deposition velocity

$$w_{dep}\, C(x', y', z; Q, H) := w_{dep}\, Q\, p(\vec{x}; \vec{X}, U).$$

Here, we have made use of the notation $(x', y') = (x - X, y - Y)$ introduced in section 3.4 and have also introduced a new function p that makes explicit the linear dependence of this expression on the emission rate Q.

Suppose now that measurements are made by accumulating the contaminant in a sequence of N_r *dustfall jars* or receptors, located at positions $\vec{x} = \vec{\xi}_r = (\xi_r, \eta_r, h_r)$ for $r = 1, 2, \ldots, N_r$. Each receptor is a cylindrical container with an opening having cross-sectional area A [m^2], and the contaminant is sampled over a time period of duration T [s], which is typically on the order of weeks in order that the receptors collect measurable quantities of contaminant particles. Then the mass of contaminant in [kg] deposited at the rth receptor can be written as

$$D_r = AT(\mathit{flux}) = w_{dep} ATQ\, p(\vec{\xi}_r; \vec{X}, U). \tag{4.1}$$

If we then consider the full set of N_r receptor measurements, this represents a system of N_r linear equations in the single unknown emission rate Q. In particular, if $N_r = 1$, then the problem has a unique solution for Q; otherwise ($N_r > 1$), the system is overdetermined and there is no unique solution in general.

If we bear in mind that the Gaussian dispersion model is only an approximation of the real world and that deposition measurements are subject to significant experimental errors, then it makes sense to search for a solution that minimizes some measure of the error between experimental data and the plume model prediction. In particular, minimizing an error measure corresponding to the root mean square of the difference leads directly to the well-known method of linear least squares, which is the approach we advocate here. In practice, some care must be taken to select both the number and location of receptors in order to obtain an accurate approximation of the emission rate.

We now present a specific example of an emissions scenario at a zinc smelter in Trail, British Columbia, Canada, which is a simplified version of the problem introduced in section 3.4 and studied in detail in the paper [24]. We consider a single source S1 and nine receptors R1–R9, where the locations of the source and receptors are given explicitly in the MATLAB file `setparams.m`. The layout of sources and receptors is also depicted in Figure 4.1. Assume that the wind is constant in time, blowing at a constant speed of 5 m/s and directed along the positive x-axis. Take the mass of zinc deposited in the nine receptors over a one-month period to be

$$\vec{D} = [8.4,\ 68,\ 33,\ 4.2,\ 11,\ 8.2,\ 2.9,\ 2.2,\ 0.93] \text{ mg}.$$

Finally, assume the receptors are cylindrical glass jars of diameter 16 cm, so that the mouth of each jar has area $A \approx 0.02$ m^2.

Based on the above description and the parameters in `setparams.m`, we employ MATLAB's `lsqlin` function to solve the corresponding linear least squares problem, which reduces to four linear equations for a single emission rate Q. Using the MATLAB routine `inverse1.m`, we obtain the estimate $Q \approx 169$ T/yr, which incidentally is within an order of magnitude of the estimates of total zinc emissions computed in [24] using a much more careful analysis. This is a surprisingly accurate result if one

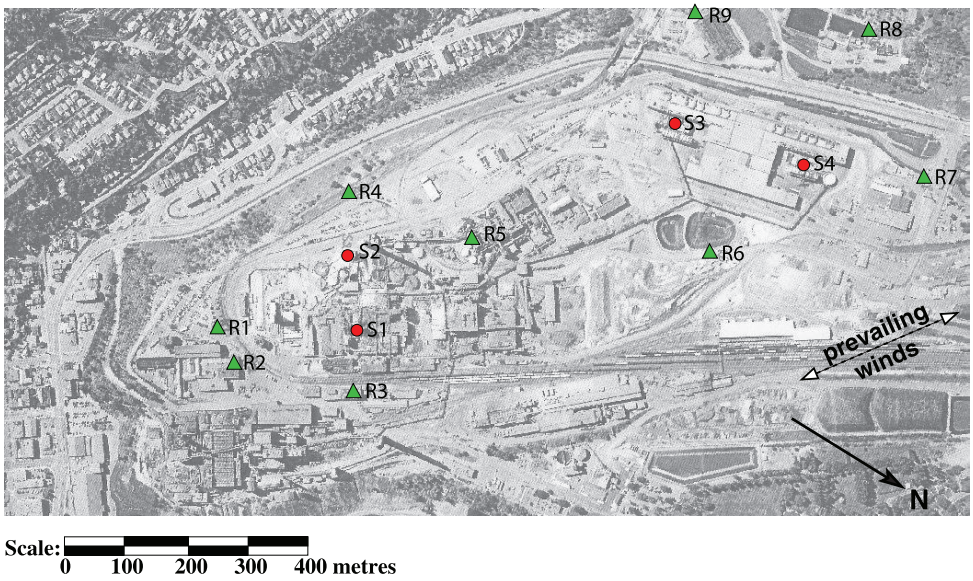


Fig. 4.1 *Aerial photo of a zinc smelter site (Teck-Cominco Ltd. in Trail, BC, Canada) indicating the location of each source Ss (circles) and receptor Rr (triangles). The size of the area depicted is roughly* 1600×800 m.

takes into account the fact that the actual problem has four emissions sources (S1–S4) at different locations and includes additional physical constraints on the variables, not to mention the errors that are inherent in the Gaussian plume model.

Exercise 14. Substitute the estimate Q determined from the example above into the Ermak solution (3.23) and determine the corresponding deposition values (in kg) at each of the nine receptor locations. Compare your results with the measured data and explain the discrepancy at the first four receptors, R1–R4. Redo the inverse and forward calculations by omitting these four receptors, and discuss your results. Hint: It may help to answer this question in combination with Exercise 15.

4.2. Multiple Sources and Receptors. We now generalize the problem from the previous section by considering the situation where there are N_r receptor measurements, but instead of a single source there are now $N_s > 1$ sources of contaminant with emission rate Q_s and location $\vec{X}_s = (X_s, Y_s, H_s)$ for $s = 1, 2, \ldots, N_s$. The total mass of contaminant deposited in the rth receptor is simply the sum of the contributions from each source, so that

$$D_r = w_{dep} AT \sum_{s=1}^{N_s} Q_s \, p(\vec{\xi}_r; \vec{X}_s, U). \tag{4.2}$$

To contrast with the previous section, (4.2) represents a system of N_r linear equations in N_s unknowns that is solvable provided $N_r \geqslant N_s$—this is a practical restriction since there are usually many more measurements than emission sources. We can rewrite (4.2) more compactly in the form

$$\vec{D} = \mathbf{P}\,\vec{Q}, \tag{4.3}$$

where $\vec{D}$ and $\vec{Q}$ are vectors (of length r and s, respectively) that contain the depositions and emission rates and $\mathbf{P}$ is an $N_r \times N_s$ matrix with entries

$$\mathsf{P}_{rs} = w_{dep} A T \, p(\vec{\xi}_r; \vec{X}_s, U). \tag{4.4}$$

Exercise 15. Repeat Exercise 14 but this time include all four zinc sources S1–S4 in the least squares inversion process. Compare and contrast your results.

4.3. Time-Varying, Unidirectional Wind. We have so far taken the wind to be constant over the time period of interest, but this is clearly not a reasonable assumption in most real emissions scenarios where the wind speed and direction can vary significantly throughout the day. Suppose therefore that the wind is allowed to be time-dependent, but that only the speed $U(t)$ varies while the direction remains fixed; this type of behavior might correspond to a long, straight valley with relatively level floor and steep sides that funnel the wind in a direction parallel to the valley walls.

The total time T is then divided into N_t subintervals of length $\Delta t = T/N_t$. Care must be taken to choose a time interval Δt that is short enough to capture the most significant variations in wind speed and yet long enough that any emissions released within that subinterval have time to reach a steady-state distribution (which incidentally relates to one of the main assumptions in the Gaussian plume model). In many atmospheric dispersion handbooks as well as studies in the literature, one encounters the "rule of thumb" that a time interval of $\Delta t = 10$ min is usually appropriate. For the site pictured in Figure 4.1, and assuming an average sustained wind speed of roughly 3–5 m/s, any contaminant plume released from one of the four sources will be advected a distance of several kilometers downwind, which extends well outside the domain of interest. Consequently, it is reasonable in this situation to assume that the air flow is uniform and steady state within each time interval of duration Δt.

If we orient the coordinate axes so that the x-axis is aligned with the prevailing wind direction, then the total amount of zinc deposited at a receptor location $\vec{\xi}_r$ may be written as

$$D_r = w_{dep} A \Delta t \sum_{s=1}^{N_s} Q_s \sum_{n=1}^{N_t} p(\vec{\xi}_r; \vec{X}_s, U^n), \tag{4.5}$$

where $U^n = U(n\Delta t)$.

4.4. Wind with Varying Time and Direction. When the direction of the wind varies in time, the Ermak solution in (3.23) can only be applied if a new set of transformed coordinates (x'_s, y'_s) is defined for each source s that not only translates the source location to the origin, but also rotates the coordinates so that the transformed x-axis is aligned parallel with the wind velocity. To this end, we generalize the coordinate transformation from section 3.4 and define

$$\begin{pmatrix} x'_s \\ y'_s \end{pmatrix} = \mathbf{R}_{-\theta} \begin{pmatrix} x - X_s \\ y - Y_s \end{pmatrix}, \tag{4.6}$$

where θ corresponds to the angle that the wind direction vector makes with the original x-axis (measured counterclockwise) and $\mathbf{R}_{-\theta}$ is the 2×2 matrix that rotates vectors through an angle $-\theta$ in the x, y-plane (see Figure 4.2). The resulting coordinates have an x'_s-axis that is aligned with the wind direction.

We close this section by mentioning that the derivation of the Gaussian plume solution used above is similar to that of Calder [3], who considered the problem of

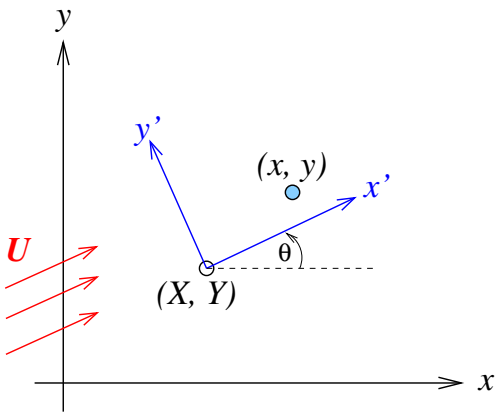


Fig. 4.2 *Relationship between the original coordinates (x, y) and transformed coordinates (x', y') for a point source at location (X, Y), in a wind having speed U and direction angle θ.*

multiple-source estimation in a time-varying wind with a rotated coordinate system aligned with the wind direction. The main difference between Calder's work and ours is that he provided a general theoretical framework for the source estimation problem that avoided providing any specific Gaussian plume approximation for the advection–diffusion equation. Finally, we point out the work of Hogan et al. [17], who estimated both location and emission rate for a single source using exactly four concentration measurements and showed that the solution could be found *exactly* given synthetic data (that is, data computed directly from the forward solution with no noise). Of course, real data always contain a significant degree of error, which is why we are advocating an approach such as the least squares method outlined here.

Exercise 16. Generalize your MATLAB code from Example 15 to handle a wind velocity whose direction and magnitude vary with time. You should make use of the wind measurements in the file `wind.mat` that can be read in using the command "`read wind`," after which you will have access to a structure variable called `wind` containing the following members:

`wind.time` – time of wind measurement (s),
`wind.vel` – wind speed (m/s),
`wind.dir` – wind direction (radians ccw from north).

Each structure member is a vector of length 4320 whose entries correspond to wind data measured at 10-minute intervals over a 30-day period.

5. Conclusions. In this paper, we provide a detailed look at the basic mathematics behind atmospheric dispersion modeling, based on Gaussian plume approximations to the advection-diffusion equation with a continuous point source. Using techniques from Green's functions and Laplace transforms, we derive various plume solutions based on a number of physically-relevant simplifying assumptions. The results are illustrated using examples from atmospheric contaminant transport in realistic emission scenarios with real data. We also discuss the inverse source estimation problem, in which multiple source emission rates are estimated from a number of ground-level contaminant measurements. This last problem is a nice application of the method of least squares to the solution of overdetermined linear systems. A number of exercises provide many opportunities for students to investigate the problem in more detail,

and suggestions are provided throughout on extensions that permit educators to explore the material further in undergraduate classes on mathematical modeling, PDEs, or numerical analysis.

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REFERENCES

[1] S. P. Arya, *Air Pollution Meteorology and Dispersion*, Oxford University Press, New York, 1999.

[2] J. Bluett, N. Gimson, G. Fisher, C. Heydenrych, T. Freeman, and J. Godfrey, *Good Practice Guide for Atmospheric Dispersion Modelling*, Ref. ME522, Ministry of the Environment, Wellington, New Zealand, 2004. Available online from http://www.mfe.govt.nz/publications/air/atmospheric-dispersion-modelling-jun04/index.html.

[3] K. L. Calder, *Multiple-source plume models of urban air pollution: Their general structure*, Atmos. Environ., 11 (1977), pp. 403–414.

[4] D. M. Cannell, *George Green: Mathematician & Physicist,* 1793–1841: *The Background to His Life and Work*, 2nd ed., SIAM, Philadelphia, 2001.

[5] H. S. Carslaw and J. C. Jaeger, *Conduction of Heat in Solids*, Clarendon Press, Oxford, 1959.

[6] C. V. Chrysikopoulos, L. M. Hildemann, and P. V. Roberts, *A three-dimensional steady-state atmospheric dispersion-deposition model for emissions from a ground-level area source*, Atmos. Environ., 26A (1992), pp. 747–757.

[7] J. Crank, *The Mathematics of Diffusion*, 2nd ed., Oxford University Press, Oxford, 1975.

[8] G. T. Csanady, *Crosswind shear effects on atmospheric diffusion*, Atmos. Environ., 6 (1972), pp. 221–232.

[9] D. G. Duffy, *Green's Functions with Applications*, Chapman & Hall/CRC, Boca Raton, FL, 2001.

[10] D. L. Ermak, *An analytical model for air pollutant transport and deposition from a point source*, Atmos. Environ., 11 (1977), pp. 231–237.

[11] B. E. A. Fisher and J. F. MacQueen, *A theoretical model for particulate transport from an elevated source in the atmosphere*, IMA J. Appl. Math., 27 (1981), pp. 359–371.

[12] R. A. Freeze and J. A. Cherry, *Groundwater*, Prentice–Hall, Englewood Cliffs, NJ, 1979.

[13] H. K. French, S. E. A. T. M. van der Zee, and A. Leijnse, *Prediction uncertainty of plume characteristics derived from a small number of measuring points*, Hydrogeol. J., 8 (2000), pp. 188–199.

[14] R. Haberman, *Applied Partial Differential Equations with Fourier Series and Boundary Value Problems*, Pearson Prentice–Hall, Upper Saddle River, NJ, 2004.

[15] C. R. Hadlock, *Mathematical Modeling in the Environment*, Mathematical Association of America, Washington, DC, 1998.

[16] S. R. Hanna, G. A. Briggs, and R. P. Hosker Jr., *Handbook on Atmospheric Diffusion*, Technical Report DOE/TIC-11223, Technical Information Center, U.S. Department of Energy, 1982.

[17] W. R. Hogan, G. F. Cooper, M. M. Wagner, and G. L. Wallstrom, *An Inverted Gaussian Plume Model for Estimating the Location and Amount of Release of Airborne Agents from Downwind Atmospheric Concentrations*, Technical Report, Realtime Outbreak and Disease Surveillance Laboratory, University of Pittsburgh, Pittsburgh, PA, 2005.

[18] H.-J. Jeong, E.-H. Kim, K.-S. Suh, W.-T. Hwang, M.-H. Han, and H.-K. Lee, *Determination of the source rate released into the environment from a nuclear power plant*, Rad. Prot. Dos., 113 (2005), pp. 308–313.

[19] S. A. Levin, H. C. Muller-Landau, R. Nathan, and J. Chave, *The ecology and evolution of seed dispersal: A theoretical perspective*, Ann. Rev. Ecology Evolution Systematics, 34 (2003), pp. 575–604.

[20] J.-S. Lin and L. M. Hildemann, *Analytical solutions of the atmospheric diffusion equation with multiple sources and height-dependent wind speed and eddy diffusivities*, Atmos. Environ., 30 (1996), pp. 239–254.

[21] J.-S. Lin and L. M. Hildemann, *A generalized mathematical scheme to analytically solve the atmospheric diffusion equation with dry deposition*, Atmos. Environ., 31 (1997), pp. 59–71.

[22] R. P. Llewelyn, *An analytical model for the transport, dispersion and elimination of air pollutants emitted from a point source*, Atmos. Environ., 17 (1983), pp. 249–256.
[23] C. Loos, R. Seppelt, S. Meier-Bethke, J. Schiemann, and O. Richter, *Spatially explicit modelling of transgenic maize pollen dispersal and cross-pollination*, J. Theoret. Biol., 225 (2003), pp. 241–255.
[24] E. Lushi and J. M. Stockie, *An inverse Gaussian plume approach for estimating contaminant emissions from multiple point sources*, Atmos. Environ., 44 (2010), pp. 1097–1107.
[25] C. MacKay, S. McKee, and A. J. Mulholland, *Diffusion and convection of gaseous and fine particulate from a chimney*, IMA J. Appl. Math., 71 (2006), pp. 670–691.
[26] R. M. M. Mattheij, S. W. Rienstra, and J. H. M. ten Thije Boonkkamp, *Partial Differential Equations: Modeling, Analysis, Computation*, SIAM Monogr. Math. Model. Comput. 10, SIAM, Philadelphia, 2005.
[27] W. Nadler and D. L. Stein, *Reaction-diffusion description of biological transport processes in general dimension*, J. Chem. Phys., 104 (1996), pp. 1918–1936.
[28] S. M. S. Nagendra and M. Khare, *Line source emission modelling*, Atmos. Environ., 36 (2002), pp. 2083–2098.
[29] H. Nitsche, W. Wergen, and K. Fraedrich, *Boundary-layer diffusion modelling: The Gaussian plume approach versus the spectral solution*, Bound. Layer Meteorol., 12 (1977), pp. 127–139.
[30] S. Okamoto, H. Ohnishi, T. Yamada, T. Mikami, S. Momose, H. Shinji, and T. Itohiya, *A model for simulating atmospheric dispersion in low wind conditions*, Int. J. Environ. Poll., 16 (2001), pp. 69–79.
[31] T. W. Peterson and J. H. Seinfeld, *Mathematical model for transport, interconversion, and removal of gaseous and particulate air pollutants: Application to the urban plume*, Atmos. Environ., 11 (1977), pp. 1171–1184.
[32] O. F. T. Roberts, *The theoretical scattering of smoke in a turbulent atmosphere*, Philos. Trans. Roy. Soc. Lond. Ser. A, 104 (1924), pp. 640–654.
[33] J. H. Seinfeld and S. N. Pandis, *Atmospheric Chemistry and Physics: From Air Pollution to Climate Change*, John Wiley & Sons, New York, 1998.
[34] G. S. Settles, *Fluid mechanics and homeland security*, Annu. Rev. Fluid Mech., 38 (2006), pp. 87–110.
[35] M. Sharan, A. K. Yadav, M. P. Singh, P. Agarwal, and S. Nigam, *A mathematical model for the dispersion of air pollutants in low wind conditions*, Atmos. Environ., 30 (1996), pp. 1209–1220.
[36] F. B. Smith, *The problem of deposition in atmospheric diffusion of particulate matter*, J. Atmospheric Sci., 19 (1962), pp. 429–435.
[37] R. J. Smith, *Dispersion of odours from ground level agricultural sources*, J. Agric. Eng. Res., 54 (1993), pp. 187–200.
[38] I. Stakgold, *Boundary Value Problems of Mathematical Physics*, Vol. II, Macmillan, New York, 1968.
[39] O. G. Sutton, *A theory of eddy diffusion in the atmosphere*, Proc. Roy. Soc. Lond. Ser. A, 135 (1932), pp. 143–165.
[40] A. B. Tayler, *Mathematical Models in Applied Mechanics*, Oxford Appl. Math. Comput. Sci. Ser., Clarendon Press, Oxford, 1986.
[41] R. Turner and T. Hurst, *Factors influencing volcanic ash dispersal from the* 1995 *and* 1996 *eruptions of Mount Ruapehu, New Zealand*, J. Appl. Meteorol., 40 (2001), pp. 56–69.
[42] U.S. Environmental Protection Agency, *Guideline on Air Quality Models*, Appendix W to Part 51, Title 40: Protection of the Environment, Code of Federal Regulations, 2010, http://ecfr.gpoaccess.gov.
[43] L. M. Wein, D. L. Craft, and E. H. Kaplan, *Emergency response to an anthrax attack*, Proc. Natl. Acad. Sci. USA, 100 (2003), pp. 4346–4351.
[44] H. F. Weinberger, *A First Course in Partial Differential Equations with Complex Variables and Transform Methods*, Blaisdell, New York, 1965.
[45] Wikipedia, *Atmospheric dispersion modeling*, http://en.wikipedia.org/wiki/Atmospheric_dispersion_modeling, 2010.
[46] Wikipedia, *Inversion (meteorology)*, http://en.wikipedia.org/wiki/Inversion_(meteorology), 2010.
[47] Y. Yang, L. T. Wilson, M. E. Makela, and M. A. Marchetti, *Accuracy of numerical methods for solving the advection-diffusion equation as applied to spore and insect dispersal*, Ecol. Model., 109 (1998), pp. 1–24.