11. Catalytic membrane reactor

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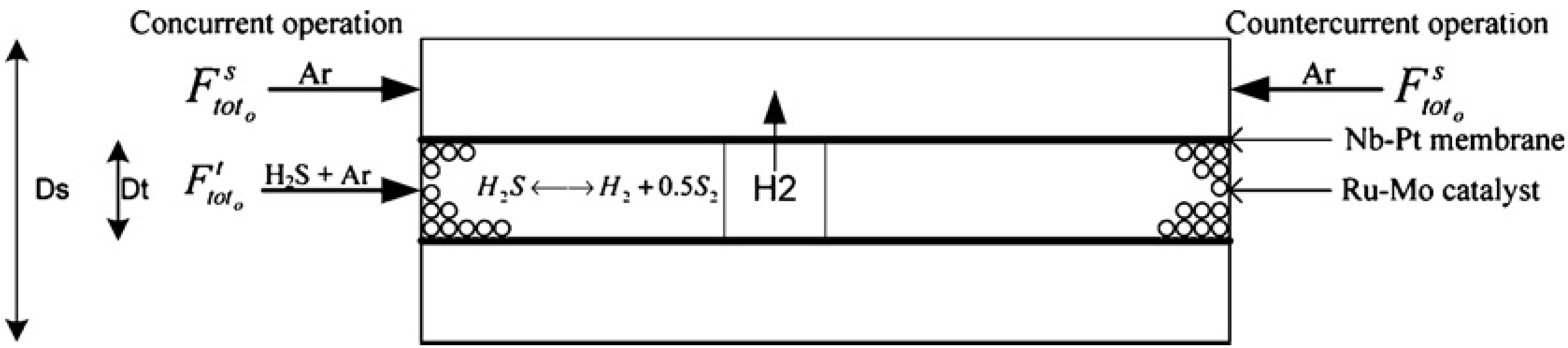
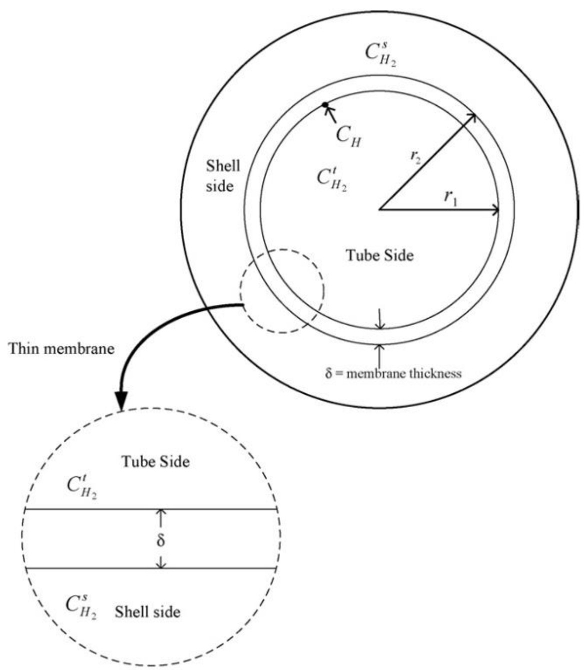
$$H_2S_{(g)} \rightleftarrows H_{2(g)} + 1/2\,S_{2(g)}$$





Dissociative chemisorption and diffusion in (Nb-Pt) membrane

$$H_{2(g)} + 2^* \rightleftarrows 2H^*$$

C_H^o – solubility of H_2 in membrane

$$K_H = \frac{C_H^2}{P_{H_2} C_*^2}$$

$$C_H + C_* = C_H^o \quad \Rightarrow \quad C_H = \frac{C_H^o \sqrt{K_H P_{H_2}}}{1 + \sqrt{K_H P_{H_2}}} \cong C_H^o \sqrt{K_H P_{H_2}}$$

Hydrogen flux through Nb-Pt membrane

$$J_{H_2}^{memb} = -D_{H_2}^{memb}\frac{dC_H}{dr}$$

$$F_{H_2}^{memb} = 2\pi r \Delta x J_{H_2}^{memb} = 2\pi r \Delta x\left[-D_{H_2}^{memb}\frac{dC_H}{dr}\right]$$

$$F_{H_2}^{memb}\int_{r_1}^{r_2}\frac{dr}{r} = 2\pi\Delta x\left[-D_{H_2}^{memb}\int_{\Theta_1}^{\Theta_2} dC_H\right]$$

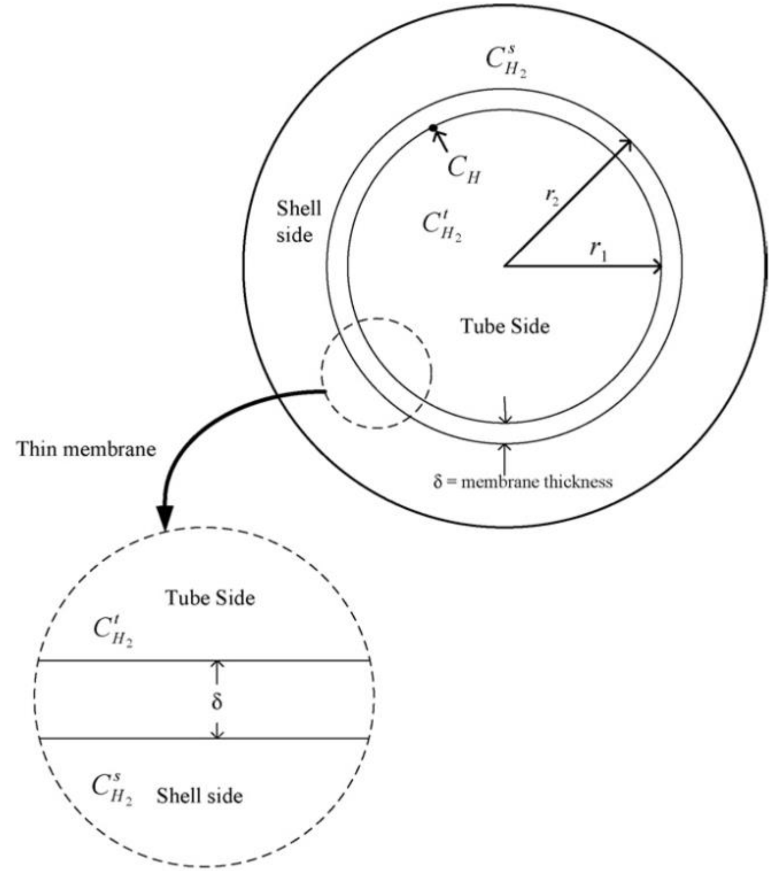
$$F_{H_2}^{memb}\ln\frac{r_2}{r_1} = 2\pi\Delta x D_{H_2}^{memb}\left(C_H(r_1) - C_H(r_2)\right)$$

$$F_{H_2}^{memb} = \frac{2\pi D_{H_2}^{memb}}{\ln\frac{r_2}{r_1}}\Delta x\left(C_H(r_1) - C_H(r_2)\right) =$$

$$= \frac{2\pi D_{H_2}^{memb} C_H^o\sqrt{K_H}}{\ln\frac{r_2}{r_1}}\Delta x\left(\sqrt{P_{H_2}(r_1)} - \sqrt{P_{H_2}(r_2)}\right)$$

$$\frac{F_{H_2}^{memb}}{2\pi r_1\Delta x} = J_{H_2}^{memb}(r_1) = \frac{D_{H_2}^{memb} C_H^o\sqrt{K_H}}{r_1\ln\frac{r_2}{r_1}}\left(\sqrt{P_{H_2}(r_1)} - \sqrt{P_{H_2}(r_2)}\right) = \frac{\Gamma_{H_2}^{(1)}}{\delta}\left(\sqrt{P_{H_2}(r_1)} - \sqrt{P_{H_2}(r_2)}\right)$$

$$\Gamma_{H_2}^{(1)} / \delta$$



$$\Gamma_{H_2}^{(1)} = \frac{0.043122}{T} - 3.0484\text{x}10^{-5} \quad (\text{mole.m}^{-1}.\text{s}^{-1}.\text{kPa}^{-0.5})$$

Balance of hydrogen in tube side (catalyst)

H_2

$$\frac{dF_{H_2}}{dx} = \nu_{H_2} r_M \rho_b \pi r_1^2 - 2\pi r_1 J_{H_2}^{memb}(r_1) = \nu_{H_2} r_M \rho_b \pi r_1^2 - 2\pi r_1 \frac{\Gamma_{H_2}^{(1)}}{\delta}\left(\sqrt{P_{H_2}(r_1)} - \sqrt{P_{H_2}(r_2)}\right)$$

other components

$$\frac{dF_i}{dx} = \nu_i r_M \rho_b \pi r_1^2$$

$$r_M = k(T)\left(P_{H_2S} - P_{H_2} P_{S_2}^{1/2} / K^{eq}(T)\right) \qquad (\text{mol.g}^{-1}.s^{-1})$$

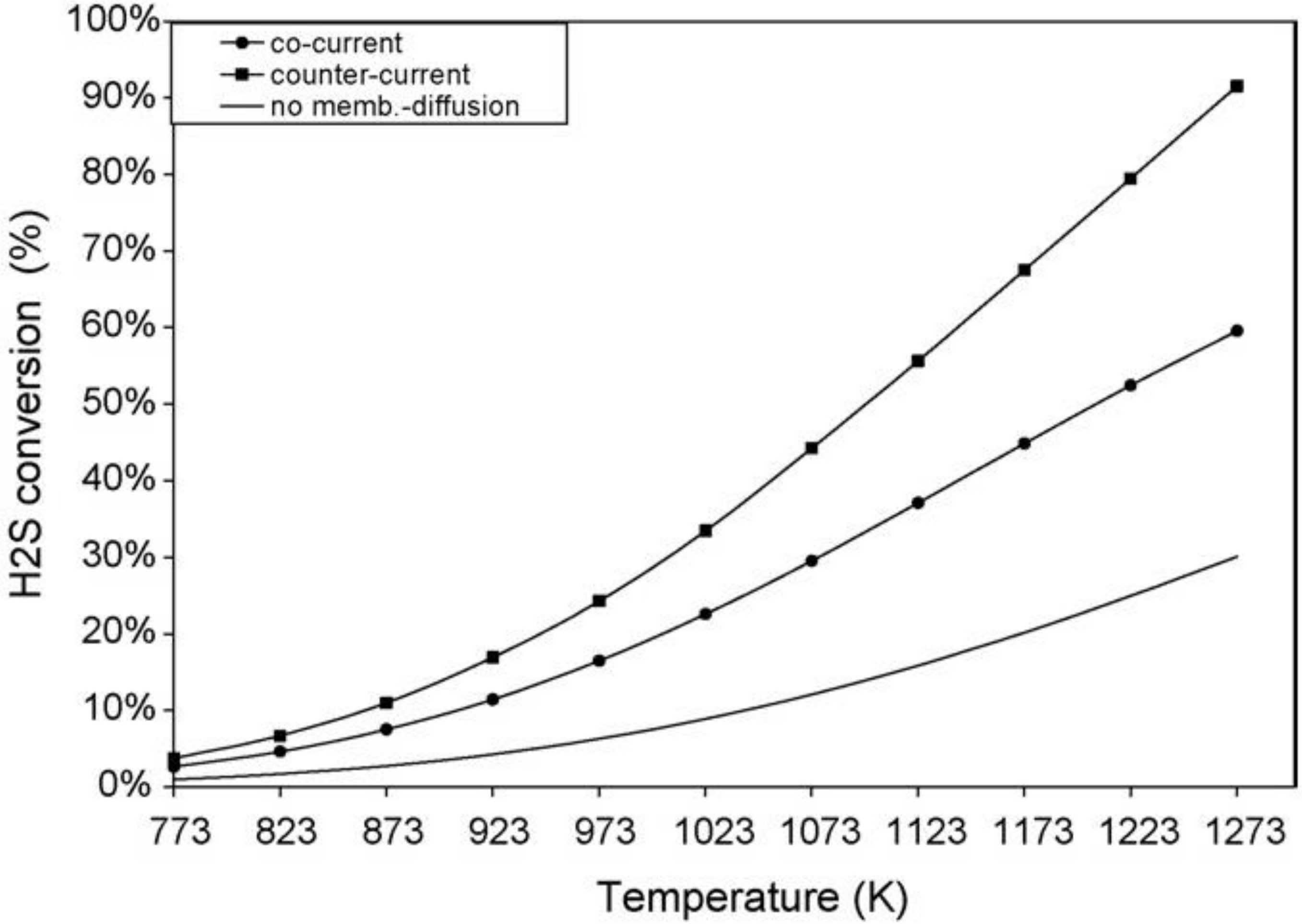
$$k(T) = 0.038505 \exp\left(-\frac{87220}{RT}\right) \qquad (\text{mol.g}^{-1}.s^{-1}.kPa^{-1})$$

$$K^{eq}(T) = 3782 \exp\left(-\frac{10871}{T}\right) \qquad (\text{kPa}^{1/2})$$

Balance of hydrogen in shell-side

co-current (+), contre-current (-)

$$\frac{dF_{H_2}}{dx} = \pm 2\pi r_2 J_{H_2}^{memb}(r_2) = \pm 2\pi r_2 \frac{\Gamma_{H_2}^{(2)}}{\delta}\left(\sqrt{P_{H_2}(r_1)} - \sqrt{P_{H_2}(r_2)}\right)$$


co-current
counter-current
no memb.-diffusion
H2S conversion (%)
100%
90%
80%
70%
60%
50%
40%
30%
20%
10%
0%
773
823
873
923
973
1023
1073
1123
1173
1223
1273
Temperature (K)

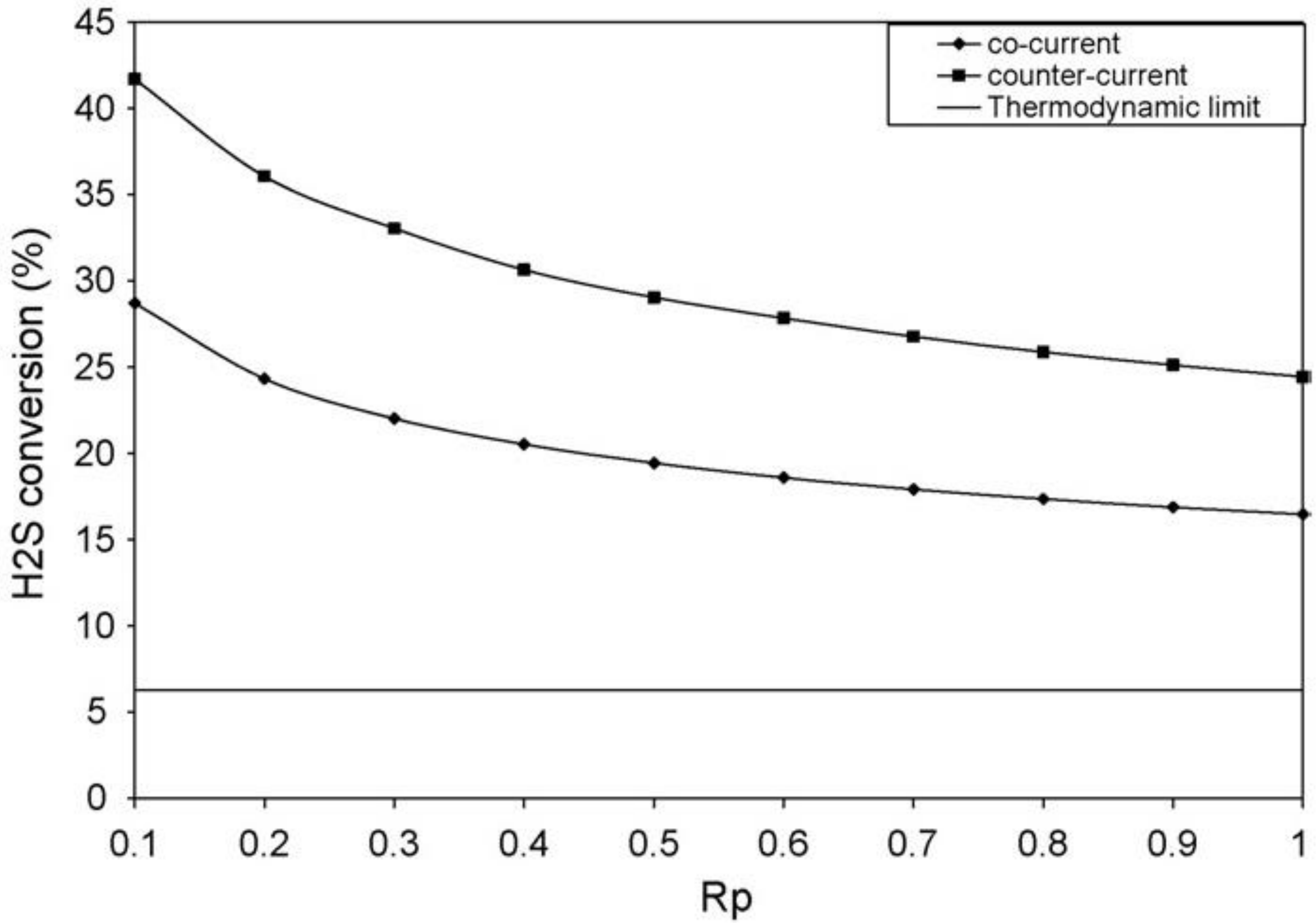


Fig. 6. Effect of shell-tube side pressure ratio on H_2S conversion at $T_o^t = 973\,K$, rtt = 600 s, rts = 600 s ($Da_o^t = 319$, $Tu_o = 3.8$).

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Catalytic decomposition of H_2S in a double-pipe packed bed membrane reactor: Numerical simulation studies

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