ChE-403 Problem Set 3.2

Week 11

Problem 1

We determined that the diffusion of molecules in a single pore was governed by the following dimensionless equation:

$$\frac{d^2 C_A{}'}{d\chi^2} - \phi^2 C_A{}' = 0$$

With boundary conditions:

$C_A{}' = 1$ @ $\chi = 0$

$\frac{dC_A{}'}{d\chi} = 0$ @ $\chi = 1$ (no flux at the end of the pore)

Can you solve this equation?

Solution:

This is a linear differential eq. of order 2 with constant coefficients of the type:

$ay'' + by' + cy = g(x)$ where: $g(x) = 0$ and $b = 0$

It's characteristic equation is therefore:

$ar^2 + c = 0$ where: $a = 1$ and $c = -\phi^2$

This leads to an equation of the type:

$r^2 - \phi^2 = 0$

$r = \pm\phi$ according to the rule, we should have a formula of the form:

$\rightarrow C_A' = cst1\; e^{+\phi\chi} + cst2\; e^{-\phi\chi}$

@ $\chi = 0$ $\quad cst1\; e^0 + cst2\; e^0 = 1 \rightarrow cst1 = 1 - cst2$

@ $\chi = 1$ $\quad \phi cst1 e^{\phi} - \phi\; cst2\; e^{-\phi} = 0 \rightarrow cst1 = cst2\; e^{-2\phi}$

$$cst2\left(1 + e^{-2\phi}\right) = 1 \rightarrow cst2 = \frac{1}{(1 + e^{-2\phi})}$$

$$cst1 = \frac{e^{-2\phi}}{(1 + e^{-2\phi})}$$

$$C_A' = \frac{e^{-2\phi}}{(1 + e^{-2\phi})}\; e^{\phi\chi} + \frac{1}{(1 + e^{-2\phi})}\; e^{-\phi\chi}$$

Multiply all fractions by e^{ϕ}:

$$C_A' = \frac{e^{-\phi}}{(e^{\phi} + e^{-\phi})}\, e^{+\phi\chi} + \frac{e^{\phi}}{(e^{\phi} + e^{-\phi})}\, e^{-\phi\chi} = \frac{1}{(e^{\phi} + e^{-\phi})}\left(e^{-\phi(1-\chi)} + e^{\phi(1-\chi)}\right)$$

Note that: $\cosh x = \frac{e^{x}+e^{-x}}{2}$

$$= \frac{1}{2\cosh\phi}\left(e^{-\phi(1-\chi)} + e^{\phi(1-\chi)}\right)$$

$$= \frac{1}{2\cosh\phi}\, 2\cosh[\phi(1-\chi)]$$

$$C_A' = \frac{\cosh[\phi(1-\chi)]}{\cosh\phi}$$

Problem 2

The isothermal first order reaction of gaseous A occurs within the pores of a spherical catalyst pellet. The reactant concentration halfway between the external surface of the pellet and the center of the pellet is equal to ¼ of the concentration at the surface of the pellet (C_{AS}). What is the concentration of A at the center of the pellet?

Solution:

For a first order reaction we have that:

$$C_A' = \frac{\sinh(\phi\, \bar{r}')}{\bar{r}' \sinh(\phi)}$$

Here at $\bar{r}' = \frac{\bar{r}}{R_p} = \frac{1}{2}$, we have $C_A' = \frac{1}{4}$

$$\frac{1}{4} = \frac{2\sinh(\phi/2)}{\sinh(\phi)} \rightarrow \sinh(\phi) = 8\ \ \sinh(\phi/2)$$

Using the identity: $\sinh(\phi) = 2\sinh(\phi/2)\cosh(\phi/2)$

We have: $8\ \ \sinh(\phi/2) = \ 2\sinh(\phi/2)\cosh(\phi/2) \rightarrow \ \cosh(\phi/2) = 4$

Or $\phi = 2\,\mathrm{arccosh}(4)$

We can use this to find ϕ: $\phi = 4.13$

Now let's calculate C_A' @ $\bar{r}' = 0$

$$C_A' = \frac{\sinh(\phi\, \bar{r}')}{\bar{r}' \sinh(\phi)}$$

Both the top and the bottom of the function equal zero. We need to use L'Hospital's rule:

$$\lim_{\bar{r}' \to 0} C_A' = \lim_{\bar{r}' \to 0} \frac{(\sinh(\phi\, \bar{r}'))'}{(\bar{r}' \sinh(\phi))'} = \frac{\phi \cosh(0)}{\sinh(\phi)} = \frac{\phi}{\sinh(\phi)} = 0.133$$

Problem 3

Demonstrate that the solution for the following differential equation seen in class for diffusion in a spherical catalyst pellet):

$$\frac{d^2C_A{}'}{d\bar{r}'^2}+\frac{2}{\bar{r}'}\frac{dC_A{}'}{d\bar{r}'}-\phi^2C_A'=0$$

With boundary conditions

$C_A{}'=1$ @ $\bar{r}'=1$

$\frac{dC_A{}'}{d\bar{r}'}=0$ @ $\bar{r}'=0$

has a solution:

$$C_A'=\frac{\sinh(\phi\,\bar{r}')}{\bar{r}'\sinh(\phi)}$$

With: $\sinh(x)=\frac{e^x-e^{-x}}{2}$

Hint: This is a second order differential equation with non-constant coefficients, which is quite difficult to solve. However, try doing a variable change (with a new variable *y*) where: $y=C_A'\bar{r}'$ or $C_A'=y/\bar{r}'$. You might get a familiar equation…

Solution:

$$\frac{dC_A{}'}{d\bar{r}'}=\frac{d(y/\bar{r}')}{d\bar{r}'}=\frac{1}{\bar{r}'}\frac{dy}{d\bar{r}'}-\frac{y}{\bar{r}'^2}$$

$$\frac{d^2C_A{}'}{d\bar{r}'^2}=\frac{d^2(y/\bar{r}')}{d\bar{r}'^2}=\frac{d}{d\bar{r}'}\left(\frac{1}{\bar{r}'}\frac{dy}{d\bar{r}'}-\frac{y}{\bar{r}'^2}\right)=\frac{1}{\bar{r}'}\left(\frac{d^2y}{d\bar{r}'^2}\right)-\frac{1}{\bar{r}'^2}\left(\frac{dy}{d\bar{r}'}\right)-\frac{1}{\bar{r}'^2}\left(\frac{dy}{d\bar{r}'}\right)+\frac{2y}{\bar{r}'^3}$$

Let's substitute this back into the original differential equation:

$$\frac{1}{\bar{r}'}\left(\frac{d^2y}{d\bar{r}'^2}\right)-\frac{2}{\bar{r}'^2}\left(\frac{dy}{d\bar{r}'}\right)+\frac{2y}{\bar{r}'^3}+\frac{2}{\bar{r}'^2}\frac{dy}{d\bar{r}'}-2\frac{y}{\bar{r}'^3}-\frac{\phi^2y}{\bar{r}'}=\frac{1}{\bar{r}'}\left(\frac{d^2y}{d\bar{r}'^2}\right)-\frac{\phi^2y}{\bar{r}'}=0$$

Which simplifies to:

$$\frac{d^2y}{d\bar{r}'^2}-\phi^2y=0$$

This is the same equation as for problem 1, with the boundary conditions switched.

$\rightarrow y = cst1\ e^{+\phi\bar{r}'} + cst2\ e^{-\phi\bar{r}'}$

@ $\bar{r}' = 0$ $\quad \frac{dC_{A'}}{d\bar{r}'} = \frac{1}{\bar{r}'}\frac{dy}{d\bar{r}'} - \frac{y}{\bar{r}'^2} = 0 = \frac{1}{\bar{r}'}(\ \phi cst1e^0 - \phi\ cst2\ e^{-0}) - \frac{cst1e^0 + cst2\ e^{-0}}{\bar{r}'^2}$

We can multiply by $\bar{r}'^2$ to get an equation that's easier to solve:

$$\bar{r}'(\ \phi cst1e^0 - \phi\ cst2\ e^{-0}) - cst1e^0 - \ cst2\ e^{-0} = -cst1e^0 - \ cst2\ e^{-0} = 0$$

$\rightarrow cst1 = -cst2$

@ $\bar{r}' = 1$ $\quad cst1e^{\phi} + \ cst2\ e^{-\phi} = cst1e^{\phi} - \ cst1\ e^{-\phi} = 1 \rightarrow cst1 = \frac{1}{e^{\phi} - e^{-\phi}}$

$$y = \frac{1}{e^{\phi} - \ e^{-\phi}}\left(e^{\phi\bar{r}'} - \ e^{-\phi\bar{r}'}\right) = \frac{2\sinh(\phi\bar{r}')}{2\sinh(\phi)}$$

$$C_A' = y/\bar{r}' = \frac{\sinh(\phi\bar{r}')}{\bar{r}'\sinh(\phi)}$$