knighting-1952 weinberger-1965 lof@mparison of measured zinc depositions with the values computed using the inverse algorithm with sources S1–S4 and receptors R5–R9.17

SOLUTIONS TO SELECTED EXERCISES FOR "THE MATHEMATICS OF ATMOSPHERIC DISPERSION MODELLING" SIAM REVIEW, 53(2):349-372, 2011

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These notes contain solutions to selected exercises from the paper. Equations that are introduced in this document are labelled as "(Ex-nn)", while all other references of the form "(nn.nn)" correspond to equations from the published paper. Helpful tables of Laplace transforms and Bessel function identities are provided at the end.

A few of the solutions are still incomplete, namely for Exercises 5 and 16. And there are a few details of the derivation in Exercise 7 that still remain to be worked out.

Exercise 1. Reformulate with a delta function source in the boundary condition.

Start by taking the steady advection-diffusion equation (2.4a) with a delta function source term

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

and integrate both sides over the interval $x \in [-d, d]$ where d > 0 to obtain

$$u\left(C(d,y,z) - C(-d,y,z)\right) = 2dK\left(\frac{\partial^2 \bar{C}_d}{\partial y^2} + \frac{\partial^2 \bar{C}_d}{\partial z^2}\right) + Q\delta(y)\delta(z-H),$$

where $\bar{C}_d(y,z) = \frac{1}{2d} \int_{-d}^d C(x,y,z) dx$ represents the average value of concentration over the interval [-d,d]and we have used the fact that $\int_{-d}^d \delta(x) dx = 1$. Consider the limit as $d \to 0^+$ in the equation above to obtain

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

making use of the assumption that C(-d, y, z) = 0. All of the other boundary conditions remain unchanged. Because we are only concerned with solving the PDE on the interval x > 0, the delta function term can be neglected and the PDE reduces to

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

as required.

Exercise 2. Nondimensionalization.

Consider the advection-diffusion equation with constant eddy diffusivity K

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

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and boundary conditions

$$\begin{split} C(0,y,z) &= \frac{Q}{u} \,\delta(y)\delta(z-H), \qquad C(\infty,y,z) = 0, \qquad C(x,\pm\infty,z) = 0, \qquad C(x,y,\infty) = 0, \\ &\quad K \frac{\partial C}{\partial z}(x,y,0) = 0. \end{split}$$

Using the change of variables

 $\widetilde{x} = (K/uH^2) x, \qquad \widetilde{y} = y/H, \qquad \widetilde{z} = z/H \qquad \text{and} \qquad \widetilde{C}(\widetilde{x}, \widetilde{y}, \widetilde{z}) = (uH^2/Q) C(x, y, z),$

derivatives transform according to

$$\frac{\partial}{\partial x} = \frac{K}{uH^2} \frac{\partial}{\partial \widetilde{x}}, \qquad \frac{\partial}{\partial y} = \frac{1}{H} \frac{\partial}{\partial \widetilde{y}}, \qquad \frac{\partial}{\partial z} = \frac{1}{H} \frac{\partial}{\partial \widetilde{z}},$$

and the partial differential equation becomes

$$\frac{\partial \widetilde{C}}{\partial \widetilde{x}} = \left(\frac{K}{uH}\right)^2 \frac{\partial^2 \widetilde{C}}{\partial \widetilde{x}^2} + \frac{\partial^2 \widetilde{C}}{\partial \widetilde{y}^2} + \frac{\partial^2 \widetilde{C}}{\partial \widetilde{z}^2}.$$
 (Ex-1)

To determine the size of the quantity multiplying the x-diffusion term, we can use typical parameter values u = 5 m/s, H = 15 m from Table 3.1, but we still require an estimate for K. Using the relationship $K = (\mu/2)\partial_x^2(\sigma^2) = (abu/2)x^{b-1}$ we find $K \approx 0.70x^{-0.14} \approx 0.37$ if we choose x = 100 m. Consequently, $(K/uH)^2 \approx 2.5 \times 10^{-5}$, which is sufficiently small that the x-diffusion term can be neglected.

Transforming the boundary conditions leads to

$$\widetilde{C}(\infty, \widetilde{y}, \widetilde{z}) = 0, \qquad \widetilde{C}(\widetilde{x}, \pm \infty, \widetilde{z}) = 0, \qquad \widetilde{C}(\widetilde{x}, \widetilde{y}, \infty) = 0, \qquad \frac{\partial C}{\partial \widetilde{z}}(\widetilde{x}, \widetilde{y}, 0) = 0, \qquad (\text{Ex-2})$$
$$\widetilde{C}(0, \widetilde{y}, \widetilde{z}) = H^2 \,\delta(H\widetilde{y}) \,\delta(H\widetilde{z} - H)$$

Applying the identity $\delta(Hx) = \delta(x)/H$ to the final boundary condition yields

$$\widetilde{C}(0,\widetilde{y},\widetilde{z}) = \delta(\widetilde{y})\,\delta(\widetilde{z}-1).$$
 (Ex-3)

Exercise 3. Derivation of Gaussian plume by separation of variables.

Start with the PDE boundary value problem

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

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

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

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

and perform the change of variables $r = \frac{1}{u} \int_0^x K(x') dx'$, under which derivatives transform according to $\partial_x = \frac{K}{u} \partial_r$. Defining c(r, y, z) = C(x, y, z) we obtain the transformed problem

$$\frac{\partial c}{\partial r} = \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2},$$

$$c(0, y, z) = (Q/u)\,\delta(y)\delta(z - H), \quad c(\infty, y, z) = 0, \quad c(r, \pm \infty, z) = 0, \quad c(r, y, \infty) = 0, \quad \frac{\partial c}{\partial z}(r, y, 0) = 0.$$

Substitute the separable solution $c(r, y, z) = \frac{Q}{u}a(r, y) b(r, z)$ into the PDE to obtain

$$a \frac{\partial b}{\partial r} + b \frac{\partial a}{\partial r} = b \frac{\partial^2 a}{\partial y^2} + a \frac{\partial^2 b}{\partial z^2}$$

Dividing by ab and collecting terms yields

$$\frac{1}{a}\left(\frac{\partial a}{\partial r} - \frac{\partial^2 a}{\partial y^2}\right) = \frac{1}{b}\left(\frac{\partial^2 b}{\partial z^2} - \frac{\partial b}{\partial r}\right).$$

Because the left hand side is a function of r and y (but not z) whereas the right hand side depends on r and z (but not y), both sides of the equation must be equal to $\lambda(r)$, an as-yet undetermined function of r; consequently,

$$\frac{\partial a}{\partial r} = \frac{\partial^2 a}{\partial y^2} + a\lambda$$
 and $\frac{\partial b}{\partial r} = \frac{\partial^2 b}{\partial z^2} - b\lambda$ (Ex-4)

We demonstrate later why it must be true that $\lambda(r) \equiv 0$, but for now we just assume that λ is constant. It is also straightforward to show that the corresponding boundary conditions separate to yield

$$a(0, y) = \delta(y) \qquad b(0, z) = \delta(z - H)$$

$$a(\infty, y) = 0 \qquad b(\infty, z) = 0$$

$$a(r, \pm \infty) = 0 \qquad b(r, \infty) = 0$$

$$\frac{\partial b}{\partial z}(r, 0) = 0$$
(Ex-5)

Notice that both problems have the same form as the familiar initial value problems for the 1D diffusion (or heat) equation where r is a "time-like" variable. The conditions at r = 0 correspond to initial values while the conditions at $r = \infty$ are redundant since any solution of the diffusion equation necessarily decays to zero as $r \to \infty$.

Why is $\lambda(r) \equiv 0$?. Consider first the case when λ is a constant. Then the solutions to Eqs. (Ex-4)–(Ex-5) can be obtained using a slightly modified version of the Laplace transform technique applied in Section 3.1 of the paper. The Laplace transform in r yields the modified equation

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

where the only difference is that the Laplace transform variable ρ is replaced by $(\rho - \lambda)$. Consequently, the solution becomes

$$\hat{a} = \frac{1}{2(\rho - \lambda)} e^{-y\sqrt{\rho - \lambda}},$$

which after applying the "frequency shift" property of the Laplace transform yields

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

In order that a(r, y) remain bounded as $y \to \pm \infty$, we require that $\lambda = 0$.

A similar argument can be applied in the case when λ is a function of r, but then the Laplace transform approach cannot be used.

Exercise 4. Cross-wind averaged concentration.

Begin with

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

and integrate over $y \in [-\infty, \infty]$. Here, we can simply make use of the following property of Gaussian-type functions

$$I = \int_{-\infty}^{\infty} e^{-y^2/4r} \, dy = 2\sqrt{\pi r},$$

to show that the cross-wind averaged concentration is given by

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

This is a nice opportunity to remind students of a neat integration trick, usually first seen in a multivariable calculus course, for determining the integral I above. It is easiest to consider the square of the integral

$$I^{2} = \left(\int_{-\infty}^{\infty} e^{-y^{2}/4r} \, dy\right)^{2} = \int_{-\infty}^{\infty} e^{-y^{2}/4r} \, dy \, \int_{-\infty}^{\infty} e^{-x^{2}/4r} \, dx,$$
$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-(x^{2}+y^{2})/4r} \, dx dy.$$

Converting to polar coordinates using $x = \rho \cos \theta$ and $y = \rho \sin \theta$, we obtain

$$I^{2} = \int_{0}^{2\pi} \int_{0}^{\infty} e^{-\rho^{2}/4r} \rho \, d\rho \, d\theta,$$

= $\int_{0}^{2\pi} d\theta \int_{0}^{\infty} e^{-\rho^{2}/4r} \rho \, d\rho,$
= $2\pi \left(-2re^{-\rho^{2}/4r} \right) \Big|_{\rho=0}^{\infty},$
= $4\pi r,$

and hence $I = 2\sqrt{\pi r}$ as required.

Exercise 5. Numerical simulations with noise.

Exercise 6. Reduction of Eq. (3.18) to the Gaussian plume solution.

Take the following expression for concentration

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

and assume that $\alpha = 0$ (constant wind velocity) and $\beta = 0$ (diffusivities are functions of x only). Then $\lambda = 2 + \alpha - \beta = 2$ and $\nu = (1 - \beta)/\lambda = 1/2$, and so the concentration becomes

$$c(r, y, z) = \frac{Q}{2u_o\sqrt{\pi r_y}} \exp\left(-\frac{y^2}{4r_y}\right) \frac{\sqrt{zH}}{2r_z} \exp\left(-\frac{(z^2 + H^2)}{4r_z}\right) I_{-1/2}\left(\frac{2zH}{4r_z}\right).$$

Applying the identity $\sqrt{2/\pi x} \cosh(x)$ to the Bessel function term yields

$$\begin{split} c(r,y,z) &= \frac{Q\sqrt{zH}}{4u_o r_z \sqrt{\pi r_y}} \exp\left(-\frac{y^2}{4r_y}\right) \exp\left(-\frac{(z^2+H^2)}{4r_z}\right) \sqrt{\frac{4r_z}{\pi zH}} \cosh\left(\frac{zH}{2r_z}\right),\\ &= \frac{Q}{2\pi u_o \sqrt{r_y r_z}} \exp\left(-\frac{y^2}{4r_y}\right) \exp\left(-\frac{(z^2+H^2)}{4r_z}\right) \cosh\left(\frac{zH}{2r_z}\right),\\ &= \frac{Q}{4\pi u_o \sqrt{r_y r_z}} \exp\left(-\frac{y^2}{4r_y}\right) \exp\left(-\frac{(z^2+H^2)}{4r_z}\right) \left[\exp\left(\frac{zH}{2r_z}\right) + \exp\left(-\frac{zH}{2r_z}\right)\right], \end{split}$$

where the final line follows from $\cosh(x) = \frac{1}{2} (e^x + e^{-x})$. The final result comes from combining the exponential terms involving z:

$$\begin{split} c(r,y,z) &= \frac{Q}{4\pi u_o \sqrt{r_y r_z}} \exp\left(-\frac{y^2}{4r_y}\right) \, \left[\exp\left(\frac{-z^2 - H^2 + 2zH}{4r_z}\right) + \exp\left(\frac{-z^2 - H^2 - 2zH}{4r_z}\right)\right],\\ &= \frac{Q}{4\pi u_o \sqrt{r_y r_z}} \, \exp\left(-\frac{y^2}{4r_y}\right) \, \left[\exp\left(\frac{-(z-H)^2}{4r_z}\right) + \exp\left(\frac{-(z+H)^2}{4r_z}\right)\right], \end{split}$$

which is identical to the formula (3.13).

Exercise 7. Derivation for height-dependent parameters.

The formula (3.18) appears in many papers that study atmospheric dispersion with height-dependent parameters (for example, [8, 5, 11, 12, 4, 6]); however, to our knowledge there is no complete derivation available for this formula in the literature. This exercise is actually more of a small project, requiring a large number of intermediate steps and fairly detailed calculations. Therefore, if this problem is to be assigned to students then it would make sense to divide it up into a number of smaller problems and provide hints at several places during the derivation.

Simplify the governing equation. Integrating Eqs. (2.5a)–(2.5d) for $y \in [-\infty, \infty]$ yields the following problem for the crosswind-averaged concentration $\bar{C}(x, z) = \int_{-\infty}^{\infty} C(x, y, z) \, dy$:

$$u(z)\frac{\partial \bar{C}}{\partial x} = \frac{\partial}{\partial z} \left(K(z)\frac{\partial \bar{C}}{\partial z} \right), \qquad (2.5a)$$

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

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

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

Take note of the following:

- The eddy diffusion coefficient depends on z and so it cannot be brought outside the z-derivative in Eq. (2.5a).
- The factor of u(H) in Eq. (2.5b) is evaluated at H and not z because the delta function term zero everywhere except at z = H.

Based on the given functional forms for $u(z) = z^{\alpha}$ and $K(z) = z^{\beta}$, we then suggest the change of independent variable $z = H\zeta^p$ so that z-derivatives transform according to

$$\frac{\partial}{\partial z} = \frac{\partial \zeta}{\partial z} \frac{\partial}{\partial \zeta} = \frac{1}{Hp} \zeta^{1-p} \frac{\partial}{\partial \zeta}.$$

Rescale the dependent variable using $\bar{C}(x, z) = QH \zeta^{\nu} C(x, \zeta)$, where the exponent ν is to be determined and the constant factor QH is chosen to simplify the form of the boundary condition (2.5b) later on.

Substituting these expressions into the PDE yields

$$H^{\alpha}\zeta^{\alpha p+\nu} \frac{\partial \mathcal{C}}{\partial x} = \frac{1}{H^2 p^2} \zeta^{1-p} \frac{\partial}{\partial \zeta} \left[\zeta^{\beta p-p+1} \frac{\partial}{\partial \zeta} \left(\zeta^{\nu} \mathcal{C} \right) \right].$$

Then

$$\begin{split} H^{2+\alpha}p^2\,\zeta^{\nu+p(1+\alpha)-1}\,\frac{\partial\mathcal{C}}{\partial x} &= \frac{\partial}{\partial\zeta}\left[\nu\zeta^{\nu+p\beta-p}\,\mathcal{C} + \zeta^{1+\nu+p\beta-p}\,\frac{\partial\mathcal{C}}{\partial\zeta}\right],\\ &= \nu(\nu+p\beta-p)\,\zeta^{\nu+p\beta-p}\,\mathcal{C} + (1+2\nu+p\beta-p)\,\zeta^{\nu+p\beta-p}\,\frac{\partial\mathcal{C}}{\partial\zeta} + \zeta^{1+\nu+p\beta-p}\,\frac{\partial^2\mathcal{C}}{\partial\zeta^2}. \end{split}$$

Dividing both sides of the equation by $\zeta^{1+\nu+p\beta-p}$, we obtain

$$H^{2+\alpha}p^{2}\zeta^{-2+p(2+\alpha-\beta)}\frac{\partial\mathcal{C}}{\partial x} = \nu(\nu+p\beta-p)\zeta^{-2}\mathcal{C} + (1+2\nu+p\beta-p)\zeta^{-1}\frac{\partial\mathcal{C}}{\partial\zeta} + \frac{\partial^{2}\mathcal{C}}{\partial\zeta^{2}},$$

which can be simplified significantly by taking $-2 + p(2 + \alpha - \beta) = 0$ and $1 + 2\nu + p\beta - p = 1$, or

$$p = \frac{2}{\lambda}$$
 and $\nu = \frac{1-\beta}{\lambda}$ where $\lambda = 2 + \alpha - \beta$.

so the PDE reduces to

$$H^{2+\alpha}p^2\frac{\partial \mathcal{C}}{\partial x} = -\frac{\nu^2}{\zeta^2}\mathcal{C} + \frac{1}{\zeta}\frac{\partial \mathcal{C}}{\partial \zeta} + \frac{\partial^2 \mathcal{C}}{\partial \zeta^2}.$$

Finally, we take the Laplace transform in x to get

$$\frac{\partial^2 \hat{\mathcal{C}}}{\partial \zeta^2} + \frac{1}{\zeta} \frac{\partial \hat{\mathcal{C}}}{\partial \zeta} - \left(H^{2+\alpha} p^2 \xi + \frac{\nu^2}{\zeta^2} \right) \hat{\mathcal{C}} = -H^{2+\alpha} p^2 \mathcal{C}(0,\zeta), \quad (\text{Ex-6})$$

where $\xi > 0$ is the Laplace transform variable.

NOTE: This last equation doesn't quite match Tayler's equation – his right-hand side is $-p \delta(\zeta - 1)$ while ours is

$$-H^{2+\alpha}p^2 \,\mathcal{C}(0,\zeta) = -\frac{H^{2+\alpha}p^2}{QH\zeta^{\nu}} \,\bar{C}(0,z) = -\frac{H^{1+\alpha}p^2}{Q\zeta^{\nu}} \,\frac{Q\,\delta(H\zeta^p - H)}{H^{\alpha}} = -p^2\,\delta(\zeta^p - 1)$$

Until this is sorted out, let's assume for the moment that the equation we are solving is Tayler's [9, p. 198] instead

$$\frac{\partial^2 \hat{\mathcal{C}}}{\partial \zeta^2} + \frac{1}{\zeta} \frac{\partial \hat{\mathcal{C}}}{\partial \zeta} - \left(\theta^2 \xi + \frac{\nu^2}{\zeta^2}\right) \hat{\mathcal{C}} = -p \,\delta(\zeta - 1), \tag{Ex-7}$$

where $\theta^2 = H^{2+\alpha} p^2$.

Derive the Laplace transform solution. The solution can be found using the *method of variation of parameters*, which proceeds as follows:

• First, determine the solution to the homogeneous equation with zero right hand side in (Ex-7). This problem has two linearly independent solutions that are given by the *modified Bessel functions of* the first and second kind, $I_{\nu}(\theta\xi^{1/2}\zeta)$ and $K_{\nu}(\theta\xi^{1/2}\zeta)$ respectively, and so the homogeneous solution can be written as

$$\hat{\mathcal{C}}_{o}(\xi,\zeta) = c_{1}I_{\nu}(\theta\xi^{1/2}\zeta) + c_{2}K_{\nu}(\theta\xi^{1/2}\zeta),$$

where c_1 and c_2 are unknown constants.

• Next, guided by the homogeneous solution, look for a solution to the non-homogeneous problem that has the form

$$\hat{\mathcal{C}}(\xi,\zeta) = A(\zeta)I_{\nu}(\theta\xi^{1/2}\zeta) + B(\zeta)K_{\nu}(\theta\xi^{1/2}\zeta).$$

• Use the fact that the Wronskian of the modified Bessel functions is $W\{I_{\nu}(x), K_{\nu}(x)\} = -x^{-1}$ to calculate the variation of parameters formulas

$$A'(\zeta) = \frac{1}{W} \det \begin{bmatrix} 0 & K_{\nu}(\theta\xi^{1/2}\zeta) \\ -p\delta(\zeta-1) & \theta\xi^{1/2}K'_{\nu}(\theta\xi^{1/2}\zeta) \end{bmatrix} = -\zeta p\delta(\zeta-1)K_{\nu}(\theta\xi^{1/2}\zeta)$$
$$B'(\zeta) = \frac{1}{W} \det \begin{bmatrix} I_{\nu}(\theta\xi^{1/2}\zeta) & 0 \\ \theta\xi^{1/2}I'_{\nu}(\theta\xi^{1/2}\zeta) & -p\delta(\zeta-1) \end{bmatrix} = \zeta p\delta(\zeta-1)I_{\nu}(\theta\xi^{1/2}\zeta)$$

These two equations can then be integrated (easily, because of the delta function terms), to obtain

$$A(\zeta) = -pK_{\nu}(\theta\xi^{1/2})\mathcal{H}(\zeta-1) + c_1 \quad \text{and} \quad B(\zeta) = pI_{\nu}(\theta\xi^{1/2})\mathcal{H}(\zeta-1) + c_2$$

where \mathcal{H} is the Heaviside function. Then the general solution is

$$\hat{\mathcal{C}}(\xi,\zeta) = c_1 I_{\nu}(\theta\xi^{1/2}\zeta) + c_2 K_{\nu}(\theta\xi^{1/2}\zeta) + p\mathcal{H}(\zeta-1) \left[-K_{\nu}(\theta\xi^{1/2})I_{\nu}(\theta\xi^{1/2}\zeta) + I_{\nu}(\theta\xi^{1/2})K_{\nu}(\theta\xi^{1/2}\zeta) \right].$$

• Finally, we determine the two constants c_1 and c_2 using the boundary conditions. The decay condition at infinity $\hat{\mathcal{C}}(\xi, \infty) = 0$ means that the coefficient of I_{ν} must be zero, since K_{ν} decays to zero at infinity but I_{ν} does not; therefore, $c_1 = pK_{\nu}(\theta\xi^{1/2})$. Consider next the no-flux condition at the ground, $\hat{\mathcal{C}}_{\zeta}(\xi, 0) = 0$ for which we require the ζ -derivative

$$\frac{\partial \mathcal{C}(\xi,\zeta)}{\partial \zeta} = p\theta\xi^{1/2}K_{\nu}(\theta\xi^{1/2})I_{\nu}'(\theta\xi^{1/2}\zeta) + c_2\theta\xi^{1/2}K_{\nu}'(\theta\xi^{1/2}\zeta),$$

where we have used the fact that $\mathcal{H}(\zeta - 1) = 0$ for ζ close to 0. Next set the derivative to zero, yielding

$$c_{2} = -pK_{\nu}(\theta\xi^{1/2}) \lim_{\zeta \to 0} \frac{I_{\nu}'(\theta\xi^{1/2}\zeta)}{K_{\nu}'(\theta\xi^{1/2}\zeta)} = pK_{\nu}(\theta\xi^{1/2}) \lim_{\zeta \to 0} \frac{I_{\nu-1}(\theta\xi^{1/2}\zeta) + I_{\nu+1}(\theta\xi^{1/2}\zeta)}{K_{\nu-1}(\theta\xi^{1/2}\zeta) + K_{\nu+1}(\theta\xi^{1/2}\zeta)},$$

and then consider the limit as $\zeta \to 0$. Using the fact that $I_{\nu}(x) \sim (x/2)^{\nu} / \Gamma(\nu+1)$ and $K_{\nu}(x) \sim \frac{1}{2}\Gamma(\nu) (x/2)^{-\nu}$, it is then easy to show that $c_2 \to 0$ as $\zeta \to 0$.

Therefore, the particular solution is

$$\hat{\mathcal{C}}(\xi,\zeta) = pK_{\nu}(\theta\xi^{1/2})I_{\nu}(\theta\xi^{1/2}\zeta)(1-\mathcal{H}(\zeta-1)) + pI_{\nu}(\theta\xi^{1/2})K_{\nu}(\theta\xi^{1/2}\zeta)\mathcal{H}(\zeta-1),$$

or alternately

$$\hat{\mathcal{C}}(\xi,\zeta) = \begin{cases} pK_{\nu}(\theta\xi^{1/2})I_{\nu}(\theta\xi^{1/2}\zeta), & \text{if } \zeta \leq 1, \\ pI_{\nu}(\theta\xi^{1/2})K_{\nu}(\theta\xi^{1/2}\zeta), & \text{if } \zeta > 1, \end{cases}$$
(Ex-8)

where $\theta = pH^{1+\alpha/2}$.

Invert the Laplace transform. A similar piecewise modified Bessel function was encountered by Carslaw & Jaeger [5, App. V(22)] while deriving the Green's function for heat flow in a cylinder, in which they made use of the following Laplace transform identity

$$\mathscr{L}\left\{\frac{1}{2t}\,e^{-(a^2+b^2)/4t}\,I_{\nu}\left(\frac{ab}{2t}\right)\right\} = \begin{cases} I_{\nu}(b\zeta^{1/2})\,K_{\nu}(a\zeta^{1/2}), & \text{if } a \ge b, \\ I_{\nu}(a\zeta^{1/2})\,K_{\nu}(b\zeta^{1/2}), & \text{if } a < b. \end{cases}$$

This can be applied directly to Eq. (Ex-8) to invert the Laplace transform, yielding

$$\mathcal{C}(x,\zeta) = \frac{p}{2x} \exp\left(-\frac{\theta^2(\zeta^2+1)}{4x}\right) I_{\nu}\left(\frac{\theta^2\zeta}{2x}\right).$$

Next, replace $p = \frac{2}{\lambda}$, $\theta^2 = p^2 H^{2+\alpha}$ and $\zeta = (z/H)^{1/p} = (z/H)^{\lambda/2}$ to obtain

$$\mathcal{C}(x,\zeta) = \frac{1}{\lambda x} \exp\left(-\frac{H^{\beta}(z^{\lambda} + H^{\lambda})}{\lambda^2 x}\right) I_{\nu}\left(\frac{2H^{\beta}(zH)^{\lambda/2}}{\lambda^2 x}\right).$$

Finally, the cross-wind averaged concentration is

$$\bar{C}(x,z) = QH \left(\frac{z}{H}\right)^{\nu/p} \mathcal{C}(x,\zeta)$$

$$= QH^{1-2\nu/p} (zH)^{\nu/p} \mathcal{C}(x,\zeta)$$

$$= \frac{QH^{\beta}(zH)^{(1-\beta)/2}}{\lambda x} \exp\left(-\frac{H^{\beta}(z^{\lambda}+H^{\lambda})}{\lambda^{2}x}\right) I_{\nu}\left(\frac{2H^{\beta}(zH)^{\lambda/2}}{\lambda^{2}x}\right).$$
(Ex-9)
(Ex-9)

This result does not match with the cross-wind averaged version of Eq. (3.18) from the paper. Using parameters $r_{y,z} = \int_0^x k_{y,z}(x')dx' \equiv x$, we obtain

$$\bar{C}(x,z) = \frac{Q(zH)^{(1-\beta)/2}}{\lambda x} \exp\left(-\frac{z^{\lambda} + H^{\lambda}}{\lambda^2 x}\right) I_{-\nu}\left(\frac{2(zH)^{\lambda/2}}{\lambda^2 x}\right).$$
(Ex-11)

NOTE 1. This is pretty close! But evidently, there remain some discrepancies to be resolved in the derivation in this exercise, namely:

- There is a discrepancy between our equation (Ex-6) and Tayler's equation (Ex-7).
- When comparing the solution we derived in (Ex-10) to that in (Ex-11) appearing in the literature, we have an extra factor of H^{β} appears wherever there is an x, the order parameter for the Bessel function is ν instead of $-\nu$.

NOTE 2. Typical values for the exponents appearing in the height dependent velocity and diffusivity functions are $\alpha \approx 0.29$ and $\beta \approx 0.45$, which corresponds to the following values for the other parameters: $\lambda = 1.84$, $\nu = 0.30$ and p = 1.09. Notice in particular that the order parameter ν is not an integer and so we cannot take advantage of any of the simplified expressions that are available for Bessel functions of integer order.

NOTE 3. When a Dirichlet boundary condition is used instead of the flux condition (2.5d), then the only change required in the solution is that $I_{-\nu}$ is replaced with I_{ν} in Eq. (Ex-11). This can be checked by simple substitution.

Exercise 8. Large-x asymptotics for the puff solution.

Begin with the Gaussian puff solution

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

and consider "summing up" all such puffs over times $t \in [0, \infty)$, which corresponds to evaluating the integral $\int_0^\infty C_{puff}(x, y, z, t) dt$. If we extract the term in C_{puff} that involves the time variable, our task reduces to that of evaluating the integral

$$I = \int_0^\infty \exp\left(-\frac{(x-ut)^2}{4r}\right) \, dt.$$

Using the change of variables $\xi = (x - ut)/2\sqrt{r}$, this reduces to

$$I = -\frac{2\sqrt{r}}{u} \int_{x/2\sqrt{r}}^{-\infty} e^{-\xi^2} d\xi,$$
$$= \frac{2\sqrt{r}}{u} \int_{-\infty}^{x/2\sqrt{r}} e^{-\xi^2} d\xi.$$

We then recognize that this integral is in the form of an *error function* $\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-\xi^2} d\xi$, which suggests splitting the domain of integration into two subintervals as follows

$$I = \frac{2\sqrt{r}}{u} \left[\int_0^{x/2\sqrt{r}} e^{-\xi^2} d\xi + \int_{-\infty}^0 e^{-\xi^2} d\xi \right],$$
$$= \frac{\sqrt{\pi r}}{u} \left[\operatorname{erf}\left(\frac{x}{2\sqrt{r}}\right) - \operatorname{erf}(-\infty) \right],$$
$$= \frac{\sqrt{\pi r}}{u} \left[\operatorname{erf}\left(\frac{x}{2\sqrt{r}}\right) + 1 \right],$$

where in the final line we have made use of the fact that $erf(\infty) = -erf(-\infty) = 1$.

It is important to realize that in integrating the Gaussian puff solution, we cannot hope to obtain exactly the same result as the Gaussian plume since the plume solution corresponds to an idealized steady-state situation in which all contaminant emitted at the origin has time to reach the boundary at infinity. However, a comparison of the puff and plume solutions is possible if we consider points sufficiently removed from the source, where we find that $I \sim 2\sqrt{\pi r}/u$ for large x. Substituting this result into the integrated concentration profile, we obtain

$$\int_0^\infty C_{puff}(x,y,z,t)\,dt \sim \frac{Q_T}{4\pi ur}\,\exp\left(-\frac{y^2}{4r}\right)\,\left[\exp\left(-\frac{(z-H)^2}{4r}\right) + \exp\left(-\frac{(z+H)^2}{4r}\right)\right],$$

which matches exactly with the plume solution (3.8).

Exercise 9. Practical application of the finite line source formula.

Take the formula for the finite line source

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

so that when z = 0 (at ground level) and y = 0 (along the centerline) the concentration reduces to

$$c(r,0,0) = \frac{Q_L}{u\sqrt{\pi r}} \operatorname{erf}\left(\frac{L}{4\sqrt{r}}\right).$$
(3.16)

Then substitute values of the remaining parameters L = 200 m, u = 2.5 m/s, $Q_L = 0.5 \times 10^{-3}$ kg/m s, and $r = 0.16x^{0.70} m^2$ to obtain the concentration in terms of downwind distance x:

$$C(x,0,0) \approx \frac{0.5 \times 10^{-3}}{x^{0.35} \sqrt{\pi}} \operatorname{erf}\left(\frac{200}{1.6 x^{0.35}}\right),$$

$$\approx 2.82 \times 10^{-4} x^{-0.35} \operatorname{erf}\left(125 x^{-0.35}\right).$$

At the two downwind locations of interest, $C(500, 0, 0) \approx 3.2 \times 10^{-5} \text{ kg/m}^3$ and $C(5000, 0, 0) \approx 1.4 \times 10^{-5} \text{ kg/m}^3$.

Next, calculate the standard plume solution in terms of r,

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

with the same parameters as above except that H = 0 m (for a ground-level source) and we have approximated the emission rate using $Q = LQ_L = 0.1$ kg/s. The concentration can then be written as a function of the downwind distance,

$$C(x,0,0) = \frac{Q}{2\pi u r} \approx 0.040 \, x^{-0.70},$$

and so $C(500, 0, 0) \approx 5.1 \times 10^{-4} \text{ kg/m}^3$ and $C(5000, 0, 0) \approx 1.0 \times 10^{-5} \text{ kg/m}^3$.

The concentration from the point source model is approximately 16 times larger than the line source at a downwind distance of 500 m, and 7 times larger at 5000 m. This result is not surprising since the line source can be expected to disperse contaminant particles over an area of much greater extent in the y-direction, and hence will leads to much lower concentrations along the plume centerline. Consequently, we conclude that the plume approximation is too inaccurate to be of much use and that the line source solution should be used in practice.

Exercise 10. Typos in Ermak's paper.

The plume solution derived by Ermak for the case of dispersion with deposition and settling is

$$\underbrace{C(x,y,z)}_{\text{kg/m}^3} = \underbrace{\frac{Q}{2\pi u \sigma_y \sigma_z}}_{\text{(m/s)} \cdot \text{m} \cdot \text{m}} = \text{kg/m}^3} \exp\left(\underbrace{-\frac{y^2}{2\sigma_y^2}}_{\frac{m^2}{\text{m} \cdot \text{m}} = 1} \exp\left(\underbrace{-\frac{w_{set} \left(z - H\right)}{2K}}_{\frac{(m/s) \cdot \text{m}}{\text{m}^2/s} = 1} - \underbrace{\frac{w_{set}^2 \sigma_z^2}{8K^2}}_{\frac{(m/s) \cdot \text{m}^2}{\text{m}^2/s^2} = 1}\right)\right) \\ \times \left[\exp\left(\underbrace{-\frac{\left(z - H\right)^2}{2\sigma_z^2}}_{\frac{m^2}{\text{m}^2} = 1}\right) + \exp\left(\underbrace{-\frac{\left(z + H\right)^2}{2\sigma_z^2}}_{\frac{m^2}{\text{m}^2} = 1}\right) - \underbrace{\frac{w_o \sigma_z \sqrt{2\pi}}{K}}_{\frac{(m/s) \cdot \text{m}}{\text{m}^2/s} = 1} \exp\left(\underbrace{\frac{w_o (z + H)^2}{K}}_{\frac{(m/s) \cdot \text{m}^2}{\text{m}^2/s} = m} - \underbrace{\frac{w_o^2 \sigma_z^2}{2K}}_{\frac{(m/s)^2 \cdot \text{m}^2}{\text{m}^2/s} = m^2/s}\right) \exp\left(\underbrace{\frac{w_o \sigma_z}{\frac{(m/s) \cdot \text{m}}{\text{m}^2/s}}_{\frac{(m/s) \cdot \text{m}}{\text{m}} = 1} + \underbrace{\frac{z + H}{\sqrt{2\sigma_z}}}_{\frac{m}{\text{m}} = 1}\right)\right],$$

where we have made the following substitutions in notation:

$$\begin{array}{c} {\rm Ermak's} & {\rm Ours} \\ U & u \\ h & H \\ W & w_{set} \\ V_1 & w_o \end{array}$$

We have calculated the corresponding units below each term in the above equation, making use of the fact that the units of the various physical quantities are as follows:

$$x, y, z, H$$
 [m], u, w_{set}, w_o [m/s], Q [kg/s], σ_y, σ_z [m], K [m²/s]

It is easy to see that all terms in the equation are dimensionally consistent except for the middle exponential term appearing in the final line; here, the quantity within the exponential must be dimensionless. Clearly,

there are two exponents incorrect in this expression and it should be replaced by

$$\exp\left(\frac{w_o(z+H)}{K} + \frac{w_o^2 \sigma_z^2}{2K^2}\right).$$

If we make the substitution $\sigma_y = \sigma_z = \sqrt{2r}$, then the corrected version of Ermak's equation becomes

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

which is exactly the expression given in Ermak's paper.

Exercise 11. Derivation of Ermak's solution with deposition.

Begin by substituting the separated solution $c(r, y, z) = \frac{Q}{u} a(r, y) b(r, z) \mathcal{E}(r, z)$ into the advection–diffusion equation with settling

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

where we have abbreviated

$$\mathcal{E}(r,z) = \exp\left[-\frac{w_{set}(z-H)}{2K} - \frac{w_{set}^2 r}{4K^2}\right].$$

Using the partial derivatives

$$\frac{\partial \mathcal{E}}{\partial r} = -\frac{w_{set}^2}{4K^2} \mathcal{E} \quad \text{and} \quad \frac{\partial \mathcal{E}}{\partial z} = -\frac{w_{set}}{2K} \mathcal{E},$$

we obtain

$$\begin{split} \left(b\frac{\partial a}{\partial r} + a\frac{\partial b}{\partial r} - ab\frac{w_{set}^2}{4K^2}\right) &- \frac{w_{set}}{K}\left(a\frac{\partial b}{\partial z} - ab\frac{w_{set}}{2K}\right) \\ &= b\frac{\partial^2 a}{\partial y^2} + \left(a\frac{\partial^2 b}{\partial z^2} + ab\frac{w_{set}^2}{4K^2} - 2a\frac{\partial b}{\partial z}\frac{w_{set}}{2K}\right), \end{split}$$

where we have cancelled a factor of \mathcal{E} from every term. A number of terms cancel leaving simply

$$b \frac{\partial a}{\partial r} + a \frac{\partial b}{\partial r} = b \frac{\partial^2 a}{\partial y^2} + a \frac{\partial^2 b}{\partial z^2},$$

which is the exact same separated equation we derived for the plume solution in Exercise 3. Hence, the PDEs governing a and b are the same as for the standard Gaussian plume solution:

$$\frac{\partial a}{\partial r} = \frac{\partial^2 a}{\partial y^2}$$
 and $\frac{\partial b}{\partial r} = \frac{\partial^2 b}{\partial z^2}$.

The source boundary condition is

$$c(0, y, z) = \frac{Q}{u} a(0, y) b(0, z) \exp\left[-\frac{w_{set}}{2K}(z - H)\right] = \frac{Q}{u} \delta(y) \delta(z - H),$$

which is only possible if

$$a(0,y) = \delta(y)$$
 and $b(0,z) = \delta(z-H)$

The boundary conditions at infinity are identical

$$a(r, \pm \infty) = 0$$
 and $b(r, \infty) = 0,$
 $a(\infty, y) = 0$ and $b(\infty, z) = 0.$

The radiation boundary condition

$$K\frac{\partial c}{\partial z}(r,0) = (w_{dep} - w_{set}) c(r,0)$$
(3.22)

becomes

$$\frac{\partial b}{\partial z}(r,0) = \gamma \, b(r,0),$$

where $\gamma = w_o/K$ and $w_o = w_{dep} - \frac{1}{2} w_{set}$. This completes the specification of the equations for a and b. The problem for a is unchanged from that for the plume solution and so we have

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

as before. The radiation boundary condition introduces a significant complication in the solution for b. Several approaches have been used to solve this problem such as [5, Sec. 14.II] and [10, p. 358-361], although we will use an approach developed by Duffy [2, Ex. 4.1.3] that generalizes in a straightforward manner the method we already applied for the standard plume solution. The problematic aspect here is the radiation condition, which can be simplified significantly using the substitution $\beta = \gamma b - \partial_z b$ or equivalently

$$b(r,z) = e^{\gamma z} \int_{z}^{\infty} \beta(r,\zeta) e^{-\gamma \zeta} d\zeta.$$
 (Ex-12)

Then the new variable β satisfies

$$\frac{\partial\beta}{\partial r} = \frac{\partial^2\beta}{\partial z^2},$$

the radiation condition $\partial_z b(r,0) = \gamma b(r,0)$ reduces to the zero Dirichlet condition $\beta(r,0) = 0$, and the boundary condition at r = 0 becomes

$$\beta(0, z) = \gamma \delta(z - H) - \delta'(z - H),$$

where the derivative δ' must be thought of in the distributional sense and represents a dipole source. The Green's function for this new problem in β is now easily found using the method of images,

$$G_{\beta}(r,z;0,\zeta) = \frac{1}{\sqrt{4\pi r}} \left[\exp\left(-\frac{(z-\zeta)^2}{4r}\right) - \exp\left(-\frac{(z+\zeta)^2}{4r}\right) \right],$$

and then the solution is given by

$$\begin{split} \beta(r,z) &= \int_0^\infty G_\beta(r,z;0,\zeta) \ \beta(0,\zeta) \ d\zeta, \\ &= \int_0^\infty G_\beta(r,z;0,\zeta) \ [\gamma \delta(\zeta - H) - \delta'(\zeta - H)] \ d\zeta, \\ &= \int_0^\infty \left[\gamma G_\beta(r,z;0,\zeta) - \frac{\partial G_\beta}{\partial \zeta}(r,z;0,\zeta) \right] \delta(\zeta - H) \ d\zeta, \end{split}$$

where in the last step we have used integration by parts to transfer the ζ -derivative onto the Green's function. Using the expression for G_{β} above, we can calculate this last integral explicitly as

$$\beta(r,z) = \frac{1}{\sqrt{4\pi r}} \left[\left(\frac{z-H}{2r} + \gamma \right) \exp\left(-\frac{(z-H)^2}{4r} \right) + \left(\frac{z+H}{2r} - \gamma \right) \exp\left(-\frac{(z+H)^2}{4r} \right) \right]$$

This expression is then substituted into Eq. (Ex-12), yielding

$$b(r,z) = \frac{e^{\gamma z}}{\sqrt{4\pi r}} \int_{z}^{\infty} \left[\left(\frac{\zeta - H}{2r} + \gamma \right) \exp\left(-\frac{(\zeta - H)^2}{4r} - \gamma \zeta \right) + \left(\frac{\zeta + H}{2r} - \gamma \right) \exp\left(-\frac{(\zeta + H)^2}{4r} - \gamma \zeta \right) \right] d\zeta.$$

Notice that the first term under the integral sign integrates exactly, while the second term can be made exact by adding and subtracting an appropriate quantity. We then obtain

$$\begin{split} b(r,z) &= \frac{e^{\gamma z}}{\sqrt{4\pi r}} \left[\exp\left(-\frac{(z-H)^2}{4r} - \gamma z\right) + \exp\left(-\frac{(z+H)^2}{4r} - \gamma z\right) \right] \\ &\quad - \frac{e^{\gamma z}}{\sqrt{\pi r}} \int_z^\infty \exp\left(\frac{-(\zeta+H)^2}{4r} - \gamma \zeta\right) d\zeta, \\ &= \frac{1}{\sqrt{4\pi r}} \left[\exp\left(-\frac{(z-H)^2}{4r}\right) + \exp\left(-\frac{(z+H)^2}{4r}\right) \right] \\ &\quad - \frac{e^{\gamma z}}{\sqrt{\pi r}} \int_z^\infty \exp\left(\frac{-(\zeta+H+2\gamma r)^2}{4r} + \gamma H + \gamma^2 r\right) d\zeta, \\ &= \frac{1}{\sqrt{4\pi r}} \left[\exp\left(-\frac{(z-H)^2}{4r}\right) + \exp\left(-\frac{(z+H)^2}{4r}\right) \right] - \gamma e^{\gamma (z+H) + \gamma^2 r} \operatorname{erfc}\left(\frac{z+H+2\gamma r}{2\sqrt{r}}\right), \end{split}$$

where in the last line we have used the definition $\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-\xi^2} d\xi$. Finally, by replacing $\gamma = w_o/K$ and substituting the expressions for a(r, y) and b(r, z) into the separable form of the solution c(r, y, z), it is straightforward to obtain the Ermak solution in Eq. (3.23) in the paper.

Exercise 12. Derive Ermak's solution when $K_y(x) \neq K_z(x)$.

We will only give an overview of the solution procedure here since the details of the derivation are so similar what we did in Exercise 11. We proceed in three main steps:

• First, replace the independent variable x with the two new variables

$$r_y(x) = \frac{1}{u} \int_0^x K_y(x') \, dx'$$
 and $r_z(x) = \frac{1}{u} \int_0^x K_z(x') \, dx'$,

while at the same time performing the substitution

$$C(x, y, z) = \frac{Q}{u} D(x, y, z) \exp\left[-\frac{w_{set}(z - H)}{2K_z} - \frac{w_{set}^2 r_z}{4K_z^2}\right],$$
 (Ex-13)

which eliminates the gravitational settling term and the constants Q and u. The resulting partial differential equation is

$$K_y \frac{\partial D}{\partial r_y} + K_z \frac{\partial D}{\partial r_z} = K_y \frac{\partial^2 D}{\partial y^2} + K_z \frac{\partial^2 D}{\partial z^2}.$$

• Next, separate variables by letting $D(x, y, z) = a(r_y, y) b(r_z, z)$ to obtain the two PDEs

$$\frac{\partial a}{\partial r_y} = \frac{\partial^2 a}{\partial y^2}$$
 and $\frac{\partial b}{\partial r_z} = \frac{\partial^2 b}{\partial z^2}$,

which are identical to what we had before except that the single parameter r is replaced by r_y and r_z . The boundary conditions for a and b remain unchanged.

• The separated solutions are obtained in exactly the same way as before, with

$$a(r_y, y) = \frac{1}{\sqrt{4\pi r_y}} e^{-y^2/4r_y}$$
 and $b(r_z, z) = \frac{1}{\sqrt{4\pi r_z}} \left[e^{-(z-H)^2/4r_z} + e^{-(z+H)^2/4r_z} \right]$

so that

$$D(x,y,z) = \frac{1}{4\pi\sqrt{r_y r_z}} \exp\left(-\frac{y^2}{4r_y}\right) \left[\exp\left(-\frac{(z-H)^2}{4r_z}\right) + \exp\left(-\frac{(z+H)^2}{4r_z}\right)\right],$$

and the concentration is given by the expression in (Ex-13).

In order to permit a direct comparison with the solution in Ermak's paper [3, Eq. (5)], we replace r_y and r_z with the standard deviation parameters $\sigma_{y,z}^2(x) = 2r_{y,z}(x)$ to obtain

$$\begin{split} C(x,y,z) &= \frac{Q}{2\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \exp\left(-\frac{w_{set}\left(z-H\right)}{2K_z} - \frac{w_{set}^2 \sigma_z^2}{8K_z^2}\right) \\ &\times \left[\exp\left(-\frac{\left(z-H\right)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{\left(z+H\right)^2}{2\sigma_z^2}\right) \\ &- \frac{\sqrt{2\pi}w_o \sigma_z}{K_z} \exp\left(\frac{w_o(z+H)}{K_z} + \frac{w_o^2 \sigma_z^2}{2K_z^2}\right) \operatorname{erfc}\left(\frac{z+H}{\sqrt{2}\sigma_z} + \frac{w_o \sigma_z}{\sqrt{2}K_z}\right)\right] \end{split}$$

It is interesting to note that this expression is identical to Eq. (3.13) when we substitute $\sigma_y = \sqrt{2r_y}$ and $\sigma_z = \sqrt{2r_z}$, and let $w_{set} = w_{dep} = w_o = 0$.

Exercise 13. Modify Matlab code for Ermak's solution.

Ermak's solution has been implemented in the following Matlab subroutines:

- setparams.m: assigns all values of the physical and numerical parameters (identical to the previous version).
- ermak.m: a modified version of the file gplume.m which requires two extra parameters, Wdep and Wsep.
- forward2.m: the main program that calculations and plots results.

The code can be found on the web page http://www.math.sfu.ca/~stockie/atmos, and sample output is provided in Fig. 1. The changes that have been required to the gplume and forward code are most easily seen by directly comparing the files. On any Unix-based operating system, this can be done using the diff command as follows:

diff -w gplume.m ermak.m

Exercise 14. Source identification (single source).

0 0

The Matlab code inverse2.m contains a modified version of the file inverse1.m that calculates the Ermak solution using the computed S1 emission rate, and then produces a bar plot that compares the measured and computed depositions. The plot is shown in Fig. 2(a), which shows that only the depositions at R6 and R7 are close to the measured values while the other estimates appear to be zero. In fact, the computed values of D_r at receptors R1–R4 are equal to zero, while those at R5, R8 and R9 are several orders of magnitude smaller than the R6 and R7 values, which is evident when printing the contents of the Matlab variable "dep":

```
dep =
1.0e-05 *
```



FIG. 1. Results from the Ermak problem in Exercise 13, with a contour plot of the ground-level zinc concentration (left) and bar plot of the deposition (right).



FIG. 2. Comparison of measured zinc depositions with the values computed using the inverse algorithm for source S1 only.

0 0.0000000000000 0.013830118629149 0.859225075474992 0.197185569631577 0.001739400324537 0.00000013382877

On closer examination, we find that dep(4) is not identically zero but rather contains the vanishingly small but still non-zero value 1.298980006683381e-214, which is exact to within round-off error.

There is clearly a major difference between the experimentally measured deposition values and those computed using our inverse algorithm. But why would the first four deposition measurements be zero? The reason for this discrepancy can be found by carefully studying the aerial photo in Fig. 4.1 showing the placement of source and receptors. If the wind is unidirectional and blows in the direction of the prevailing winds, then the Gaussian plume solution returns a value that is identically zero for any value of $x \leq 0$ (that is, for any point lying upwind of the source). And it is clear from the figure that R1, R2 and R3 lie upwind

of S1, while R4 is so close to the line x = 0 that the Gaussian plume solution is essentially zero at that point. Consequently, it is not possible for the linear least squares solver to compute a non-zero value at these four receptors.

We might then ask the question: Does the quality of the approximation improve if receptors R1–R4 are removed from the computation? This is easily checked by modifying the **rlist** variable, after which we obtain the plot in Fig. 2(b). Along with the Matlab output below:

```
dep =
    1.0e-05 *
    0.013830118629149
    0.859225075474992
    0.197185569631577
    0.001739400324537
    0.00000013382877
```

it is clear that the two computed solutions are identical to each other, within round-off error. It turns out that there are two problems with our approach:

- The deposition measurements were actually made under conditions when the wind is varying in both speed and direction, which we cannot deal with properly until Section 4.4.
- The measurements derive from all four sources S1–S4, which is addressed in the solution to the next exercise.

Exercise 15. Source identification (multiple sources).

Including the additional sources in the inversion process implemented in the code inverse2.m from the previous exercise can be done by simply modifying the variable slist to contain a list of sources. The estimated source emission rates are then given by

```
Zn emission rates (T/yr):
    S1: 155.1727
    S2: 41.5757
    S3: 82.5734
    S4: 36.0550
    ______
Total: 315.3768 T/yr
LSQLIN residual = 7.878078e-18
```

from which we observe that there is a slight reduction in the value of Q_1 to 155 T/yr (compared to the value of 169 T/yr with only S1). However, there are now also significant emissions from the other three sources which lead to a total zinc emission rate from all four sources of 315 T/yr. This value is considerably above the total emissions for the actual smelter operation reported in [7], but let's press on nonetheless and investigate the corresponding plot of the computed deposition values. After substituting the above values of Q_s into the Ermak solution, we find in Fig. 3 that (with the exception of R9) the computed depositions are now indistinguishable from the measured values; in fact,

dep =

```
1.0e-04 *
0.110000231049631
0.081999996425827
0.02900000000000
0.02200000000000
0.000002702121734
```

As in the previous question, it is not possible to obtain non-zero values at receptors R1–R4 because they are upwind of the four emissions sources.

It is now natural to ask: Why is the R9 deposition estimate so far away from the measured value? This has to do with the funny behaviour of solutions to overdetermined systems of equations – in our case, the



FIG. 3. Comparison of measured zinc depositions with the values computed using the inverse algorithm with sources S1-S4 and receptors R5-R9.

problem consists of solving 5 equations in 4 unknowns. The measured data are such that the minimumresidual solution from the linear least squares algorithm has $D_9 = 0$, and any deviation from that value generates a much larger residual. In fact, if we attempt to remove one more data point and solve the resulting 4×4 problem – which incidentally has a unique solution! – then we find the following:

- Omitting R9 yields essentially the same solution as above.
- Omitting any of the receptors R5–R8 yields non-physical solutions with negative emission rates. In other words, it is not possible to satisfy the equations if any of these other receptor measurements is left out of the least squares optimization approach.

This suggests that perhaps there is some problem (e.g., a large measurement error?) with the value of the deposition measured at R9.

Exercise 16. Inverse problem with time-varying wind.

This question is a bit more involved in terms of programming, mostly because of the rotation of coordinates, and some trickiness in ensuring that the wind angle is converted correctly ...

Appendix A. Table of Laplace transforms.

We summarize a number of Laplace transforms used in the derivation of the plume solution. Here, f(t) represents the original function, $\hat{f}(s) = \mathscr{L}_t\{f(t)\} := \int_0^\infty e^{-st} f(t) dt$ denotes its Laplace transform, and $\mathcal{H}(t)$ is the Heaviside step function. In this document, we restrict ourselves to the case where the constants appearing below $(a, b, \nu, ...)$ are *real-valued*, and any other restrictions on the constants are indicated in the respective table entry.

	f(t)	$\hat{f}(s)$
1.	$\delta(t)$	1
2.	$\sinh(at)$	$\frac{a}{s^2 - a^2}$
3.	$\cosh(at)$	$\frac{s}{s^2 - a^2}$
4.	$\frac{1}{\sqrt{\pi t}} e^{-a^2/4t}$	$\frac{1}{\sqrt{s}}e^{-a\sqrt{s}}$ $(a \ge 0)$
5.	f'(t)	$s\hat{f}(s) - \hat{f}(0)$
6.	f''(t)	$s^2\hat{f}(s) - sf(0) - f'(0)$
7.	$f(t-a) \mathcal{H}(t-a)$	$e^{-as}\hat{f}(s)$ $(a \ge 0)$
8.	$e^{at}f(t)$	$\hat{f}(s-a)$
9.	$\frac{1}{2t} e^{-(a^2+b^2)/4t} I_{\nu}\left(\frac{ab}{2t}\right)$	$I_{\nu}\left(a\sqrt{s}\right)K_{\nu}\left(b\sqrt{s}\right)$ $(b \ge a \ge 0)$

Appendix B. Bessel Function Identities.

We state next a number of identities involving the Bessel functions of the first and second kind $-J_{\nu}(z)$ and $Y_{\nu}(z)$ – as well as the modified Bessel functions of the first and second kind $-I_{\nu}(z)$ and $K_{\nu}(z)$. Here, the quantities x and ν are real, while z is complex and $i = \sqrt{-1}$ represents the imaginary unit.

$$J_{\nu}(z) = \frac{z}{2\nu} \Big[J_{\nu-1}(z) + J_{\nu+1}(z) \Big]$$
(Ex-14)

$$Y_{\nu}(z) = \frac{z}{2\nu} \Big[Y_{\nu-1}(z) + Y_{\nu+1}(z) \Big]$$
(Ex-15)

$$I_{\nu}(x) = i^{-\nu} J_{\nu}(ix)$$
 (Ex-16)

$$K_{\nu}(x) = \frac{\pi}{2\sin(\nu\pi)} \left[I_{-\nu}(x) - I_{\nu}(x) \right]$$
(Ex-17)

Derivatives of Bessel functions:

$$J_{\nu}'(z) = J_{\nu-1}(z) - \frac{\nu}{z} J_{\nu}(z)$$
(Ex-18)

$$= -J_{\nu+1}(z) + \frac{\nu}{z} J_{\nu}(z)$$
 (Ex-19)

$$= \frac{1}{2} \Big[J_{\nu-1}(z) - J_{\nu+1}(z) \Big]$$
(Ex-20)

$$I'_{\nu}(x) = \frac{1}{2} \Big[I_{\nu-1}(x) + I_{\nu+1}(x) \Big]$$
(Ex-21)

$$= I_{\nu-1}(x) - \frac{\nu}{x} I_{\nu}(x)$$
 (Ex-22)

$$= I_{\nu+1}(x) + \frac{\nu}{x} I_{\nu}(x)$$
 (Ex-23)

$$K'_{\nu}(x) = -\frac{1}{2} \Big[K_{\nu-1}(x) + K_{\nu+1}(x) \Big]$$
(Ex-24)

$$= -K_{\nu-1}(x) - \frac{\nu}{x} K_{\nu}(x)$$
 (Ex-25)

$$= -K_{\nu+1}(x) + \frac{\nu}{x} K_{\nu}(x)$$
 (Ex-26)

Wronskian:

$$W\{I_{\nu}(x), K_{\nu}(x)\} = \det \begin{bmatrix} I_{\nu}(x) & K_{\nu}(x) \\ I'_{\nu}(x) & K'_{\nu}(x) \end{bmatrix} = -I_{\nu}(x)K_{\nu+1}(x) - I_{\nu+1}(x)K_{\nu}(x) = -\frac{1}{x}$$
(Ex-27)

Asymptotic behaviour as $x \to 0$:

$$I_{\nu}(x) \sim \frac{\left(\frac{x}{2}\right)^{\nu}}{\Gamma(\nu+1)}$$
 $(\nu \neq -1, -2, ...)$ (Ex-28)

$$K_{\nu}(x) \sim \frac{1}{2} \Gamma(\nu) \left(\frac{x}{2}\right)^{-\nu} \qquad (Re(\nu) > 0)$$
 (Ex-29)

$$\frac{\left(\frac{x}{2}\right)^{\nu}}{\Gamma(\nu+1)} \qquad (\nu \neq -1, -2, \dots)$$

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