ChE 4063 Final Dec 6, 2001

Solution

I. $M \rightarrow (1/n) P_N$

A. $0.7 = A e^{-25000/1.987(248)}$

$A = 1.518 \times 10^{18}$

@ 30°C = 30K

$k_{20°C} = 1.518 \times 10^{18} e^{-25000/1.987 * 303}$

$k_{30°C} = 1.405 \text{ lt}^{1/2}/\text{mole}^{1/2}\text{-min}$

$$\tau = \frac{2500 \text{ lt}}{1000 \text{ lt/min}} = 2 \int_0^{f_A} \frac{df_A}{(1.405)(2^{1/2})(1-f_A)^{3/2}}$$

$$(2.5)(1.405)(2^{1/2}) = \int_0^{f_A} \frac{df_A}{(1-f_A)^{3/2}} = (1-f_A)^{-3/2+1}(-1) \Big/ (-3/2+1) \Big]_0^{f_A}$$

$$4.9674 = \frac{2}{(1-f_A)^{1/2}} \Big]_0^{f_A} = \frac{2}{(1-f_A)^{1/2}} - 2$$

$$6.9674 = \frac{2}{\sqrt{1-f_A}}$$

$$48.545(1-f_A) = 4$$

$$-48.545 f_A = -44.545$$

$$\boxed{f_A = 0.9176}$$

B. $$\tau = 2.5 = \frac{C_{A0}(f_{A,out} - f_{A,in})}{k C_{A0}^{3/2}(1-f_A)^{3/2}} = \frac{2 f_M}{k 2^{3/2}(1-f_M)^{3/2}}$$

$$2.5 = \frac{f_M}{k\sqrt{2}(1-f_M)^{3/2}}$$

$$2.5 = \frac{f_M}{A e^{-E/RT} \sqrt{2} (1-f_M)^{3/2}}$$

$$T = 298 + \frac{3180 f_M}{(600 - 35 f_M)}$$

1) only variable then is f_M.

Solve for f_M

f_M (guess)	T (eqn 1)	k	$f_M/(k\sqrt{2}(1-f_M)^{3/2}$
0.9	303.03	1.411	14.2
0.8	302.45	1.302	4.86
0.7	301.87	1.202	2.505
0.69	301.81	1.193	2.3700
(interpolate) 0.6996	301.87	1.202	2.499917

pretty close

f_M ↑ T_{OUT} ↑

c. $$2.5 = 2 \int_0^{f_A} \frac{df_A}{k 2^{3/2} (1-f_A)^{3/2}}$$

$$3.5355 = \int_0^{f_A} \frac{df_A}{k (1-f_A)^{3/2}}$$

solve:

$f_M = 0.89$
$T_{out} = 302.98$

} see attached

Adiabatic CSTR

fm	T	k	RHS
0.6996	301.86564	1.2018391	2.49999174

Adiabatic PFR:

fm	T	k	1/k(1-fm)^3/2	[1/k(1-fm)^3/2]avg*dfm	Sum
0.00	298.00	0.6999	1.4288		
0.05	298.27	0.7267	1.4861	0.0729	0.0729
0.10	298.53	0.7547	1.5519	0.0759	0.1488
0.15	298.80	0.7839	1.6279	0.0795	0.2283
0.20	299.07	0.8143	1.7162	0.0836	0.3119
0.25	299.34	0.8461	1.8197	0.0884	0.4003
0.30	299.62	0.8792	1.9421	0.0940	0.4944
0.35	299.89	0.9137	2.0884	0.1008	0.5951
0.40	300.17	0.9498	2.2654	0.1088	0.7040
0.45	300.45	0.9874	2.4828	0.1187	0.8227
0.50	300.73	1.0268	2.7547	0.1309	0.9536
0.55	301.01	1.0678	3.1024	0.1464	1.1000
0.60	301.30	1.1107	3.5590	0.1665	1.2666
0.65	301.58	1.1554	4.1797	0.1935	1.4600
0.70	301.87	1.2022	5.0621	0.2310	1.6911
0.75	302.16	1.2511	6.3944	0.2864	1.9775
0.80	302.45	1.3022	8.5858	0.3745	2.3520
0.85	302.74	1.3556	12.6980	0.5321	2.8841
0.86	302.80	1.3666	13.9695	0.1333	3.0174
0.87	302.86	1.3776	15.4866	0.1473	3.1647
0.88	302.92	1.3888	17.3218	0.1640	3.3288
0.89	**302.98**	**1.4001**	**19.5779**	**0.1845**	**3.5133**
0.90	303.03	1.4114	22.4050	0.2099	3.7232
0.91	303.09	1.4229	26.0296	0.2422	3.9653
0.92	303.15	1.4345	30.8090	0.2842	4.2495
0.93	303.21	1.4461	37.3376	0.3407	4.5903
0.94	303.27	1.4579	46.6705	0.4200	5.0103

II. $-r_A = 0.5C_A$

$r_B = 0.3C_A - 0.05C_BC_C$

$r_C = 0.2C_A - 0.05C_BC_C$

$$\tau = \frac{C_{A0} - C_A}{-r_A} = \frac{C_B}{r_B} = \frac{C_C}{r_C} = \frac{C_D}{r_D}$$

$4 = 3 - C_A / 0.5C_A$

$\boxed{C_A = 1 \text{ mole/lt}}$

$$\frac{C_B}{0.3C_A - 0.05C_BC_C} = 4 = \frac{C_C}{0.2C_A - 0.05C_BC_C}$$

$C_B = 1.2C_A - 0.2C_BC_C \qquad C_C = 0.8C_A - 0.2C_BC_C$

subtract

$C_B - C_C = 0.4C_A = 0.4$

$$\frac{C_B}{(0.3)(1) - (0.05)(C_B)(C_B - 0.4)} = 4$$

$C_B = 1.2 - 0.2C_B^2 + 0.08C_B \Rightarrow 0.2C_B^2 + 0.92C_B - 1.2 = 0$

$\boxed{C_B = 1.06}$

$\boxed{C_C = 1.06 - 0.4 = 0.66}$

$$\frac{C_D}{(0.05)(0.66)(1.06)} = 4$$

$\boxed{C_D = 0.14}$

Check C_A reacted $= 3 - 1 = 2 = C_B + C_C + 2C_D \stackrel{?}{=} 1.06 + 0.66 + 2(0.14)$ ✓