REB, The Book
Example 3.6.1 Solution

The synthesis of ammonia, reaction (1), is one of the highest production chemical processes in the world. (One reason for this is that ammonia is used to make fertilizer.) It is a heterogeneous catalytic reaction. The ammonia synthesis catalyst takes the form of pellets that pack into the the reactor with an apparent density of 155 lb_m ft^{-3}. Rase[1] provides the expression in equation (2) for the rate of generation of ammonia via reaction (1). In that expression, E_1 is the activation energy, $K_{1,eq}$ is the equilibrium constant and a_i represents the thermodynamic activity of reagent i.

$$3\ H_2 + N_2 \rightleftarrows 2\ NH_3 \tag{1}$$

$$\begin{aligned} r_{NH_3,1} &= 1.54 \times 10^{15} \exp\left(\frac{-E_1}{RT}\right) \\ &\times \left[K_{1,eq}^2\left(\frac{a_{N_2}a_{H_2}^{1.5}}{a_{NH_3}}\right) - \left(\frac{a_{NH_3}}{a_{H_2}^{1.5}}\right)\right] \frac{\text{kmol NH}_3}{\text{m}^3_{\text{bed}}\text{h}} \end{aligned} \tag{2}$$

Write an expression for the general rate of reaction (1), r_1, that is normalized per lb_m of catalyst.

Equation (2) is an expression for the rate of ammonia generation, and the units show it is normalized per cubic meter of catalyst. The general reaction rate is related to the rate of ammonia synthesis as indicated in equation (3).

$$r_{i,j} = \nu_{i,j} r_j \quad \Rightarrow \quad r_j = \frac{r_{i,j}}{\nu_{i,j}} \quad \Rightarrow \quad r_1 = \frac{r_{NH_3,1}}{\nu_{NH_3,1}} = \frac{r_{NH_3,1}}{2} \tag{3}$$

The apparent density provided in the assignment narrative can then be used to change the normalization factor from the catalyst bed volume to the catalyst mass as

[1] Rase, H. F. 1977. *Chemical Reactor Design for Process Plants*. Vol. 2. New York: John Wiley.

shown in equation (4) where r_1 is the rate per catalyst volume and r_1' is the rate per catalyst mass.

$$r'_1 = \frac{r_1}{\rho_{bed}} \tag{4}$$

Substitution of the provided rate expression into equation (3) followed by substitution of the result into equation (4) yields the requested rate expression shown in equation (5). It should be noted that the kmol in equation (5) is kmol of extent of reaction and not kmol of NH_3.

$$r'_1 = \frac{1.54 \times 10^{15}}{2\left(155 \frac{\text{lb}_\text{m}}{\text{m}_\text{bed}{}^3}\right)} \exp\left(\frac{-E_1}{RT}\right)$$
$$\times \left[K_{1,eq}^2 \left(\frac{a_{N_2} a_{H_2}^{1.5}}{a_{NH_3}}\right) - \left(\frac{a_{NH_3}}{a_{H_2}^{1.5}}\right)\right] \frac{\text{kmol NH}_3}{\text{m}_\text{bed}^3\text{h}}$$

$$r'_1 = 1.76 \times 10^{14} \exp\left(\frac{-E_1}{RT}\right)$$
$$\times \left[K_{1,eq}^2 \left(\frac{a_{N_2} a_{H_2}^{1.5}}{a_{NH_3}}\right) - \left(\frac{a_{NH_3}}{a_{H_2}^{1.5}}\right)\right] \frac{\text{kmol}}{\text{lb}_\text{m}\text{ h}} \tag{5}$$