One Dimensional Diffusion Calculations

Addendum to the Musterlösung for Übungsblatt 3 from 05.03.2017

Description of the problem

Two liquids (or gases) are placed into a tube of length L. The first liquid is occupying length L_1 ($L_1 \leq \frac{L}{2}$) and has a solute with the concentration C_0 and the second liquid has no solute in it. At $t = 0$ one-dimensional diffusion starts. The diffusion coefficient for the solute in the solvent (D) is assumed to have no dependency on the solute concentration. We want to determine the concentration of solute at a given time and at a given position along the tube.

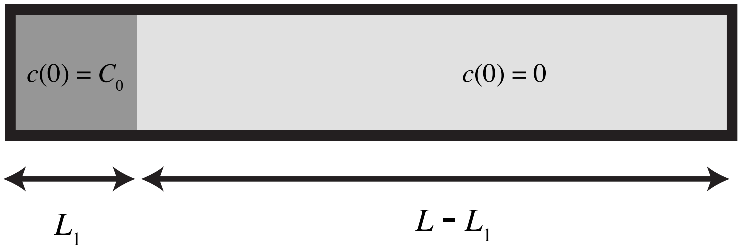

Figure 1:

Recipe

1. Calculate the diffusion length L_{diff} for a given time t.

$$L_{\text{diff}} = \sqrt{2Dt}$$

2. Determine which formula below is suitable for the task.

Case A) $L_{\text{diff}} \leq \frac{L_1}{2\sqrt{2}}$

Exact solution: $c(x) = \frac{C_0}{2}\texttt{Erfc}\left(\frac{x}{\sqrt{2}L_{\text{diff}}}\right)$ is not suitable for "easy" calculations. Therefore you can use one of the approximations below.

$$c(x) = \begin{cases} C_0 & \text{if} \quad x \leq -\frac{\sqrt{2}\,\pi L_{\text{diff}}}{2} \\ C_0\left(\frac{1}{2} - \frac{1}{2}\sin\left(\frac{x}{\sqrt{2}L_{\text{diff}}}\right)\right) & \text{if} \quad -\frac{\sqrt{2}\,\pi L_{\text{diff}}}{2} < x < \frac{\sqrt{2}\,\pi L_{\text{diff}}}{2} \\ 0 & \text{if} \quad x \geq \frac{\sqrt{2}\,\pi L_{\text{diff}}}{2} \end{cases} \tag{1}$$

or

$$c(x) = \begin{cases} C_0 & \text{falls} \quad x \leq -\frac{\sqrt{2\pi}L_{\text{diff}}}{2} \\ C_0\left(\frac{1}{2} - \left(\frac{x}{\sqrt{2\pi}L_{\text{diff}}}\right)\right) & \text{falls} \quad -\frac{\sqrt{2\pi}L_{\text{diff}}}{2} < x < \frac{\sqrt{2\pi}L_{\text{diff}}}{2} \\ 0 & \text{falls} \quad x \geq \frac{\sqrt{2\pi}L_{\text{diff}}}{2} \end{cases} \tag{2}$$

The "Quality" of the approximations are visible in the plot below. The color coding corresponds to font color of equations.

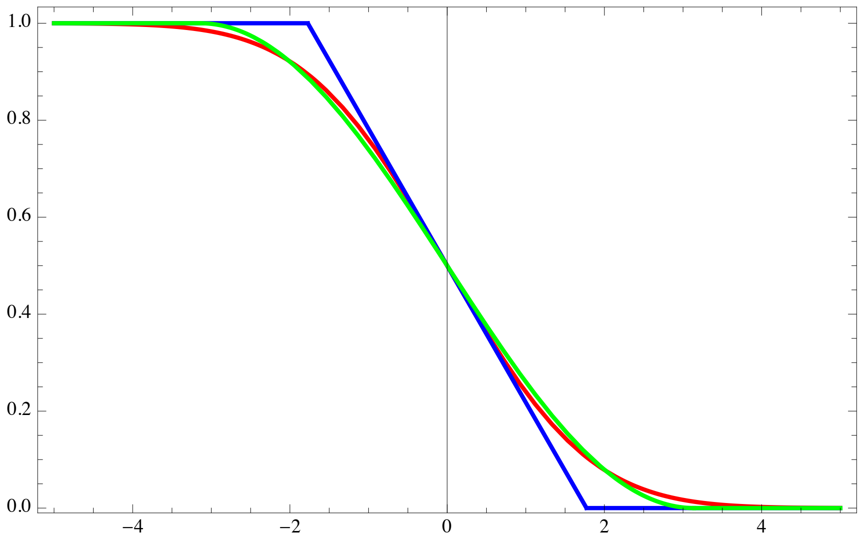

Figure 2:

NOTE: $x = 0$ corresponds to the initial interface between the two solutions.

REMARKS:
- "Green" formula gives an error of less than 2%.
- "Blue" (linear) formula is perfect for short distances but gives and error of 10% at $x = \frac{\sqrt{2\pi}L_{\text{diff}}}{2}$.
- Both formulas can also be used when $L_1 = \infty$ and/or $L = \infty$ (infinite or semi-infinite diffusion).

Case B) $\sqrt{2}\,L_1 \leq L_{\text{diff}} \leq \frac{L-L_1}{2\sqrt{2}}$

Exact solution: $c(x) = \frac{C_0}{2}\left(\texttt{Erfc}\left(\frac{x-1}{\sqrt{2}L_{\text{diff}}}\right) - \texttt{Erfc}\left(\frac{x+1}{\sqrt{2}L_{\text{diff}}}\right)\right)$ is not suitable for "easy" calculations but can be approximated by the Gauss function below.

$$c(x) = \frac{2\,C_0\,L_1}{\sqrt{2\pi}\,L_{\text{diff}}}\,e^{-\frac{1}{2}\left(\frac{x}{L_{\text{diff}}}\right)^2} \tag{3}$$

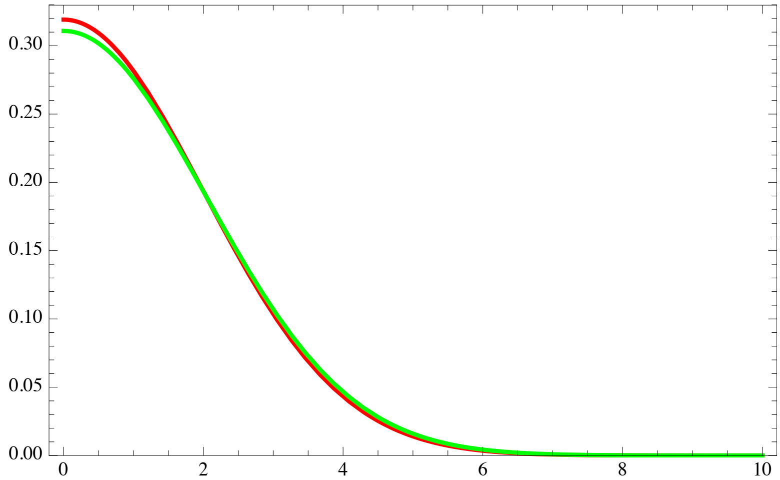

Figure 3:

NOTE: $x = 0$ corresponds to the left end of the tube.

REMARKS:
- The formula is identical to the exact solution for sufficiently large values of L_{diff}.
- The formula can be used also when $L = \infty$ (semi-infinite diffusion).
- Valid only for $L > 5\,L_1$.

Case C) $L_{\text{diff}} \geq 0.7\,(L - L_1)$

Exact solution is an infinite sum of Erfcs and is not suitable for "easy" calculations, but can be approximated by:

$$c(x) = C_0 \left(\frac{L_1}{L} + \frac{2}{\pi} e^{-\left(\frac{\sqrt{2}\pi L_{\text{diff}}}{2L}\right)^2} \sin\left(\frac{\pi L_1}{L}\right) \cos\left(\frac{\pi x}{L}\right) \right) \tag{4}$$

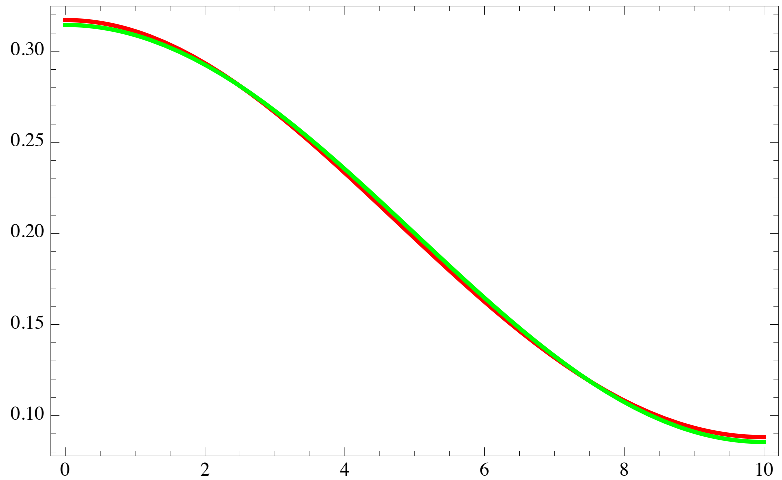

Figure 4:

NOTE: $x = 0$ corresponds to the left end of the tube.

REMARKS:
- The formula is identical to the exact solution for sufficiently large values of L_{diff}.
- In this case the diffusing solute has reached the right end of the tube, and therefore, both ends of the tube (physical boundaries) need to be accounted for in the formula.

Case D) $L_{\text{diff}} \geq 1.5L$
Concentration is almost uniform throughout the tube.

$$c(x) = \frac{L_1}{L} C_0 \tag{5}$$

REMARK:
- This is the limit case of formula 4