

The Temkin-Pyzhev kinetics gives:

$$r = \frac{r_{NH_3}}{2} = \frac{f}{\rho_{bulk}} \left(k_1 \frac{p_{N_2} p_{H_2}^{1.5}}{p_{NH_3}} - k_{-1} \frac{p_{NH_3}}{p_{H_2}^{1.5}} \right) \quad (kmol \text{ kg}_{cat}^{-1} \text{ h}^{-1})$$

With $f = 4.75$, $\rho_{cat} = 2200$, $\varphi = 0.33$, $\rho_{bulk} = (1 - \varphi)\rho_{cat} = (1 - 0.33)2200 = 1474 \text{ kg m}^{-3}$, $k_1 = 1.79 \times 10^4 e^{-87090/RT}$, $k_{-1} = 2.57 \times 10^{16} e^{-198464/RT}$, and pressures p_i in bar.

Aspen requires:

$$r_f = k_f e^{-87090/RT} \frac{p'_{N_2} p'^{1.5}_{H_2}}{p'_{NH_3}}$$

$$r_r = k_r e^{-198464/RT} \frac{p'_{NH_3}}{p'^{1.5}_{H_2}}$$

With pressures p'_i in Pa. Therefore,

$$k_f = 1.79 \times 10^4 \frac{f}{\rho_{bulk}} \frac{(10^{-5})^{1.5}}{3600} = 5.067 \times 10^{-10} \text{ kmol kg}_{cat}^{-1} \text{ s}^{-1} \text{ Pa}^{-1.5}$$

$$k_r = 2.57 \times 10^{16} \frac{f}{\rho_{bulk}} \frac{1}{3600(10^{-5})^{0.5}} = 7.275 \times 10^{12} \text{ kmol kg}_{cat}^{-1} \text{ s}^{-1} \text{ Pa}^{0.5}$$

The values in the Aspen model are off by a factor of $2\rho_{bulk}$. Therefore, the pre-exponential constants of the Aspen distribution are about 3000 too high which means that equilibrium is approached but so does with the re-calculated values. As an illustration (see Figure 1), we show below one simulation under feed flow rate at 252,000 kg/h, feed temperature at 250 °C, feed pressure at 200 bar, and mass fraction of ammonia at 0.08, corresponding to the upper steady state from Morud and Skogestad, 1995 (Morud, J. C. and Skogestad, S. Analysis of Instability in an Industrial Ammonia Reactor. AIChE Journal, Vol. 44, No. 4, 1995.).

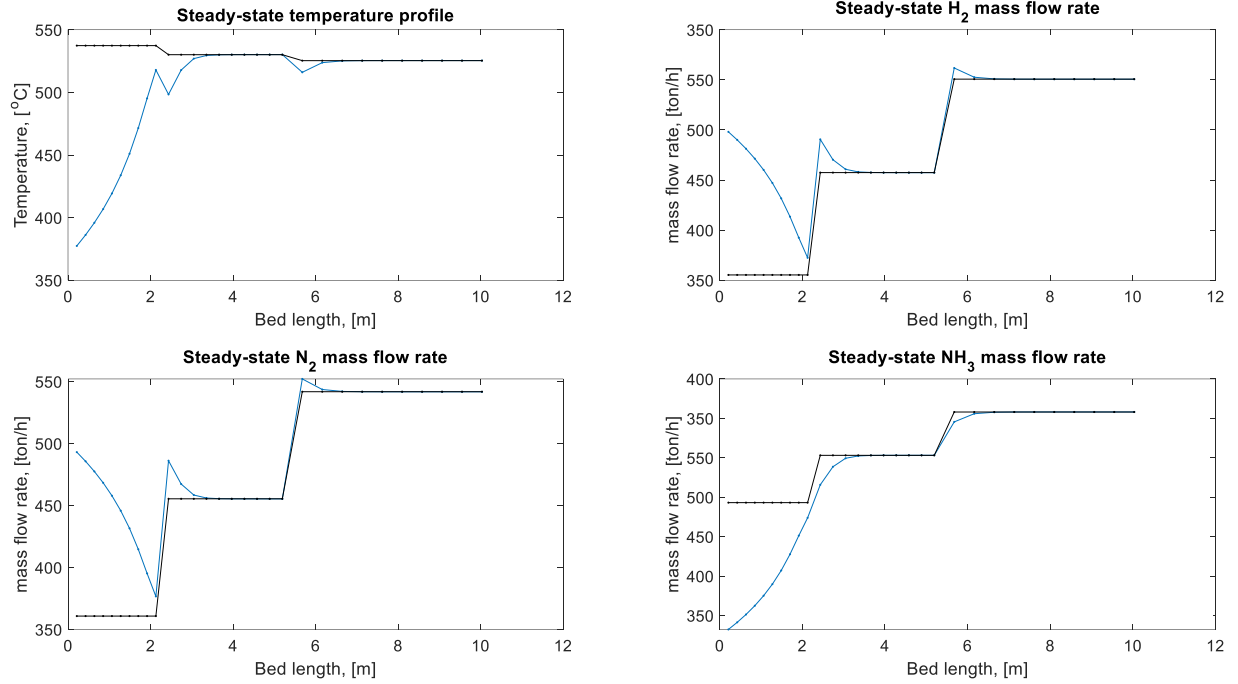


Figure 1 – Corrected parameters (blue line); publication's parameters (black line).

Since equilibrium is always reached, particularly in the last bed, the steady state computations are not likely to change.