Radial Diffusion From a Point Source

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1. Introduction

This is a solution to the transient diffusion problem with a point source. Assume a binary diffusion system in which a species A diffuses in a stagnant species B. Assume no chemical reactions occur within the mass transfer zone. Transient 1-D diffusion in the $x-$direction is governed by the following partial differential equation [1]

$$\frac{\partial C_A}{\partial t} = D_{AB}\left(\frac{\partial^2 C_A}{\partial x^2}\right), \quad -\infty < x < \infty, \quad C_A(x,0) = M\delta(x) \tag{1}$$

where x has an infinite domain and the initial condition is described by the Dirac delta function $\delta(x)$ modeling the point source. Here M is an amount (e.g. mol, gram, etc.).

2. Fourier Transform Solution

Since the system has an impulsive/localized initial condition and an infinite boundary, Fourier transforms can be used.

Initial condition: $C_A(x,0) = M\delta(x)$
Boundary conditions: $C_A(\infty,t) = 0$ and no flux at the origin

Fourier transforms and transformed equations [1] give

$$\begin{aligned}
&\hat{C_A}(k,t) = \int_{-\infty}^{\infty} C_A(x,t)e^{-ikx}dx \\
&\frac{\partial C_A}{\partial t} = \frac{\partial \hat{C_A}}{\partial t} \\
&\frac{\partial^2 C_A}{\partial x^2} = (ik)^2\hat{C_A} = -k^2\hat{C_A}
\end{aligned}$$

Plugging into equation (1),

$$\frac{\partial C_A}{\partial t} = D_{AB}\left(\frac{\partial^2 C_A}{\partial x^2}\right) \implies \frac{\partial \hat{C_A}}{\partial t} = -D_{AB}k^2\hat{C_A}$$

Solving the differential equation above using separation of variables,

$$\int_{\hat{C_A}(k,0)}^{\hat{C_A}(k,t)} \frac{\partial \hat{C_A}}{\cancel{\partial t}} \frac{1}{\hat{C_A}} \cancel{dt} = \int_0^t -D_{AB}k^2 dt \implies \ln\left(\frac{\hat{C_A}(k,t)}{\hat{C_A}(k,0)}\right) = -D_{AB}k^2 t \implies$$

$$\hat{C_A}(k,t) = \hat{C_A}(k,0)e^{\left(-D_{AB}k^2 t\right)}$$

From the initial condition

$$\hat{C_A}(k,0) = \int_{-\infty}^{\infty} M\delta(x)e^{-ikx}dx$$

By definition, $\int_{-\infty}^{\infty} \delta(x)f(x)\,dx = f(0)$. Here $f(x) = e^{-ikx} \implies \int_{-\infty}^{\infty} \delta(x)e^{-ikx}\,dx = e^0 \implies \hat{C_A}(k,0) = M \implies \hat{C_A}(k,t) = Me^{-D_{AB}k^2 t}$

From the Fourier Inversion Theorem 1. [2]

$$\begin{aligned}
C_A(x,t) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} \hat{C_A}(k,t)e^{-ikx}dk \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} Me^{(-D_{AB}k^2 t)}e^{(-ikx)}dk \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} Me^{\left(-D_{AB}t\left(k^2 - \frac{ix}{D_{AB}t}k\right)\right)}dk \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} Me^{\left(-D_{AB}t\left(\left(k-\frac{ix}{2D_{AB}t}\right)^2 + \left(\frac{x}{2D_{AB}t}\right)^2\right)\right)}dk \\
&= \frac{1}{2\pi}Me^{\left(-\frac{x^2}{4D_{AB}t}\right)}\int_{-\infty}^{\infty} e^{\left(-D_{AB}t\left(k-\frac{ix}{2D_{AB}t}\right)^2\right)}dk \\
&= \frac{1}{2\pi}Me^{\left(-\frac{x^2}{4D_{AB}t}\right)}\sqrt{\frac{\pi}{D_{AB}t}} \\
&= \frac{1}{\sqrt{4\pi D_{AB}t}}Me^{\left(-\frac{x^2}{4D_{AB}t}\right)}
\end{aligned}$$

Thus

$$\boxed{C_A(x,t) = \frac{M}{\sqrt{4\pi D_{AB}t}}e^{\left(-\frac{x^2}{4D_{AB}t}\right)}}$$

where M is amount (e.g. mol, gram, etc.), D_{AB} is the diffusivity of A in B in length^2/time, x and t are distance and time respectively. In 1-D, C_A has units (amount / length).

3. Extension to Three Dimensions

The diffusion equation (1) extended to 3-D becomes $\frac{\partial C_A}{\partial t} = D_{AB}\left(\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2}\right)$ which is a linear, homogeneous partial differential equation and separable in Cartesian coordinates. The boundary conditions are symmetric and hold when extended to the x, y, z directions. The initial condition becomes $C_A(x, y, z, 0) = M\delta(x)\delta(y)\delta(z)$. Therefore the same steps to obtain equation (2) can be taken to obtain concentration profiles in the y and z directions, omitting M from the initial condition, (i.e. $C_A(0,t) = \delta(y), C_A(0,t) = \delta(z)$ for y, z-directions respectively) and the resulting becomes

$$C_A(x,y,z,t) = \left(\frac{M}{\sqrt{4\pi D_{AB} t}} e^{\left(-\frac{x^2}{4D_{AB}t}\right)}\right)\left(\frac{1}{\sqrt{4\pi D_{AB} t}} e^{\left(-\frac{y^2}{4D_{AB}t}\right)}\right)\left(\frac{1}{\sqrt{4\pi D_{AB} t}} e^{\left(-\frac{z^2}{4D_{AB}t}\right)}\right)$$
$$C_A(x,y,z,t) = \frac{M}{(4\pi D_{AB} t)^{3/2}} e^{\left(-\frac{(x^2+y^2+z^2)}{4D_{AB}t}\right)}$$

In spherical coordinates, $x^2 + y^2 + z^2 = r^2$ and so

$$\boxed{C_A(r,t) = \frac{M}{(4\pi D_{AB} t)^{3/2}} e^{\left(-\frac{r^2}{4D_{AB}t}\right)}}$$

Where M is amount (e.g. mol, gram, etc.), D_{AB} is the diffusivity of A in B in length^2/time, r and t are radius and time respectively. In 3-D, C_A has units (amount / length^3).

This work would not be possible without the aid of [3, 4] for clarity, coding in LaTeX, and solutions to similar partial differential equations and steps involved throughout this document. A special thanks to Professor Mohraz for fruitful discussions.

4. References

[1] Walter A. Strauss. *Partial Differential Equations: An Introduction*. 2nd. Wiley, 2007.

[2] H. F. Weinberger. *A First Course in Partial Differential Equations with Complex Variables and Transform Methods*. 1st. Dover Publications, 1995.

[3] OpenAI. *ChatGPT*. AI language model. Version GPT-4. 2023. URL: `https://chat.openai.com`.

[4] DeepSeek. *DeepSeek Chat*. AI language model. Version DeepSeek-V3. 2024. URL: `https://www.deepseek.com`.