

Lecture 19

# Penetration Theory

(unsteady-state mass transfer model / surface renewal model)

$$(N) = C[\beta][k][\Xi](y_0 - y_\delta)$$

## 1.0 Answers needed:

1.1 what is the correction factor?

1.2 what is  $[k]$  in terms of binary  $k$ 's?

1.3 can also give  $k_{ij}$

## 2.0 What is the Model? (section 9.1)

2.1 surface renewal idea?

2.2 transient model

2.3 exposure time ( $t_e$ )

2.4 Higbie (1935)

all surface elements have same exposure time

$$\psi(t) = \frac{1}{t_e}$$

2.5 Danckwerts (1951)

chance of surface element being replaced with fresh fluid is independent of the time for which it has been exposed

$$\psi(t) = s e^{-st}$$

where  $s$  is the fraction of the surface area that is replaced with fresh fluid in unit time

## 3.0 Binary Analysis (section 9.2):

3.1 Higbie low mass flux mass transfer coefficient  $k$ :

$$k = 2 \sqrt{\frac{D}{\pi t_e}}$$

3.2 Danckwerts low mass flux mass transfer coef.  $k$ :

$$k = \sqrt{Ds}$$

3.3 Correction factor  $\Xi$  :

$$\Xi = \frac{\exp(-\Phi^2/\pi)}{\{1 + \operatorname{erf}(\Phi/(\sqrt{\pi}))\}}$$

$$\text{where } \Phi = N_t/(c_t k)$$

3.4 'A priori' need for  $t_e$  or  $s$

3.5 iterative method needed

## 4.0 Multicomponent Analysis (sec. 9.3)

- 4.1 exact analytic solution of this approximate model is not useful (too cumbersome).
- 4.2 Linearized theory approximation useful
- 4.3 assuming constant  $[D]$ ,  
evaluated at average properties
  - 4.3.1 form for multicomponent  $[k]$ :
    - 4.3.1.1 Higbie model: equation 9.3.33
    - 4.3.1.2 Danckwerts model: equation 9.3.34
  - 4.3.2 form for correction factor for both models  
given in equations 9.3.31 and 9.3.32
- 4.4 using modal matrix approach  
equations 8.4.25, 9.3.37-39

## 5.0 Limitation of Penetration<sub>(classical)</sub> Theory

5.1 boundary condition (eq. 9.1.6):

$$z \rightarrow \infty \quad t > 0 \quad x_i = x_{i\infty}$$

5.1.1 the penetrating, or diffusing component does not see the bulk fluid

5.1.2 strictly true only for short contact times

$$Fo = \frac{Dt}{\delta^2} < 0.20$$

5.2 for long contact times and/or short distances between the interface and the core ( $\delta$ ) of the fluid phase  $\Rightarrow$  need improved penetration theory!

5.3 thus is the case for many bubbles, drops, jets:

## 6.0 Fractional Approach (section 9.4.1)

6.1 define the fractional approach to equilibrium:

$$F \equiv \frac{(x_{10} - \langle x_1 \rangle)}{(x_{10} - x_{1I})}$$

6.2 find the Sherwood Number for spherical particle at time  $t$  by taking the driving force to be  $(x_{10} - \langle x_1 \rangle)$

$$Sh = \frac{2}{3(1-F)} \cdot \frac{\partial F}{\partial Fo}$$

where  $Fo = \frac{Dt}{r_0^2}$

6.3 When substituted and solved to give  $Sh$  as a function of time:

$$Sh = \frac{2}{3}\pi^2 \cdot \left( \sum_{m=1}^{\infty} \exp\{-m^2 \pi^2 Fo\} / \sum_{m=1}^{\infty} \frac{1}{m^2} \exp\{-m^2 \pi^2 Fo\} \right)$$

6.4 Or averaged across time to give:

$$\bar{Sh} = -2 \ln(1-F)/(3Fo) \text{ or } \bar{k} = -\ln(1-F)/(a't)$$

where  $a'$  is the surface area per unit volume and  $t$  is the contact time.

- 6.5 Note: this results in  $Sh$  at large  $Fo$  approaching a limit where  $k$  varies with  $D$  (as in the film model) as opposed to  $D^{1/2}$  as in the classical penetration model.
- 6.6 This model has also been revised for internal circulation (see eqns. 9.4.9 and 9.4.10)
- 6.7 The solution for cylinders (jets) is also shown (see eqns. 9.4.12 - 9.4.14)

## 7.0 Multicomponent Analysis (sec. 9.4.2)

- 7.1 analysis with constant  $[D]$ .
- 7.2 solution using Sylvester's formula: eqn. 9.4.26
- 7.3 solution using modal matrix of the Fick matrix  $[D]$
- 7.4 see example 9.4.1  
which shows sensitivity to  $Fo$ .  
this revised method improves the multicomponent analysis significantly  
(can even change the direction of the mass transfer)