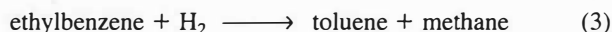


**P8-26<sub>C</sub>** (Comprehensive Problem on multiple reactions with heat effects) Styrene can be produced from ethylbenzene by the following reaction:



However, several irreversible side reactions also occur:



[J. Snyder and B. Subramaniam, *Chem. Eng. Sci.*, 49, 5585 (1994)]. Ethylbenzene is fed at a rate of 0.00344 kmol/s to a 10.0-m<sup>3</sup> PFR (PBR) along with inert steam at a total pressure of 2.4 atm. The steam/ethylbenzene molar ratio is initially [i.e., parts (a) to (c)] 14.5:1 but can be varied. Given the following data, find the exiting molar flow rates of styrene, benzene, and toluene along with  $S_{St/EB}$  for the following inlet temperatures when the reactor is operated adiabatically.

- $T_0 = 800 \text{ K}$
- $T_0 = 930 \text{ K}$
- $T_0 = 1100 \text{ K}$
- Find the ideal inlet temperature for the production of styrene for a steam/ethylbenzene ratio of 58:1. (Hint: Plot the molar flow rate of styrene versus  $T_0$ . Explain why your curve looks the way it does.)
- Find the ideal steam/ethylbenzene ratio for the production of styrene at 900 K. [Hint: See part (d).]
- It is proposed to add a counter current heat exchanger with  $Ua = 100 \text{ kJ/m}^2\text{-min/K}$  where  $T_a$  is virtually constant at 1000 K. For an entering steam to ethylbenzene ratio of 20, what would you suggest as an entering temperature? Plot the molar flow rates and  $S_{St/EB}$ .



Additional information:

Heat capacities

Methane	68 J/mol·K	Styrene	273 J/mol·K
Ethylene	90 J/mol·K	Ethylbenzene	299 J/mol·K
Benzene	201 J/mol·K	Hydrogen	30 J/mol·K
Toluene	249 J/mol·K	Steam	40 J/mol·K

$\rho_c = 2137 \text{ kg/m}^3$  of pellet

$\phi = 0.4 \rightarrow \text{Bed porosity} \} \rho_B = \rho_c (1 - \phi)$

$\Delta H_{R1EB}^\circ = 118,000 \text{ kJ/kmol ethylbenzene}$

$\Delta H_{R2EB}^\circ = 105,200 \text{ kJ/kmol ethylbenzene}$

$\Delta H_{R3EB}^\circ = -53,900 \text{ kJ/kmol ethylbenzene}$

Experimentally determined Equilibrium constant for  $r_{1st}$

$$K_{p1} = \exp \left\{ b_1 + \frac{b_2}{T} + b_3 \ln(T) + [(b_4 T + b_5) T + b_6] T \right\}_{\text{atm}}$$

$$\left. \begin{array}{ll} b_1 = -17.34 & b_4 = -2.314 \times 10^{-10} \\ b_2 = -1.302 \times 10^4 & b_5 = 1.302 \times 10^{-6} \\ b_3 = 5.051 & b_6 = -4.931 \times 10^{-3} \end{array} \right\}$$

The kinetic rate laws for the formation of styrene (St), benzene (B), and toluene (T), respectively, are as follows. (EB = ethylbenzene)

$$r_{1st} = \underbrace{\rho(1-\phi)}_{\rho_B} \exp \left( \underbrace{-0.08539 - \frac{10,925}{T}}_{k_1'} \right) \left( P_{EB} - \frac{P_{St} P_{H_2}}{K_{p1}} \right) \quad (\text{kmol/m}^3 \cdot \text{s})$$

$$r_{2B} = \underbrace{\rho(1-\phi)}_{\rho_B} \exp \left( \underbrace{13.2392 - \frac{25,000}{T}}_{k_2'} \right) (P_{EB}) \quad (\text{kmol/m}^3 \cdot \text{s})$$

$$r_{3T} = \underbrace{\rho(1-\phi)}_{\rho_B} \exp \left( \underbrace{0.2961 - \frac{11,000}{T}}_{k_3'} \right) (P_{EB} P_{H_2}) \quad (\text{kmol/m}^3 \cdot \text{s})$$

The temperature  $T$  is in Kelvin and  $P_i$  is in atm.

$$\rightarrow = \left( \frac{F_i}{F_T} \right) P_{Tot}$$

Not enough info for E&G.W.  $\Rightarrow \Delta P_{Tot} = 0$   
Can you solve if  $\frac{dP}{dV} \neq 0$  ??