

ChE-403 Problem Set 3.4

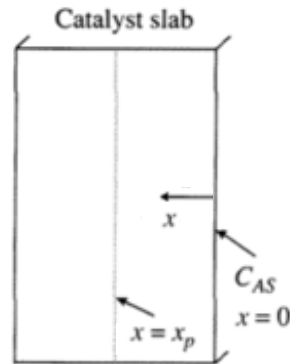
Week 13

Problem 1

Consider a reaction with kinetics:

$$r = k \text{ (zero order)}$$

Occurring in catalyst pellets in the form of slabs:



Assume that we are at low conversion and that there is no external mass transfer limitations so that $C_{A,0} = C_{AS}$.

Equimolar counter-diffusion can also be assumed.

Write the internal mass transfer balance for this reaction, determine the Thiele modulus after putting it in dimensionless form and propose appropriate boundary conditions.

Note: because it's a zero order reaction, you have to assume that in certain conditions, the concentration will be zero before the middle of the particle. You can assume that this occurs at χ_0 where we will have a no flux conditions $\left(\frac{dC_A'}{d\chi} \right)_{\chi=\chi_0} = 0$ instead of at the center. With the two boundary conditions and the property $C_A'(\chi_0) = 0$ you can solve for χ_0 and the integration constants.

Problem 2

Solve the problem of combined internal and external transport we saw in class for a slab for the case where we have a first order RX and an isothermal slab.

The general form of the equation was:

$$\frac{d^2 \bar{C}'_A}{d\chi^2} = \phi^2 \exp \left[-\gamma \left(\frac{1}{\bar{T}'} - 1 \right) \right] \bar{C}'_A$$

$$\frac{d^2 \bar{T}'}{d\chi^2} = -\phi^2 \beta \exp \left[-\gamma \left(\frac{1}{\bar{T}'} - 1 \right) \right] \bar{C}'_A$$

With boundary conditions:

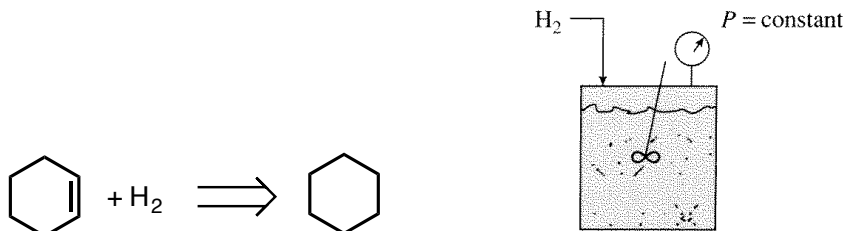
$$\left. \frac{d\bar{C}'_A}{d\chi} \right|_{\chi=1} = Bi_m [1 - \bar{C}'_A] \quad @ \chi = 1$$

$$\left. \frac{d\bar{T}'}{d\chi} \right|_{\chi=1} = Bi_h [1 - \bar{T}'] \quad @ \chi = 1$$

$$\frac{d\bar{C}'_A}{d\chi} = \frac{d\bar{T}'}{d\chi} = 0 \quad @ \chi = 0 \text{ No flux through the center}$$

Problem 3

Consider the liquid phase hydrogenation of cyclohexene to cyclohexane (in an inert solvent) that happens in the presence of a solid catalyst dispersed in the liquid. The reaction is semi-batch in hydrogen (i.e. hydrogen pressure is kept constant during the entire reaction).



These are the data we measure for this reaction. Can you interpret each of the figures?

Figure 1: We observe a linear relationship between the time and the cyclohexene concentration given below. This relationship is also present for the data collected in Figures 2 and 3.

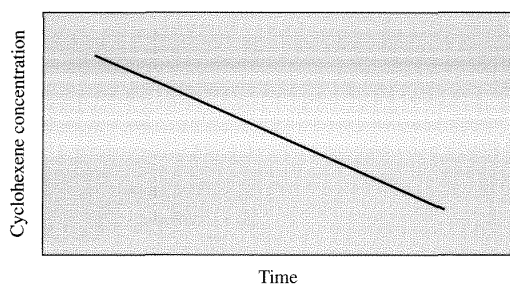


Figure 2: Effect of the catalyst weight (total catalyst added to the solution at a single metal loading) on the reaction rate.

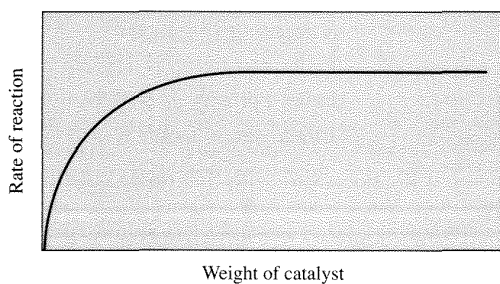


Figure 3: Evaluation of temperature effects and stirring speed on the reaction rate.

