B. Solutions to the Advective Reacting Diffusion Equation

This appendix presents solutions to the advective reacting diffusion equation given by

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = E_x\frac{\partial^2 C}{\partial x^2} + E_y\frac{\partial^2 C}{\partial y^2} + E_z\frac{\partial^2 C}{\partial z^2} - kC \tag{B.1}$$

for homogeneous, anisotropic turbulence with the steady velocity $\boldsymbol{u} = (u, v, w)$. The E_i's are the anisotropic turbulent diffusion coefficients, and k is a constant first-order decay rate. In previous chapters we denoted the turbulent diffusion coefficient by D_t. We use $D_t = E$ here so that the subscripts do not get too complicate and to expose the reader to another notation for the turbulent diffusion coefficient common in the literature.

B.1 Instantaneous point source

An instantaneous point source has an injection of mass, M, at the point $\boldsymbol{x} = (x_1, y_1, z_1)$ at time $t = 0$. The following solutions cover different ambient conditions.

B.1.1 Steady, uni-directional velocity field

For a steady velocity field $\boldsymbol{u} = (U, 0, 0)$, the solutions is

$$\begin{aligned} C(x,y,z,t) = \frac{M}{4\pi t\sqrt{4\pi E_x E_y E_z t}} \exp\Bigg(&-\frac{((x-x_1)-Ut)^2}{4E_x t} \\ &- \frac{(y-y_1)^2}{4E_y t} - \frac{(z-z_1)^2}{4E_z t} - kt\Bigg). \end{aligned} \tag{B.2}$$

B.1.2 Fluid at rest with isotropic diffusion

For isotropic diffusion, $E_x = E_y = E_z = E$, and, in a stagnant ambient without decay, (B.2) simplifies to

$$C(x,y,z,t) = \frac{M}{(4\pi E t)^{3/2}} \exp\left(-\frac{r^2}{4Et}\right) \tag{B.3}$$

where $r = \sqrt{x^2 + y^2 + z^2}$ and $x_1 = y_1 = z_1 = 0$.

B.1.3 No-flux boundary at $z = 0$

The no-flux boundary condition at $z = 0$ is enforced by an image source at $\boldsymbol{x} = (x_1, y_1, -z_1)$, giving the solution for $z > 0$ neglecting decay and crossflow as

$$\begin{aligned} C(x,y,z,t) = & \frac{M}{4\pi t\sqrt{4\pi E_x E_y E_z t}} \cdot \\ & \exp\left(-\frac{(x-x_1)^2}{4E_x t} - \frac{(y-y_1)^2}{4E_y t} - \frac{(z-z_1)^2}{4E_z t}\right) \\ + & \frac{M}{4\pi t\sqrt{4\pi E_x E_y E_z t}} \cdot \\ & \exp\left(-\frac{(x-x_1)^2}{4E_x t} - \frac{(y-y_1)^2}{4E_y t} - \frac{(z+z_1)^2}{4E_z t}\right). \end{aligned} \tag{B.4}$$

B.1.4 Steady shear flow

The following solution, presented in Okubo & Karweit (1969), is for the special shear flow given by $\boldsymbol{u} = (u_0(t) + \lambda_y y + \lambda_z z, 0, 0)$, where λ_y and λ_z are the velocity gradients defined by

$$\lambda_y = \frac{\partial u}{\partial y} \tag{B.5}$$

$$\lambda_z = \frac{\partial u}{\partial z}. \tag{B.6}$$

The solution is

$$\begin{aligned} C(x,y,z,t) = & \frac{M}{4\pi t\sqrt{4\pi E_x E_y E_z t}\sqrt{1+\phi^2 t^2}} \cdot \\ & \exp\left(-\frac{\left(x - \int_0^t u_0(t')dt' - \frac{1}{2}(\lambda_y y + \lambda_z z)t\right)^2}{4E_x t(1+\phi^2 t^2)}\right. \\ & \left. -\frac{y^2}{4E_y t} - \frac{z^2}{4E_z t} - kt\right), \end{aligned} \tag{B.7}$$

where the injection is at $(0, 0, 0)$ and ϕ^2 is given by

$$\phi^2 = \frac{1}{12}\left(\lambda_y^2 \frac{E_y}{E_x} + \lambda_z^2 \frac{E_z}{E_x}\right). \tag{B.8}$$

B.2 Instantaneous line source

An instantaneous line source has an injection of mass, m', per unit length along the line through $\boldsymbol{x} = (x_1, y_1)$ for $z = \pm\infty$ at time $t = 0$. The following solutions cover different ambient conditions.

B.2.1 Steady, uni-directional velocity field

For a steady velocity field $\boldsymbol{u} = (U, 0, 0)$, the solutions is

$$C(x,y,z,t) = \frac{m'}{4\pi t\sqrt{E_x E_y}} \cdot \exp\left(-\frac{((x-x_1)-Ut)^2}{4E_x t} - \frac{(y-y_1)^2}{4E_y t} - kt\right). \tag{B.9}$$

B.2.2 Truncated line source

For the line source along the line $\boldsymbol{x} = (0, 0)$ for $z = \pm z_2$, the solution is

$$C(x,y,z,t) = \frac{m'}{8\pi t\sqrt{E_x E_y}} \left(\mathrm{erf}\left(\frac{z+z_2}{\sqrt{4E_z t}}\right) - \mathrm{erf}\left(\frac{z-z_2}{\sqrt{4E_z t}}\right)\right) \cdot \exp\left(-\frac{(x-Ut)^2}{4E_x t} - \frac{y^2}{4E_y t} - kt\right). \tag{B.10}$$

B.3 Instantaneous plane source

An instantaneous plane source has an injection of mass, m'', per unit area distributed uniformly on the y-z plane passing through x_1. The solution for the uni-directional velocity field given by $\boldsymbol{u} = (U, 0, 0)$ is

$$C(x,y,z,t) = \frac{m''}{\sqrt{4\pi E_x t}} \exp\left(-\frac{((x-x_1)-Ut)^2}{4E_x t} - kt\right). \tag{B.11}$$

B.4 Continuous point source

The solution for a *continuous* point source is obtained by the time-integration of the solution for an *instantaneous* point source. The injection duration is t_1, and the general form of the solution is

$$C(x,y,z,t) = \gamma \int_0^{t_1} \frac{1}{(t-\tau)^{3/2}} \exp\left(-\frac{\alpha}{(t-\tau)} - \beta(t-\tau)\right) d\tau \tag{B.12}$$

where

$$\alpha = \frac{(x-x_1)^2}{4E_x} + \frac{(y-y_1)^2}{4E_y} + \frac{(z-z_1)^2}{4E_z} \tag{B.13}$$

$$\beta = \frac{U^2}{4E_x} + k \tag{B.14}$$

$$\gamma = \frac{\dot{m}\exp\left(\frac{(x-x_1)U}{2E_x}\right)}{4\pi\sqrt{4\pi E_x E_y E_z}} \tag{B.15}$$

and $\dot{m}$ is the time rate of mass injection $\partial M/\partial t$.

B.4.1 Times after injection stops

Assuming an injection period from $t = 0$ to $t = t_1$, the solution for times greater than t_1 (i.e. after injection stops) is

$$C(x,y,z,t) = \frac{\gamma\sqrt{\pi}}{2\sqrt{\alpha}}\left\{\exp(2\sqrt{\alpha\beta})\left(\operatorname{erf}\left(\sqrt{\frac{\alpha}{(t-t_1)}}+\sqrt{\beta(t-t_1)}\right)\right.\right.$$
$$\left.-\operatorname{erf}\left(\sqrt{\frac{\alpha}{t}}+\sqrt{\beta t}\right)\right)$$
$$+\exp(-2\sqrt{\alpha\beta})\left(\operatorname{erf}\left(\sqrt{\frac{\alpha}{(t-t_1)}}-\sqrt{\beta(t-t_1)}\right)\right.$$
$$\left.\left.-\operatorname{erf}\left(\sqrt{\frac{\alpha}{t}}-\sqrt{\beta t}\right)\right)\right\} \tag{B.16}$$

B.4.2 Continuous injection

A continuous injection in an injection from time $t = 0$ to the current time t, and the solution is

$$C(x,y,z,t) = \frac{\gamma\sqrt{\pi}}{2\sqrt{\alpha}}\left\{\exp(2\sqrt{\alpha\beta})\operatorname{erfc}\left(\sqrt{\frac{\alpha}{t}}+\sqrt{\beta t}\right)+\right.$$
$$\left.\exp(-2\sqrt{\alpha\beta})\operatorname{erfc}\left(\sqrt{\frac{\alpha}{t}}-\sqrt{\beta t}\right)\right\}. \tag{B.17}$$

The steady-state solution is found for $t \to \infty$ to be

$$C(x,y,z) = \frac{\gamma\sqrt{\pi}}{\sqrt{\alpha}}\exp(-2\sqrt{\alpha\beta}). \tag{B.18}$$

For the special case of a homogeneous, isotropic diffusion at steady state, we have

$$C(x,y,z) = \frac{\dot{m}}{4\pi E r}\exp\left(-\frac{r\sqrt{U^2+4Ek}-xU}{2E}\right) \tag{B.19}$$

where $r = \sqrt{x^2+y^2+z^2}$.

B.4.3 Continuous point source neglecting longitudinal diffusion

The steady-state solution for homogeneous turbulence and neglecting longitudinal diffusion is found from the governing equation

$$U\frac{\partial C}{\partial x} = E_y\frac{\partial^2 C}{\partial y^2}+E_z\frac{\partial^2 C}{\partial z^2}-kC. \tag{B.20}$$

For an infinite domain, the solution is

$$C(x,y,z) = \frac{\dot{m}}{4\pi x\sqrt{E_y E_z}}\exp\left(-\frac{y^2U}{4xE_y}-\frac{z^2U}{4xE_z}-\frac{kx}{U}\right). \tag{B.21}$$

B.4.4 Continuous point source in uniform flow with anisotropic, non-homogeneous turbulence

Here, we treat a special type of non-homogeneous turbulence, where the turbulent diffusion coefficients are functions of x, only, and where we will neglect longitudinal diffusion. The governing equation at steady state is

$$U\frac{\partial C}{\partial x} = E_y(x)\frac{\partial^2 C}{\partial y^2} + E_z(x)\frac{\partial^2 C}{\partial z^2}. \tag{B.22}$$

where the diffusivities are taken from Walters (1962) as

$$E_y = a_y x^\alpha \tag{B.23}$$

$$E_z = a_z x^\beta. \tag{B.24}$$

The solution for this special case is

$$C(x,y,z) = \frac{\dot{m}}{2\pi}\sqrt{\frac{(1+\alpha)(1+\beta)}{a_y a_z}}\,x^{-\left(1+\frac{\alpha+\beta}{2}\right)} \cdot \exp\left(-\frac{(1+\alpha)U}{4x^{1+\alpha}}\frac{y^2}{a_y} - \frac{(1+\beta)U}{4x^{1+\beta}}\frac{z^2}{a_z}\right). \tag{B.25}$$

B.4.5 Continuous point source in shear flow with non-homogeneous, isotropic turbulence

Smith (1957) investigated the specific case of a shear flow of the from

$$u(z) = a_0 z^\mu \tag{B.26}$$

where a_0 is a constant and $\mu = 1/2$. For this case the turbulent diffusion coefficient can be taken as

$$E_z(z) = b_0 z^{1-\mu} \tag{B.27}$$

where b_0 is another constant. The governing equation at steady state is

$$u(z)\frac{\partial C}{\partial x} = E_z(z)\frac{\partial^2 C}{\partial y^2} + \frac{\partial}{\partial z}\left(E_z(z)\frac{\partial C}{\partial z}\right), \tag{B.28}$$

and the solution is found to be

$$C(x,y,z) = \frac{\dot{m}a_0^{1/4}}{2(b_0 x)^{5/4}\sqrt{3\pi}}\exp\left(-\frac{a_0(y^2+z^2)}{4b_0 x}\right). \tag{B.29}$$

B.5 Continuous line source

The solution for a continuous line-source injection is obtained by integrating the solution of an instantaneous line-source (B.9). Taking the line source along the z-axis and assuming a uniform crossflow in the x-direction, the solution is derived by integrating

$$C(x,y,t) = \int_0^t \frac{\dot{m}'}{4\pi(t-\tau)\sqrt{E_x E_y}} \cdot \exp\left(-\frac{(x-U(t-\tau))^2}{4E_x(t-\tau)} - \frac{y^2}{4E_y(t-\tau)} - k(t-\tau)\right) d\tau \quad \text{(B.30)}$$

where $\dot{m}'$ is the time rate of mass injection per unit length.

B.5.1 Steady state solution

The solution to (B.30) for $t \to \infty$ is given by

$$C(x,y) = \frac{\dot{m}'}{2\pi\sqrt{E_x E_y}} \exp\left(\frac{Ux}{2E_x}\right) K_0(2\beta_2) \quad \text{(B.31)}$$

where K_0 is the modified Bessel function of second kind of order zero and

$$\beta_2 = \frac{\sqrt{(E_y x^2 + E_x y^2)(U^2 E_y + 4E_x E_y k)}}{4E_x E_y}. \quad \text{(B.32)}$$

B.5.2 Continuous line source neglecting longitudinal diffusion

For the special case where we can neglect longitudinal diffusion, E_x, the solution becomes

$$C(x,y) = \frac{\dot{m}'}{\sqrt{4\pi x U E_y}} \exp\left(-\frac{Uy^2}{4E_y x} - \frac{kx}{U}\right). \quad \text{(B.33)}$$

B.6 Continuous plane source

The time integral solution for a continuous infinite (in the y- and z-directions) plane source is given by integrating the solution for an instantaneous plane, namely:

$$C(x,t) = \int_0^{t_1} \frac{\dot{m}''}{\sqrt{4\pi E_x(t-\tau)}} \cdot \exp\left(-\frac{(x-U(t-\tau))^2}{4E_x(t-\tau)} - k(t-\tau)\right) d\tau, \quad \text{(B.34)}$$

where $\dot{m}''$ is the time rate of mass injection per unit area.

B.6.1 Times after injection stops

Assuming an injection period from $t = 0$ to $t = t_1$, the solution for times greater than t_1 is

$$C(x,t) = \frac{\dot{m}'' e^{Ux/(2E_x)}}{2\Omega} \left(\exp\left(\frac{x\Omega}{2E_x}\right) \left\{ \mathrm{erf}\left(\frac{x+\Omega t}{\sqrt{4E_x t}}\right) - \mathrm{erf}\left(\frac{x+\Omega(t-t_1)}{\sqrt{4E_x(t-t_1)}}\right) \right\} - \exp\left(\frac{-x\Omega}{2E_x}\right) \cdot \left\{ \mathrm{erf}\left(\frac{x-\Omega t}{\sqrt{4E_x t}}\right) - \mathrm{erf}\left(\frac{x-\Omega(t-t_1)}{\sqrt{4E_x(t-t_1)}}\right) \right\} \right), \tag{B.35}$$

where $\Omega = \sqrt{U^2 + 4kE_x}$.

B.6.2 Continuous injection

For an injection from time $t = 0$ to the current time t, the solution is

$$C(x,t) = \frac{\dot{m}'' e^{Ux/(2E_x)}}{2\Omega} \left(\exp\left(\frac{x\Omega}{2E_x}\right) \left\{ \mathrm{erf}\left(\frac{x+\Omega t}{\sqrt{4E_x t}}\right) \mp 1 \right\} - \exp\left(\frac{-x\Omega}{2E_x}\right) \left\{ \mathrm{erf}\left(\frac{x-\Omega t}{\sqrt{4E_x t}}\right) \mp 1 \right\} \right). \tag{B.36}$$

For the location $x = 0$, the solution simplifies to

$$C(0,t) = \frac{\dot{m}''}{\Omega} \mathrm{erf}\left(\frac{\Omega t}{\sqrt{4E_x t}}\right). \tag{B.37}$$

For the limiting case where the system reaches steady state ($t \to \infty$), the solution becomes

$$C(x) = \frac{\dot{m}''}{\Omega} \exp\left(\frac{x}{2E_x}(U \mp \Omega)\right). \tag{B.38}$$

B.6.3 Continuous plane source neglecting longitudinal diffusion in downstream section

If we neglect longitudinal diffusion (diffusion in the flow direction) downstream of the injection plane, then the solution at steady state for $x > 0$ simplifies to

$$C(x) = \frac{\dot{m}''}{U} \exp\left(-\frac{kx}{U}\right). \tag{B.39}$$

B.6.4 Continuous plane source neglecting decay in upstream section

If we neglect decay upstream of the injection plane, then the solution at steady state for $x < 0$ simplifies to

$$C(x) = \frac{\dot{m}''}{U} \exp\left(\frac{Ux}{E_x}\right). \tag{B.40}$$

B.7 Continuous plane source of limited extent

B.7.1 Semi-infinite continuous plane source

For a source over the region $-\infty < y < 0$, $-\infty < z < \infty$, the governing differential equation for steady state is

$$U\frac{\partial C}{\partial x} = E_y \frac{\partial^2 C}{\partial y^2} - kC, \tag{B.41}$$

and the solution is

$$C(x, y) = \frac{\dot{m}'' e^{kx/U}}{2U} \operatorname{erfc}\left(\frac{y}{2}\sqrt{\frac{U}{E_y x}}\right). \tag{B.42}$$

B.7.2 Rectangular continuous plane source

For a continuous plane source over the domain $-b/2 < y < b/2$, $-\infty < z < \infty$, Brooks (1960) gives the steady-state solution for a series of cases.

Homogeneous turbulence. For homogeneous turbulence (E_y = constant), the solution is

$$\frac{C(x, y)}{C_0} = \frac{e^{kx/U}}{2}\left(\operatorname{erf}\left(\frac{y + b/2}{2}\sqrt{\frac{U}{E_y x}}\right) - \operatorname{erf}\left(\frac{y - b/2}{2}\sqrt{\frac{U}{E_y x}}\right)\right), \tag{B.43}$$

where C_0 is the concentration at the source. The solution for $y = 0$ simplifies to

$$\frac{C(x, 0)}{C_0} = e^{kx/U} \operatorname{erf}\left(\frac{b}{4}\sqrt{\frac{U}{E_y x}}\right). \tag{B.44}$$

The relationship for the plume width, defined by $L(x) = 2\sqrt{3}\sigma_y(x)$ is given by

$$\frac{L}{b} = \sqrt{1 + \frac{24 E_y x}{U b^2}}. \tag{B.45}$$

Non-homogeneous turbulence. For non-homogeneous turbulence of the form $E_y = E_{y0}(L/b)$, the center-line solution and plume width are given by

$$\frac{C(x, 0)}{C_0} = e^{kx/U} \operatorname{erf}\sqrt{\frac{3/2}{\left(1 + \frac{12 E_{y0} x}{U b^2}\right)^2 - 1}} \tag{B.46}$$

and

$$\frac{L}{b} = 1 + \frac{12 E_{y0} x}{U b^2}, \tag{B.47}$$

respectively.

For non-homogeneous turbulence of the form $E_y = E_{y0}(L/b)^{4/3}$ (the so-called 4/3-power law), the center-line solution and plume width are given by

$$\frac{C(x, 0)}{C_0} = e^{kx/U} \operatorname{erf}\sqrt{\frac{3/2}{\left(1 + \frac{8 E_{y0} x}{U b^2}\right)^3 - 1}} \tag{B.48}$$

and

$$\frac{L}{b} = \left(1 + \frac{8E_{y0}x}{Ub^2}\right)^{3/2}, \tag{B.49}$$

respectively.

B.8 Instantaneous volume source

For the one-dimensional case of an instantaneous injection of mass M over the range $L_1 < x < L_2$, producing the initial concentration C_i given by

$$C_i = \frac{M}{A(L_2 - L_1)}, \tag{B.50}$$

where A is a cross-sectional area perpendicular to the x-axis, the solution is

$$\frac{C(x,t)}{C_i} = \frac{e^{-kt}}{2}\left(\mathrm{erf}\left(\frac{(x - L_1) - Ut}{\sqrt{4E_x t}}\right) - \mathrm{erf}\left(\frac{(x - L_2) - Ut}{\sqrt{4E_x t}}\right)\right). \tag{B.51}$$

For the special case of $L_1 = -\infty$ and $L_2 = 0$, the solution is

$$\frac{C(x,t)}{C_i} = \frac{1}{2}\left(1 - \mathrm{erf}\left(\frac{x - Ut}{\sqrt{4E_x t}}\right)\right). \tag{B.52}$$