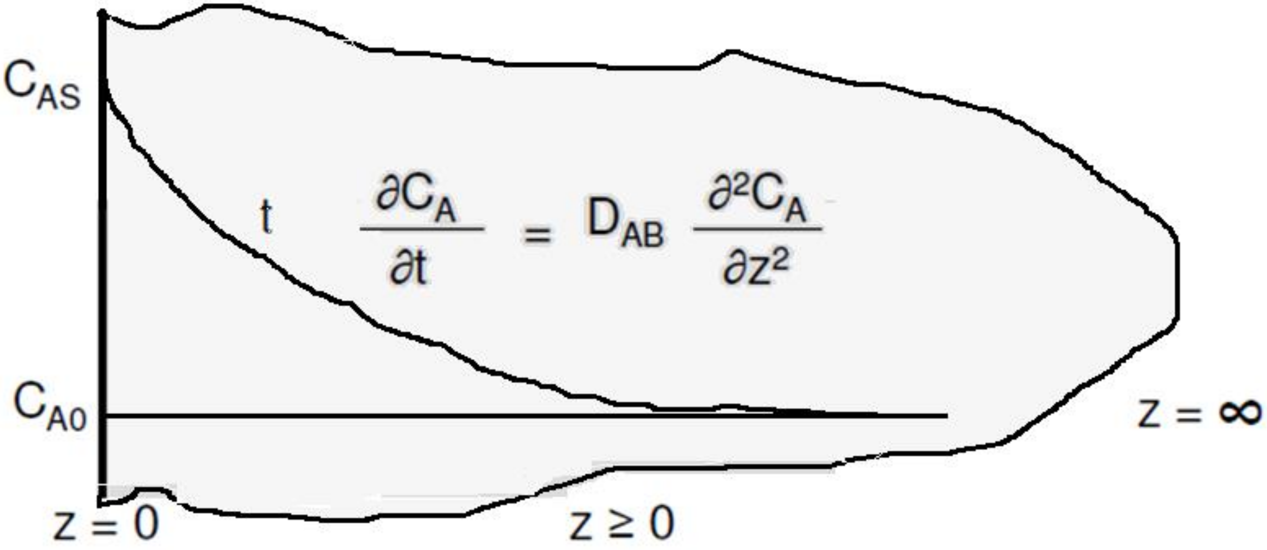
Unsteady-state diffusion in semi-infinite medium

Summary

Unsteady-state diffusion in semi-infinite medium with constant surface concentration



Initial condition:

$C_A = C_{A0}$ at $t \leq 0$ and $z \geq 0$

Boundary condition:

$C_A = C_{AS}$ at $t \geq 0$ and $z = 0$

$C_A = C_{A0}$ at $t \geq 0$ and $z \to \infty$

Introducing dimensionless concentration change:

Use $Y = \dfrac{C_A - C_{A0}}{C_{AS} - C_{A0}}$

and transform equation the equation to the following:

$$\frac{\partial Y}{\partial t} = D_{AB} \frac{\partial^2 Y}{\partial z^2}$$

where $\dfrac{\partial Y}{\partial t} = \dfrac{\partial C_A / \partial t}{C_{AS} - C_{A0}}$

$$\frac{\partial^2 Y}{\partial z^2} = \frac{\partial^2 C_A / \partial z^2}{C_{AS} - C_{A0}}$$

Introducing dimensionless concentration change:

Use $Y = \dfrac{C_A - C_{A0}}{C_{AS} - C_{A0}}$

and transform the initial and boundary conditions to the following:

Initial condition:

$C_A = C_{A0}$ becomes $Y = 0$ at $t \leq 0$ and $z \geq 0$

Boundary condition:

$C_A = C_{AS}$ becomes $Y = 1$ at $t \geq 0$ and $z = 0$

$C_A = C_{A0}$ becomes $Y = 0$ at $t \geq 0$ and $z \rightarrow \infty$

Solving for Y as a function of z and t:

$$\frac{\partial Y}{\partial t} = D_{AB} \frac{\partial^2 Y}{\partial z^2}$$

Initial condition: $Y = 0$ at $t \le 0$ and $z \ge 0$

Boundary condition: $Y = 1$ at $t \ge 0$ and $z = 0$

$Y = 0$ at $t \ge 0$ and $z \to \infty$

Since the PDE (Partial Differential Equation), its initial condition and boundary conditions are all linear in the dependent variable Y, an exact solution exists.

Non-dimensional concentration change (Y) is given by:

$$Y = \frac{C_A - C_{A0}}{C_{AS} - C_{A0}} = \mathrm{erfc}\left(\frac{z}{2\sqrt{D_{AB}\, t}} \right)$$

where the complimentary error function, erfc, is related to the error function, erf, by:

$$\mathrm{erfc}(x) = 1 - \mathrm{erf}(x) \qquad = 1 - \frac{2}{\sqrt{\pi}} \int_0^x \exp(-\sigma^2)\, d\sigma$$

Gaussian Error Function

w	erf w	w	erf w	w	erf w
0.00	0.00000	0.36	0.38933	1.04	0.85865
0.02	0.02256	0.38	0.40901	1.08	0.87333
0.04	0.04511	0.40	0.42839	1.12	0.88679
0.06	0.06762	0.44	0.46622	1.16	0.89910
0.08	0.09008	0.48	0.50275	1.20	0.91031
0.10	0.11246	0.52	0.53790	1.30	0.93401
0.12	0.13476	0.56	0.57162	1.40	0.95228
0.14	0.15695	0.60	0.60386	1.50	0.96611
0.16	0.17901	0.64	0.63459	1.60	0.97635
0.18	0.20094	0.68	0.66378	1.70	0.98379
0.20	0.22270	0.72	0.69143	1.80	0.98909
0.22	0.24430	0.76	0.71754	1.90	0.99279
0.24	0.26570	0.80	0.74210	2.00	0.99532
0.26	0.28690	0.84	0.76514	2.20	0.99814
0.28	0.30788	0.88	0.78669	2.40	0.99931
0.30	0.32863	0.92	0.80677	2.60	0.99976
0.32	0.34913	0.96	0.82542	2.80	0.99992
0.34	0.36936	1.00	0.84270	3.00	0.99998

[1]The Gaussian error function is defined as

$$\operatorname{erf} w = \frac{2}{\sqrt{\pi}} \int_0^w e^{-v^2}\, dv$$

The complementary error function is defined as

$$\operatorname{erfc} w \equiv 1 - \operatorname{erf} w$$

Determine the flux!

$$J_A = - D_{AB} \left. \frac{\partial C_A}{\partial z} \right|_{at\ z}$$

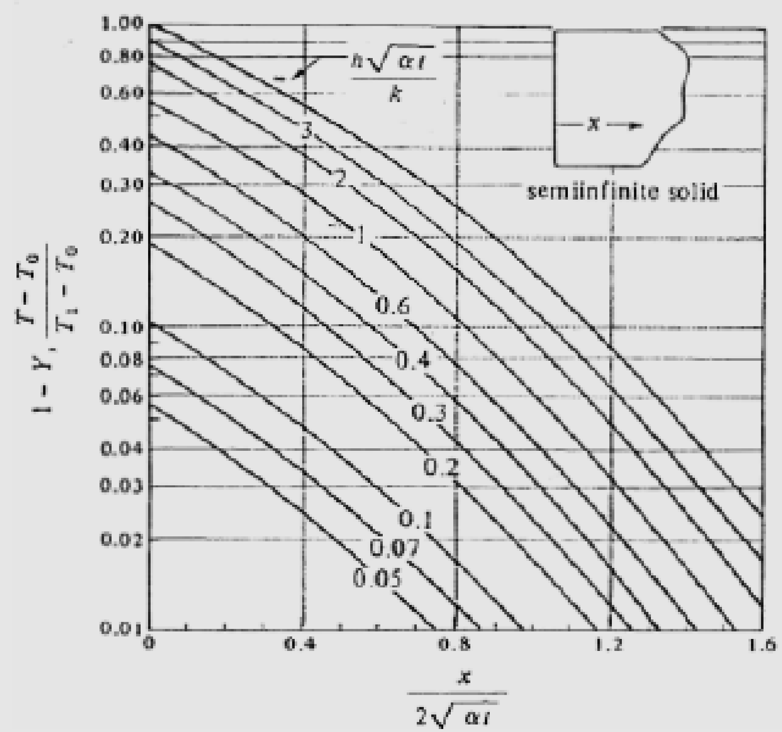
$$J_A = \sqrt{D_{AB} / \pi t} \ \exp(-z^2/4D_{AB}t) \ (C_{AS}-C_{A0})$$

Flux across the interface at $z = 0$ is

$$\left. J_A \right|_{at\ z\ =\ 0} = \sqrt{D_{AB} / \pi t} \quad (C_{AS}-C_{A0})$$

Semi-infinite slab _ Chart method _ General solution

For a semi-infinite slab:



*Relation Between Mass- and Heat-Transfer Parameters for Unsteady-State Diffusion**

	Mass Transfer	
Heat Transfer	$K = c_L/c = 1.0$	$K = c_L/c \neq 1.0$
$Y, \frac{T_1 - T}{T_1 - T_0}$	$\frac{c_1 - c}{c_1 - c_0}$	$\frac{c_1/K - c}{c_1/K - c_0}$
$1 - Y, \frac{T - T_0}{T_1 - T_0}$	$\frac{c - c_0}{c_1 - c_0}$	$\frac{c - c_0}{c_1/K - c_0}$
$X, \frac{\alpha t}{x_1^2}$	$\frac{D_{AB} t}{x_1^2}$	$\frac{D_{AB} t}{x_1^2}$
$\frac{x}{2\sqrt{\alpha t}}$	$\frac{x}{2\sqrt{D_{AB} t}}$	$\frac{x}{2\sqrt{D_{AB} t}}$
$m, \frac{k}{h x_1}$	$\frac{D_{AB}}{k_c x_1}$	$\frac{D_{AB}}{K k_c x_1}$
$\frac{h}{k}\sqrt{\alpha t}$	$\frac{k_c}{D_{AB}}\sqrt{D_{AB} t}$	$\frac{K k_c}{D_{AB}}\sqrt{D_{AB} t}$
$n, \frac{x}{x_1}$	$\frac{x}{x_1}$	$\frac{x}{x_1}$

* x is the distance from the center of the slab, cylinder, or sphere; for a semiinfinite slab, x is the distance from the surface. c_0 is the original uniform concentration in the solid, c_1 the concentration in the fluid outside the slab, and c the concentration in the solid at position x and time t.