sebacic acid and no compound II, the number of abrasive cut-off pieces was only 10000. By use of our new griding fluid coolant (sample C, compound II), loading did not occur after 20 min. However, by use of a sodium nitrite solution system (sample D), loading occurred after 14 min.

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CORRESPONDENCE

Comments on "Simulation and Optimization of an Industrial Ammonia Reactor"

Sir: In a recent paper on the simulation of an industrial ammonia reactor, Elnashaie et al. (1988) used the Wilke effective diffusivity formula (cf. their eq 16)

$$D_i^0 = \frac{1 - X_{ig}}{\sum_{j=1, j\neq i}^{n} \frac{X_{jg}}{D_{ji}^0}} \qquad i = 1\text{–}3 \qquad (1)$$

in the calculation of the effectiveness factor inside the catalyst particle. However, eq 1 is strictly applicable for the determination of the effective diffusivity of a transferring component, i, in a mixture of stagnant (i.e., nontransferring) components. In the ammonia synthesis process, none of the three components present in the gaseous mixture, N_2 (1), H_2 (2), and NH_3 (3), can be considered to have a vanishing flux. Indeed, the ratio of the molar flux of component i, N_i, to the mixture molar flux

$$z_i = N_i/(N_1 + N_2 + N_3) \qquad i = 1\text{–}3 \qquad (2)$$

is determined by the reaction stoichiometry to be

$$z_1 = 1/2; \quad z_2 = 3/2; \quad z_3 = -1 \qquad (3)$$

The appropriate expression for the effective diffusivity of any component with stoichiometrically constrained fluxes can be easily derived from the Maxwell–Stefan diffusion equations (cf. Kubota et al. (1969)):

$$D_i^0 = \frac{1}{\sum_{j=1, j\neq i}^{n} \frac{1}{D_{ji}^0}\left[X_{jg} - X_{ig}\frac{z_j}{z_i}\right]} \qquad i = 1\text{–}3 \qquad (4)$$

Equation 4 in general will give significantly different values for the effective diffusivity than the Wilke formula (eq 1). To demonstrate this, let us calculate the effective diffusivities by the two formulas at the following compositions:

$$X_{1g} = 0.15, \quad X_{2g} = 0.65, \quad X_{3g} = 0.20 \qquad (5)$$

With the pair diffusivities values (at 298 K and 100 kPa) of

$$D_{12}^0 = 78, \quad D_{13}^0 = 23, \quad D_{23}^0 = 78 \text{ mm}^2/\text{s} \qquad (6)$$

we find from the Wilke formula (eq 1) that

$$D_1^0 = 50, \quad D_2^0 = 78, \quad D_3^0 = 54 \text{ mm}^2/\text{s} \qquad (7)$$

while from the Kubota et al. formulation (eq 4) we get

$$D_1^0 = 41, \quad D_2^0 = 138, \quad D_3^0 = 43 \text{ mm}^2/\text{s} \qquad (8)$$

In particular, the effective diffusivity of hydrogen is significantly higher because of stoichiometry considerations, and the reaction rates will consequently be altered to a significant extent. It is to be noted that intraparticle diffusion effects are apparently important in ammonia synthesis as witnessed by an effectiveness factor of 0.4 at the entrance to the reactor. We conclude that, for a proper simulation of the ammonia synthesis reactor, the appropriate expression (eq 4) for the effective diffusivity has to be used.

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