A First Course on Kinetics and Reaction Engineering

Activity 38.1

Consider the situation where a gas stream flows over a flat solid whereupon a 0.5 mm thick porous, catalytic layer has been applied. The system is isothermal (no temperature gradients anywhere) and within the porous layer the first order catalytic reaction A → B takes place with a rate coefficient equal to 1.5×10^{-3} min^{-1}. There are no concentration gradients in the gas phase, but they may exist within the porous layer. If the effective diffusion coefficient for the Fickian diffusion of A within the porous layer is 1.8×10^{-7} cm^2 s^{-1} and the gas phase concentration is 1 mol L^{-1}, calculate the effectiveness factor using a pseudo-homogeneous model for the porous layer.

Problem Solution

- Let S represent the surface area of the flat solid and L the thickness of the porous overlayer. Define the z direction as perpendicular to the solid surface with z = 0 being the interface between the solid and the porous layer and z = L being the interface between the porous layer and the gas phase.
- Write a mole balance on a differentially thick section of the porous layer (parallel to the solid surface) and take the limit as its thickness goes to zero to generate a mole balance for the catalyst phase

- Substitute the rate expression into the mole balance

- The mole balance is a second order ordinary differential equation
  - Write two boundary conditions that can be used to solve it

  - What type of ODE is the mole balance, initial value or boundary value?

  - Is there a singularity within the range of z where the ODE is valid?

- In order to use MATLAB to solve this second order, boundary value ODE, it must be converted into an equivalent set of 2 first order ODEs
  - Define 2 new dependent variables for this purpose

  - Generate two first order ODEs in terms of those new dependent variables that are equivalent to the original second order ODE

  - Re-write the boundary conditions in terms of these new dependent variables

  - What else will you need to provide in order to solve these new equations numerically?

  - What new information would you obtain by solving these 2 ODEs numerically?

- Show how to use the results of solving the ODEs to calculate the effectiveness factor
  - Flux of A from the gas phase into the surface of the porous layer
  - Equivalent rate of consumption of A per unit catalyst volume
  - Rate of consumption of A if there were no gradients in the porous solid
  - Effectiveness factor is the ratio of these rates
- Go back and solve the mole balance analytically