P8-26$_C$ *(Comprehensive Problem on multiple reactions with heat effects)* Styrene can be produced from ethylbenzene by the following reaction:

$$\text{ethylbenzene} \longleftrightarrow \text{styrene} + H_2 \qquad (1)$$

However, several irreversible side reactions also occur:

$$\text{ethylbenzene} \longrightarrow \text{benzene} + \text{ethylene} \qquad (2)$$

$$\text{ethylbenzene} + H_2 \longrightarrow \text{toluene} + \text{methane} \qquad (3)$$

Member

Hall of Fame

[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^3 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 $\tilde{S}_{St/BT}$ for the following inlet temperatures when the reactor is operated adiabatically.

(a) $T_0 = 800$ K
(b) $T_0 = 930$ K
(c) $T_0 = 1100$ K

(d) 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.)
(e) Find the ideal steam/ethylbenzene ratio for the production of styrene at 900 K. [*Hint:* See part (d).]
(f) It is proposed to add a counter current heat exchanger with Ua = 100 kJ/m^3/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 $\tilde{S}_{St/BT}$.

Additional information:

Average $\bar{C}_P$ values, For $\Delta \bar{C}_{P_{RX}}$

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

$\rho_c = 2137$ kg/m^3 of pellet
$\phi = 0.4 \rightarrow$ Bed porosity $\} \; \rho_B = \rho_c(1-\phi)$

$\Delta H^\circ_{Rx1EB} = 118{,}000$ kJ/kmol ethylbenzene

$\Delta H^\circ_{Rx2EB} = 105{,}200$ kJ/kmol ethylbenzene

$\Delta H^\circ_{Rx3EB} = -53{,}900$ kJ/kmol ethylbenzene

Experimentally determined Equilibrium constant for r_{1ST}

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

$b_1 = -17.34$ $\qquad b_4 = -2.314 \times 10^{-10}$
$b_2 = -1.302 \times 10^4$ $\qquad b_5 = 1.302 \times 10^{-6}$
$b_3 = 5.051$ $\qquad b_6 = -4.931 \times 10^{-3}$

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

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

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

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

Not enough info for ERGUN. $\Rightarrow \Delta P_{TOT} = 0$
Can you solve if $\frac{dP}{dV} \neq 0$??

The temperature T is in Kelvin and $\boxed{P_i}$ is in atm.

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