A. Point-source Diffusion in an Infinite Domain: Boundary and Initial Conditions

In this appendix we discuss how the boundary and initial conditions for a point source in an infinite, one-dimensional domain are applied to find the solution of the diffusion equation. The governing equation is

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \tag{A.1}$$

with boundary conditions $C(\pm\infty, t) = 0$ and initial condition $C(x, 0) = (M/A)\delta(x)$ (for more detail, refer to Chapter 1).

In this case we will use the Fourier exponential transform instead of the similary method to obtain our result. Although each method is equally valid, it is easier to see how the boundary conditions are applied using the Fourier transform. Since the governing equations that is obtained after applying the boundary conditions will be the same using either method, applying the Fourier transform method here is the better approach. For this method we use the Fourier exponential transformation defined by

$$\mathcal{F}(\alpha, t) = \int_{-\infty}^{\infty} F(x, t)e^{-i\alpha x}dx \tag{A.2}$$

where $\mathcal{F}(\alpha, t)$ is the Fourier transformation of $F(x, t)$, α is a transformation variable, and i is the imaginary number. This method implicitly satisfies the boundary conditions at $\pm\infty$. This is called a behavioral boundary condition (see e.g. Boyd 1989), and it is not necessary to apply the boundary to fix the values of integration constants—the solution implicitely obeys the boundary conditions because of our use of the Fourier transform. The following application of this method to the diffusion equation is taken from Mei (1997).

The Fourier transform of the governing diffusion equation gives

$$\frac{d\mathcal{C}}{dt} + D\alpha^2\mathcal{C} = 0. \tag{A.3}$$

The power of the Fourier transform is that it converts partial differential equations into ordinary differential equations, this time a simple, first-order ODE with solution

$$\mathcal{C}(\alpha, t) = \mathcal{F}(\alpha)\exp(-D\alpha^2 t). \tag{A.4}$$

$\mathcal{F}(\alpha)$ is found by applying the initial condition. Applying the Fourier transform to the initial condition gives

$$\begin{aligned}\mathcal{F}(\alpha) &= \mathcal{C}(\alpha, 0)\\ &= \int_{-\infty}^{\infty}(M/A)\delta(x)e^{-i\alpha x}dx\end{aligned}$$

$$= M/A. \tag{A.5}$$

The drawback of the Fourier transform method is that the inverse transform to get back to our desired dimensional space is sometimes a difficult integral.

We stop here to take a look at what we have done so far. The Fourier transform method implicitly satisfies the boundary conditions; therefore, we do not have to think about them anymore. Further, the initial condition was used to find the solution to the ODE obtained after the Fourier transform. Thus, our solution

$$\mathcal{C}(\alpha, t) = (M/A)\exp(-D\alpha^2 t) \tag{A.6}$$

satisfies all our boundary and initial conditions. The remaining task is to perform a Fourier inverse transform on this solution.

The Fourier inverse transform is defined in general as

$$F(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathcal{F}(\alpha,t)e^{i\alpha x}d\alpha. \tag{A.7}$$

For our problem, the inverse transform becomes

$$C(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} (M/A)\exp(-D\alpha^2 t)e^{i\alpha x}d\alpha. \tag{A.8}$$

We can simplify a little by recognizing that $e^{i\alpha x} = \cos(\alpha x) + i\sin(\alpha x)$. Since $e^{-D\alpha^2 t}$ is an even function and $i\sin(\alpha x)$ is an odd function, we can neglect the sin-contribution, leaving us with the integral

$$C(x,t) = \frac{M}{2\pi A}\left(2\int_0^{\infty} e^{-D\alpha^2 t}\cos(\alpha x)d\alpha\right) \tag{A.9}$$

which we still must solve.

The first step in solving (A.9) is to simplify the exponential using the change of variable

$$\alpha = \frac{x}{\sqrt{Dt}} \tag{A.10}$$

$$d\alpha = \frac{dx}{\sqrt{Dt}} \tag{A.11}$$

(note, this in an arbitrary change of variable that puts the integral in a form more likely to be found in integral tables). Further, we define a new variable

$$\eta = \frac{x}{\sqrt{Dt}} \tag{A.12}$$

(note, this is also an arbitrary decision). Substituting these definitions leaves us with

$$C(x,t) = \frac{M}{\pi A\sqrt{Dt}}\int_0^{\infty} e^{-x^2}\cos(\eta x)dx. \tag{A.13}$$

Thus, our solution simplifies to having to solve the integral

$$I(\eta) = \int_0^{\infty} e^{-x^2}\cos(\eta x)dx. \tag{A.14}$$

The integral in (A.14) is not a trivial integral, but can be solved by employing the following tricks. Basically, we need to find the derivative of I with respect to η and then put it in a useful form. We begin with

$$\frac{dI}{d\eta} = \int_0^\infty -xe^{-x^2}\sin(\eta x)dx. \tag{A.15}$$

Next, recognize that $xdx = (1/2)d(x^2)$, giving

$$\frac{dI}{d\eta} = -\frac{1}{2}\int_0^\infty e^{-x^2}\sin(\eta x)d(x^2). \tag{A.16}$$

Similarly, we make use of the identity $e^{-x^2}d(x^2) = -d(e^{-x^2})$, which lets us write

$$\frac{dI}{d\eta} = \frac{1}{2}\int_0^\infty \sin(\eta x)d(e^{-x^2}). \tag{A.17}$$

Now, we integrate by parts (where $u = \sin(\eta x)$ and $dv = d(e^{-x^2})$) yielding

$$\begin{aligned}\frac{dI}{d\eta} &= \frac{1}{2}(e^{-x^2}\sin(\eta x))\Big|_0^\infty - \frac{1}{2}\int_0^\infty e^{-x^2}d(\sin(\eta x))\\ &= 0 - \frac{\eta}{2}\int_0^\infty e^{-x^2}\cos(\eta x)dx\\ &= -\frac{\eta}{2}I(\eta).\end{aligned} \tag{A.18}$$

We can rearrange the last line as follows

$$\frac{dI}{d\eta} + \frac{\eta}{2}I(\eta) = 0 \tag{A.19}$$

which looks remarkably like (1.49) if C_0 is taken as zero. The initial condition necessary to solve the above ODE is given by

$$I(0) = \int_0^\infty e^{-x^2}dx. \tag{A.20}$$

If we convert I in the previous two equations to our variables used in the similarity solution, we obtain

$$\frac{df}{d\eta} + \frac{\eta}{2}f(\eta) = 0 \tag{A.21}$$

with initial condition

$$\int_{-\infty}^\infty f(\eta)d\eta = 1. \tag{A.22}$$

Therefore, we have shown through a rigorous application of the Fourier transform method, that the above two equations give the solution to the diffusion equation that we seek in an infinite domain for an instantaneous point source *after* having applied the appropriate boundary and initial conditions.