(*) Solution:

$A \xrightarrow{K_1} B$

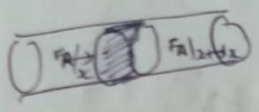
$B \xrightarrow{K_2} A$

$A \xrightarrow{K_3} C.$

$\left[A \underset{K_2}{\overset{K_1}{\rightleftharpoons}} B \quad ; \quad A \xrightarrow{K_3} C. \right] \left[\frac{\gamma_{1A}}{1} = \frac{\gamma_{1B}}{1} \right]$

→ In PBR Reactor.

Mole balance:-



$F_A|_x - F_A|_{x+\Delta x} + (-\gamma_A)\Delta W = 0$

Here **

$\gamma_A = \frac{\text{moles of A}}{(\text{time})(\text{mass of catalyst})}$

$$\boxed{\frac{dF_A}{dW} = \gamma_A} \quad \text{—(1)}$$

Ily we write mole balance equation for B, C.

$$\boxed{\frac{dF_B}{dW} = \gamma_B} \quad \text{—(2)}$$

$$\boxed{\frac{dF_C}{dW} = \gamma_C} \quad \text{—(3)}$$

and

$\gamma_A = -\gamma_{1A} + \gamma_{2B} - \gamma_{3A}$

$\gamma_B = +\gamma_{1A} - \gamma_{2B}$

$\gamma_C = +\gamma_{3A}$

where $\gamma_{1A} = +K_1 C_a$

$\gamma_{2B} = +K_2 C_b$

$\gamma_{3A} = +K_3 C_a$

→ for $P = P_0$

$$C_A = C_T \left(\frac{F_A}{F_T}\right)\left(\frac{T_0}{T}\right)$$

$$C_B = C_T \left(\frac{F_B}{F_T}\right)\left(\frac{T_0}{T}\right)$$

$$\rightarrow k_1 = 0.5 \exp\left(2\left(1 - \frac{320}{T}\right)\right)$$

$$\rightarrow k_c = 10 \exp\left[4.8\left(\frac{432}{T} - 1.5\right)\right]$$

$$\rightarrow k_2 = k_1 / k_c$$

$$\rightarrow k_3 = 0.005 \exp\left[4.6\left(1 - \frac{460}{T}\right)\right]$$

→ Constant value.

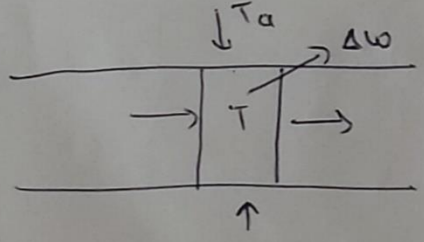
$T_0 = 330$ $\quad T_a = 500$ $\quad C_T = 2$ $\quad F_T = 2$

$\frac{UA}{\rho} = 16$ $\quad \Delta h_{rxn1} = -1800$ $\quad C_{PA} = 100$

$\Delta h_{rxn2} = 1800$ $\quad C_{PB} = 100$

$\Delta h_{rxn3} = -1100$ $\quad C_{PC} = 100$

→ Energy Balance.



$$Q = \frac{UA}{\rho}(T_a - T)\,\Delta Q$$

$$(\Sigma F_i h_i)|_w - \Sigma [F_i h_i)|_{w+\Delta w} + UA(T_a - T)\Delta w = 0$$

$$UA(T_a - T) = \frac{d}{dw}[\Sigma F_i h_i]$$

$$\Sigma F_i \frac{dh_i}{dw} + \Sigma h_i \left(\frac{dF_i}{dw}\right) = UA(T_a - T)$$

$$\left\{ \Sigma dF_i \frac{dh_i}{dw} = \Sigma F_i \left(\frac{dh_i}{dT}\right)\left(\frac{dT}{dw}\right) = \left(\frac{dT}{dw}\right) \Sigma F_i C_p \right\}$$

$$\left\{ \Sigma h_i \frac{dF_i}{dw} = \Sigma h_i \left(\sum_{j=1}^{r} \gamma_{ij}\right) \right\}$$

γ_i = moles of i / (time)(mass of catalyst) **

$$\frac{dT}{dw} = \frac{\frac{UA}{g}(T_a - T) + \sum_{j=1}^{r} \gamma_j (\Delta h_{rxn})_j}{\sum_{i=1}^{i} F_i C_{pi}} \quad -(4)$$

$$\frac{dF_A}{dw} = \gamma_A \quad -(1) \qquad \frac{dF_B}{dw} = \gamma_B \quad -(2) \qquad \frac{dF_C}{dw} = \gamma_C \quad -(3)$$

** variable = F_A, F_B, F_C, T

** for coding = y_1, y_2, y_3, y_4

$$\gamma_A = -\gamma_{1A} + \gamma_{2B} - \gamma_{3A}$$

$$\gamma_B = +\gamma_{1A} - \gamma_{2B}$$

$$\gamma_C = +\gamma_{3A}$$

$$\gamma_{1A} = +k_1 C_A$$

$$\gamma_{2B} = +k_2 C_B$$

$$\gamma_{3A} = +k_3 C_A$$

$$C_A = C_T \left(\frac{F_A}{F_T}\right)\left(\frac{T_0}{T}\right) \qquad C_B = C_T \left(\frac{F_B}{F_T}\right)\left(\frac{T_0}{T}\right)$$

→ for coding purpose F_A, F_B, F_C, T → changes to y_1, y_2, y_3, y_3

then ODEs changes.

$$\frac{dy_1}{dW} = \gamma_A \qquad \frac{dy_2}{dW} = \gamma_B \qquad \frac{dy_3}{dW} = \gamma_C$$

$$\frac{dy_4}{dW} = \frac{\frac{U_a}{S}(T_a - T_0) + (-\gamma_{1A})(-\Delta H_{RXN1}) + (\gamma_{2A})(-\Delta H_{RXN2}) + (-\gamma_{3A})(-\Delta H_{RXN3})}{\gamma_1 C_{PA} + y_2 C_{PB} + y_3 C_{PC}}$$

and we put $\gamma_A, \gamma_B, \gamma_C, -\gamma_{1A}, \gamma_{2B}, -\gamma_{3A}$ in terms of y_1, y_2, y_3, y_4 in order to solve with ODE 45 solver tool.

→ **Part 1**

- $F_{A0} = 1$ mol/min $\qquad F_{B0} = 1$ mol/min
- $T_0 = 330$ $\qquad F_{C0} = 0$

means initial conditions:

$y_{10} = 1 \qquad y_{20} = 1 \qquad y_{30} = 0 \qquad y_{40} = 330$

→ we solve this ODE with Matlab Software with ODE45 solver tool.

```
to = 330;
ta = 500;
ct = 2;
ft = 2;
uabyrho = 16;
hrxn1 = -1800;
hrxn2 = 1800;
hrxn3 = -1100;
cpa = 100;
cpb = 100;
cpc = 100;
%k1 = 0.5*exp(2*(1-(320/T)));
%kc = 10*exp(4.8*((432/T)-1.5));
%k2 = (0.5*exp(2*(1-(320/T))))/(10*exp(4.8*((432/T)-1.5)));
%k3 = 0.005*exp(4.6*(1-(460/T)));
%ca = ct*(fa/ft)*(to/T);
%cb = ct*(fb/ft)*(to/T);
%r1a = (0.5*exp(2*(1-(320/y(4)))))*(ct*(y(1)/ft)*(to/y(4)));
%r2b = (0.5*exp(2*(1-(320/y(4)))))/(10*exp(4.8*((432/y(4))-
1.5)))*(ct*(y(2)/ft)*(to/y(4)));
%r3a = 0.005*exp(4.6*(1-(460/y(4))))*(ct*(y(1)/ft)*(to/y(4)));
%ra = -((0.5*exp(2*(1-(320/y(4)))))*(ct*(y(1)/ft)*(to/y(4))))+((0.5*exp(2*(1-
(320/y(4)))))/(10*exp(4.8*((432/y(4))-1.5)))*(ct*(y(2)/ft)*(to/y(4))))-
(0.005*exp(4.6*(1-(460/y(4))))*(ct*(y(1)/ft)*(to/y(4))));
%rb = ((0.5*exp(2*(1-(320/y(4)))))*(ct*(y(1)/ft)*(to/y(4))))-((0.5*exp(2*(1-
(320/y(4)))))/(10*exp(4.8*((432/y(4))-1.5)))*(ct*(y(2)/ft)*(to/y(4))));
%rc = (0.005*exp(4.6*(1-(460/y(4))))*(ct*(y(1)/ft)*(to/y(4))));

f =@(w,y) [-((0.5*exp(2*(1-(320/y(4)))))*(ct*(y(1)/ft)*(to/y(4))))+((0.5*exp(2*(1-
(320/y(4)))))/(10*exp(4.8*((432/y(4))-1.5)))*(ct*(y(2)/ft)*(to/y(4))))-
(0.005*exp(4.6*(1-(460/y(4))))*(ct*(y(1)/ft)*(to/y(4)))); ((0.5*exp(2*(1-
(320/y(4)))))*(ct*(y(1)/ft)*(to/y(4))))-((0.5*exp(2*(1-
(320/y(4)))))/(10*exp(4.8*((432/y(4))-1.5)))*(ct*(y(2)/ft)*(to/y(4))));
(0.005*exp(4.6*(1-(460/y(4))))*(ct*(y(1)/ft)*(to/y(4)))); (uabyrho*(ta-y(4))+(-
((0.5*exp(2*(1-(320/y(4)))))*(ct*(y(1)/ft)*(to/y(4)))))*(-hrxn1)+(((0.5*exp(2*(1-
(320/y(4)))))/(10*exp(4.8*((432/y(4))-1.5)))*(ct*(y(2)/ft)*(to/y(4)))))*(-
hrxn2)+(-(0.005*exp(4.6*(1-(460/y(4))))*(ct*(y(1)/ft)*(to/y(4)))))*(-
hrxn3))/((y(1)*cpa)+(y(2)*cpb)+(y(3)*cpc))];
[w,y] = ode45(f,[0 100],[1; 1; 0; 330])
figure(1)
plot(w,y(:,1),'-o',w,y(:,2),'-o',w,y(:,3),'-o')
xlabel('w weight')
ylabel('y flowrate')
figure(2)
plot(w,y(:,4),'-o')
xlabel('w weight')
ylabel('y(4) tempearture')
```

w =

0
0.0615
0.1231
0.1846
0.2461
0.5537
0.8614
1.1690
1.4766
1.7733
2.0699
2.3666
2.6633
2.9914
3.3196
3.6478
3.9759
4.3283
4.6806
5.0330
5.3854
5.7927
6.2001
6.6075
7.0148
7.5033
7.9918
8.4803
8.9687

9.5965

10.2242

10.8520

11.4797

12.4825

13.4853

14.4880

15.4908

16.4275

17.3641

18.3008

19.2374

19.9943

20.7511

21.5079

22.2648

22.9486

23.6325

24.3163

25.0002

25.7760

26.5517

27.3275

28.1033

29.0392

29.9752

30.9111

31.8470

32.8199

33.7928

34.7656

35.7385

36.5631

37.3878

38.2124

39.0371

39.7263

40.4156

41.1048

41.7941

42.5008

43.2074

43.9141

44.6208

45.4771

46.3334

47.1897

48.0460

49.0283

50.0107

50.9930

51.9753

52.8821

53.7889

54.6956

55.6024

56.3342

57.0660

57.7978

58.5297

59.1967

59.8637

60.5308

61.1978

61.9666

62.7354

63.5043

64.2731

65.2105

66.1479

67.0852

68.0226

68.9924

69.9622

70.9320

71.9018

72.7097

73.5175

74.3253

75.1331

75.8024

76.4716

77.1409

77.8101

78.5043

79.1985

79.8927

80.5868

81.4409

82.2950

83.1491

84.0032

84.9869

85.9705

86.9542

87.9378

88.6517

89.3656

90.0794

90.7933

91.5072

92.2210

92.9349

93.6488

94.5051

95.3615

96.2179

97.0742

97.8057

98.5371

99.2686

100.0000

y =

1.0000	1.0000	0.0000	330.0000
0.9760	1.0240	0.0000	330.4697
0.9529	1.0470	0.0001	330.9411
0.9309	1.0690	0.0001	331.4140
0.9097	1.0901	0.0002	331.8881
0.8170	1.1825	0.0004	334.2681
0.7436	1.2558	0.0006	336.6477
0.6865	1.3127	0.0008	339.0068

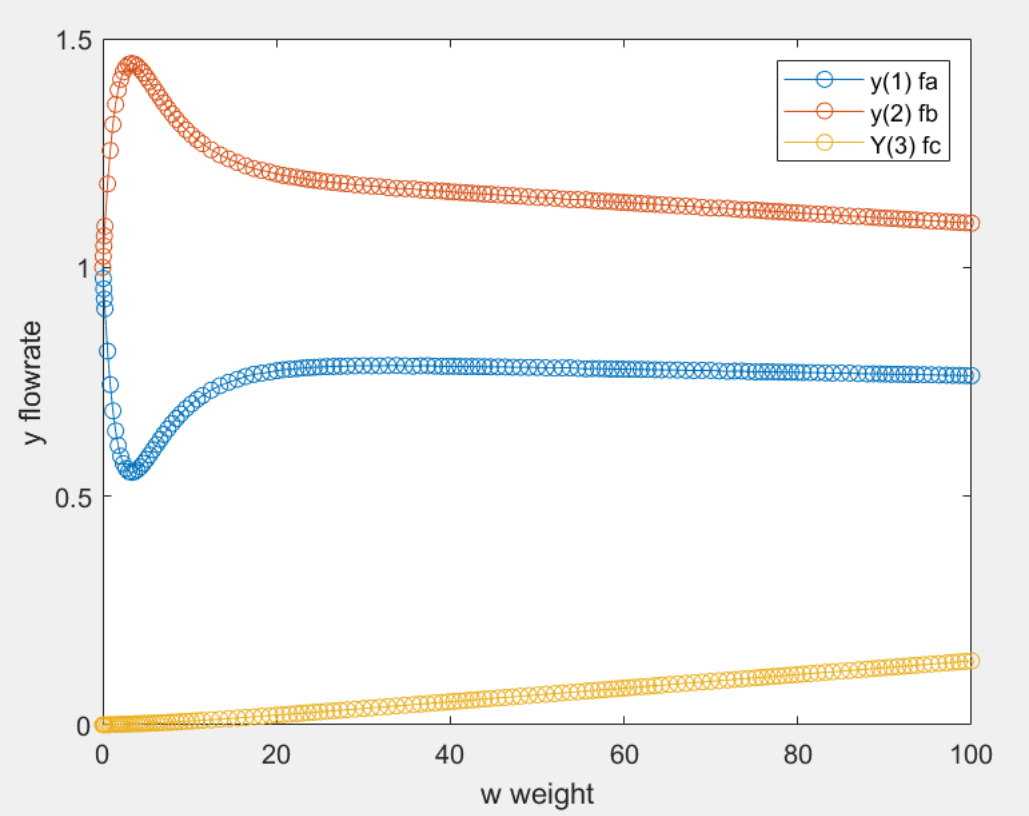
0.6427	1.3563	0.0010	341.3274
0.6107	1.3881	0.0012	343.5154
0.5873	1.4113	0.0014	345.6466
0.5710	1.4274	0.0016	347.7149
0.5604	1.4378	0.0018	349.7148
0.5539	1.4441	0.0020	351.8428
0.5519	1.4459	0.0022	353.8810
0.5534	1.4442	0.0024	355.8290
0.5574	1.4399	0.0026	357.6866
0.5638	1.4334	0.0029	359.5815
0.5716	1.4253	0.0031	361.3765
0.5806	1.4160	0.0034	363.0749
0.5901	1.4062	0.0037	364.6801
0.6014	1.3946	0.0040	366.4243
0.6128	1.3829	0.0043	368.0558
0.6240	1.3713	0.0047	369.5811
0.6349	1.3600	0.0051	371.0064
0.6472	1.3472	0.0056	372.5918
0.6588	1.3351	0.0060	374.0525
0.6697	1.3237	0.0065	375.3983
0.6798	1.3132	0.0071	376.6381
0.6915	1.3008	0.0077	378.0890
0.7020	1.2895	0.0085	379.3949
0.7114	1.2794	0.0092	380.5706
0.7199	1.2702	0.0099	381.6294
0.7318	1.2570	0.0112	383.1091
0.7415	1.2460	0.0124	384.3622
0.7491	1.2372	0.0138	385.4226
0.7554	1.2295	0.0151	386.3236
0.7615	1.2221	0.0164	387.0467
0.7662	1.2162	0.0176	387.6679

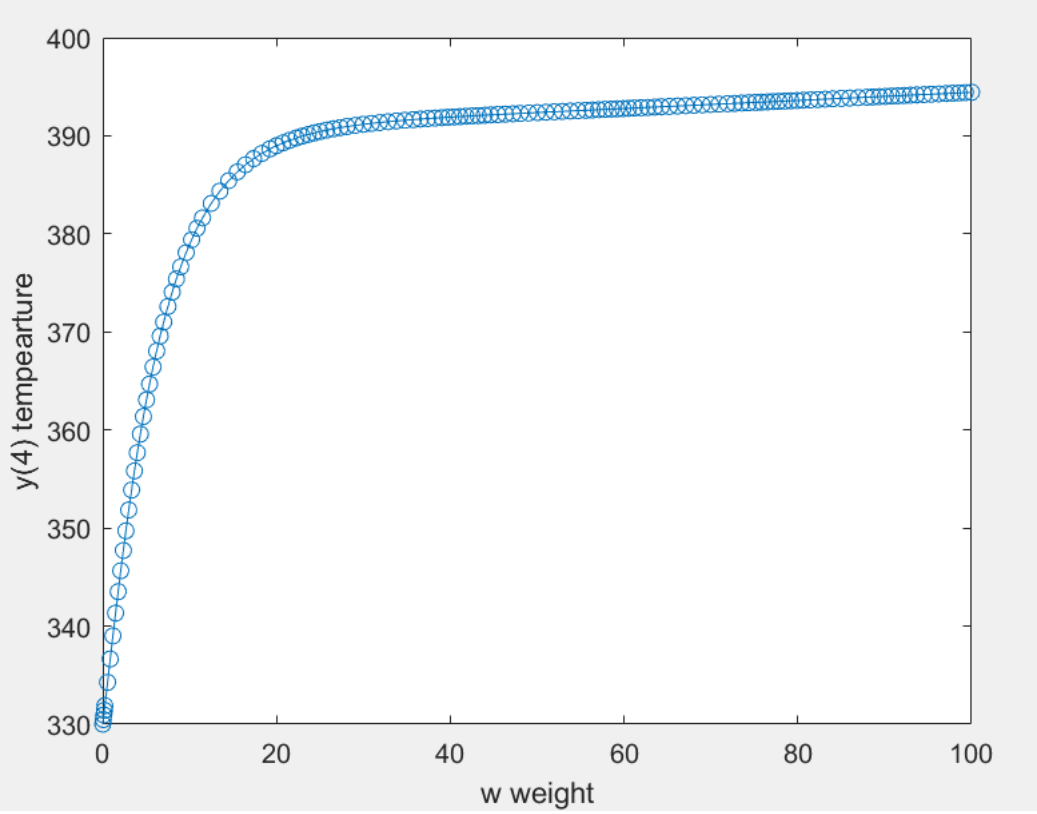
0.7689	1.2122	0.0189	388.2003
0.7713	1.2084	0.0203	388.6608
0.7742	1.2044	0.0213	388.9902
0.7764	1.2012	0.0224	389.2829
0.7775	1.1990	0.0235	389.5424
0.7785	1.1969	0.0246	389.7746
0.7799	1.1945	0.0256	389.9649
0.7810	1.1925	0.0265	390.1371
0.7817	1.1908	0.0275	390.2930
0.7823	1.1892	0.0285	390.4349
0.7831	1.1873	0.0297	390.5814
0.7837	1.1855	0.0308	390.7137
0.7840	1.1841	0.0319	390.8332
0.7842	1.1827	0.0331	390.9418
0.7848	1.1807	0.0344	391.0612
0.7851	1.1791	0.0358	391.1684
0.7850	1.1778	0.0372	391.2645
0.7849	1.1765	0.0386	391.3523
0.7856	1.1744	0.0400	391.4377
0.7857	1.1728	0.0415	391.5153
0.7848	1.1723	0.0429	391.5848
0.7842	1.1714	0.0443	391.6503
0.7850	1.1694	0.0456	391.7053
0.7852	1.1680	0.0468	391.7566
0.7843	1.1677	0.0480	391.8032
0.7836	1.1672	0.0492	391.8485
0.7839	1.1658	0.0503	391.8870
0.7840	1.1647	0.0513	391.9238
0.7836	1.1641	0.0523	391.9589
0.7833	1.1634	0.0533	391.9931
0.7833	1.1623	0.0544	392.0282

0.7832	1.1614	0.0554	392.0624
0.7829	1.1606	0.0565	392.0956
0.7826	1.1598	0.0575	392.1283
0.7826	1.1586	0.0588	392.1678
0.7823	1.1576	0.0601	392.2064
0.7819	1.1567	0.0613	392.2441
0.7815	1.1558	0.0626	392.2814
0.7817	1.1543	0.0641	392.3249
0.7815	1.1530	0.0655	392.3673
0.7806	1.1524	0.0670	392.4080
0.7799	1.1516	0.0685	392.4489
0.7806	1.1496	0.0698	392.4889
0.7806	1.1483	0.0712	392.5274
0.7792	1.1482	0.0725	392.5631
0.7783	1.1478	0.0739	392.5994
0.7788	1.1462	0.0749	392.6313
0.7789	1.1451	0.0760	392.6622
0.7783	1.1446	0.0771	392.6916
0.7777	1.1441	0.0782	392.7211
0.7778	1.1430	0.0792	392.7492
0.7777	1.1421	0.0802	392.7769
0.7774	1.1414	0.0812	392.8041
0.7771	1.1408	0.0822	392.8313
0.7770	1.1397	0.0833	392.8632
0.7768	1.1388	0.0845	392.8948
0.7764	1.1380	0.0856	392.9261
0.7761	1.1372	0.0867	392.9575
0.7760	1.1359	0.0881	392.9964
0.7757	1.1347	0.0895	393.0350
0.7751	1.1340	0.0909	393.0728
0.7746	1.1331	0.0923	393.1109

0.7750	1.1313	0.0938	393.1521
0.7749	1.1299	0.0952	393.1924
0.7736	1.1297	0.0966	393.2303
0.7727	1.1292	0.0981	393.2691
0.7734	1.1273	0.0993	393.3042
0.7735	1.1260	0.1005	393.3381
0.7724	1.1259	0.1017	393.3698
0.7716	1.1255	0.1029	393.4020
0.7719	1.1242	0.1039	393.4305
0.7719	1.1232	0.1049	393.4586
0.7715	1.1226	0.1059	393.4858
0.7712	1.1220	0.1069	393.5131
0.7711	1.1210	0.1079	393.5421
0.7709	1.1201	0.1089	393.5710
0.7706	1.1194	0.1100	393.5994
0.7703	1.1187	0.1110	393.6280
0.7702	1.1176	0.1123	393.6636
0.7699	1.1165	0.1135	393.6990
0.7695	1.1157	0.1148	393.7340
0.7691	1.1149	0.1161	393.7692
0.7692	1.1133	0.1175	393.8108
0.7690	1.1120	0.1190	393.8519
0.7680	1.1115	0.1205	393.8916
0.7673	1.1107	0.1219	393.9317
0.7675	1.1095	0.1230	393.9622
0.7674	1.1085	0.1240	393.9922
0.7670	1.1079	0.1251	394.0215
0.7666	1.1073	0.1262	394.0509
0.7665	1.1063	0.1272	394.0811
0.7663	1.1054	0.1283	394.1110
0.7660	1.1047	0.1294	394.1405

0.7656	1.1039	0.1304	394.1702
0.7655	1.1028	0.1317	394.2063
0.7653	1.1017	0.1330	394.2422
0.7648	1.1010	0.1342	394.2776
0.7644	1.1001	0.1355	394.3132
0.7643	1.0991	0.1366	394.3441
0.7641	1.0982	0.1377	394.3749
0.7637	1.0975	0.1388	394.4053
0.7634	1.0967	0.1399	394.4359





→ Part 2

$F_{A0} = 2$ mol/min $\quad F_{B0} = 0$

$T_0 = 330$ $\quad F_{C0} = 0$

means initial conditions

$y_{10} = 1$ $\quad y_{20} = 0$ $\quad y_{30} = 0$ $\quad y_{40} = 330$

→ we solve this ODE with Matlab Software with ODE45 solver tool

```
to = 330;
ta = 500;
ct = 2;
ft = 2;
uabyrho = 16;
hrxn1 = -1800;
hrxn2 = 1800;
hrxn3 = -1100;
cpa = 100;
cpb = 100;
cpc = 100;
%k1 = 0.5*exp(2*(1-(320/T)));
%kc = 10*exp(4.8*((432/T)-1.5));
%k2 = (0.5*exp(2*(1-(320/T))))/(10*exp(4.8*((432/T)-1.5)));
%k3 = 0.005*exp(4.6*(1-(460/T)));
%ca = ct*(fa/ft)*(to/T);
%cb = ct*(fb/ft)*(to/T);
%r1a = (0.5*exp(2*(1-(320/y(4)))))*(ct*(y(1)/ft)*(to/y(4)));
%r2b = (0.5*exp(2*(1-(320/y(4)))))/(10*exp(4.8*((432/y(4))-
1.5)))*(ct*(y(2)/ft)*(to/y(4)));
%r3a = 0.005*exp(4.6*(1-(460/y(4))))*(ct*(y(1)/ft)*(to/y(4)));
%ra = -((0.5*exp(2*(1-(320/y(4)))))*(ct*(y(1)/ft)*(to/y(4))))+((0.5*exp(2*(1-
(320/y(4)))))/(10*exp(4.8*((432/y(4))-1.5)))*(ct*(y(2)/ft)*(to/y(4))))-
(0.005*exp(4.6*(1-(460/y(4))))*(ct*(y(1)/ft)*(to/y(4))));
%rb = ((0.5*exp(2*(1-(320/y(4)))))*(ct*(y(1)/ft)*(to/y(4))))-((0.5*exp(2*(1-
(320/y(4)))))/(10*exp(4.8*((432/y(4))-1.5)))*(ct*(y(2)/ft)*(to/y(4))));
%rc = (0.005*exp(4.6*(1-(460/y(4))))*(ct*(y(1)/ft)*(to/y(4))));

f =@(w,y) [-((0.5*exp(2*(1-(320/y(4)))))*(ct*(y(1)/ft)*(to/y(4))))+((0.5*exp(2*(1-
(320/y(4)))))/(10*exp(4.8*((432/y(4))-1.5)))*(ct*(y(2)/ft)*(to/y(4))))-
(0.005*exp(4.6*(1-(460/y(4))))*(ct*(y(1)/ft)*(to/y(4)))); ((0.5*exp(2*(1-
(320/y(4)))))*(ct*(y(1)/ft)*(to/y(4))))-((0.5*exp(2*(1-
(320/y(4)))))/(10*exp(4.8*((432/y(4))-1.5)))*(ct*(y(2)/ft)*(to/y(4))));
(0.005*exp(4.6*(1-(460/y(4))))*(ct*(y(1)/ft)*(to/y(4)))); (uabyrho*(ta-y(4))+(-
((0.5*exp(2*(1-(320/y(4)))))*(ct*(y(1)/ft)*(to/y(4)))))*(-hrxn1)+(((0.5*exp(2*(1-
(320/y(4)))))/(10*exp(4.8*((432/y(4))-1.5)))*(ct*(y(2)/ft)*(to/y(4)))))*(-
hrxn2)+(-(0.005*exp(4.6*(1-(460/y(4))))*(ct*(y(1)/ft)*(to/y(4)))))*(-
hrxn3))/((y(1)*cpa)+(y(2)*cpb)+(y(3)*cpc))];
[w,y] = ode45(f,[0 100],[2; 0; 0; 330])
figure(1)
plot(w,y(:,1),'-o',w,y(:,2),'-o',w,y(:,3),'-o')
xlabel('w weight')
ylabel('y flowrate')
figure(2)
plot(w,y(:,4),'-o')
xlabel('w weight')
ylabel('y(4) tempearture')
```

w =

0

0.0000

0.0001

0.0001

0.0002

0.0004

0.0007

0.0009

0.0011

0.0023

0.0035

0.0047

0.0059

0.0118

0.0177

0.0236

0.0295

0.0591

0.0886

0.1182

0.1477

0.2955

0.4432

0.5910

0.7388

0.9923

1.2459

1.4995

1.7531

2.0474

2.3417

2.6360

2.9303

3.2387

3.5471

3.8554

4.1638

4.4865

4.8091

5.1318

5.4545

5.8112

6.1679

6.5246

6.8814

7.2981

7.7147

8.1314

8.5481

9.0549

9.5617

10.0685

10.5752

11.2383

11.9014

12.5645

13.2276

14.3693

15.5109

16.6525

17.7941

18.4657

19.1373

19.8089

20.4805

21.1521

21.8237

22.4953

23.1669

24.0597

24.9525

25.8453

26.7381

27.7891

28.8402

29.8913

30.9424

31.6411

32.3397

33.0384

33.7370

34.4357

35.1344

35.8330

36.5317

37.4134

38.2951

39.1769

40.0586

41.0770

42.0955

43.1139

44.1323

44.8390

45.5457

46.2525

46.9592

47.6659

48.3726

49.0793

49.7860

50.6586

51.5313

52.4039

53.2765

54.2722

55.2679

56.2636

57.2593

57.9721

58.6848

59.3975

60.1103

60.8230

61.5357

62.2485

62.9612

63.8265

64.6918

65.5571

66.4224

67.3995

68.3765

69.3535

70.3306

71.2167

72.1027

72.9888

73.8749

74.5917

75.3085

76.0253

76.7421

77.4092

78.0763

78.7433

79.4104

80.1892

80.9679

81.7467

82.5254

83.4675

84.4096

85.3517

86.2938

87.2482

88.2026

89.1569

90.1113

90.8983

91.6853

92.4724

93.2594

93.9208

94.5822

95.2436

95.9050

96.6061

97.3071

98.0082

98.7093

99.0320

99.3546

99.6773

100.0000

y =

2.0000	0.0000	0.0000	330.0000
1.9999	0.0001	0.0000	330.0002
1.9999	0.0001	0.0000	330.0004
1.9998	0.0002	0.0000	330.0006
1.9998	0.0002	0.0000	330.0008
1.9995	0.0005	0.0000	330.0017
1.9993	0.0007	0.0000	330.0027
1.9990	0.0010	0.0000	330.0036
1.9988	0.0012	0.0000	330.0046
1.9975	0.0025	0.0000	330.0093
1.9963	0.0037	0.0000	330.0141
1.9950	0.0050	0.0000	330.0189
1.9938	0.0062	0.0000	330.0237
1.9875	0.0125	0.0000	330.0477
1.9813	0.0187	0.0000	330.0718

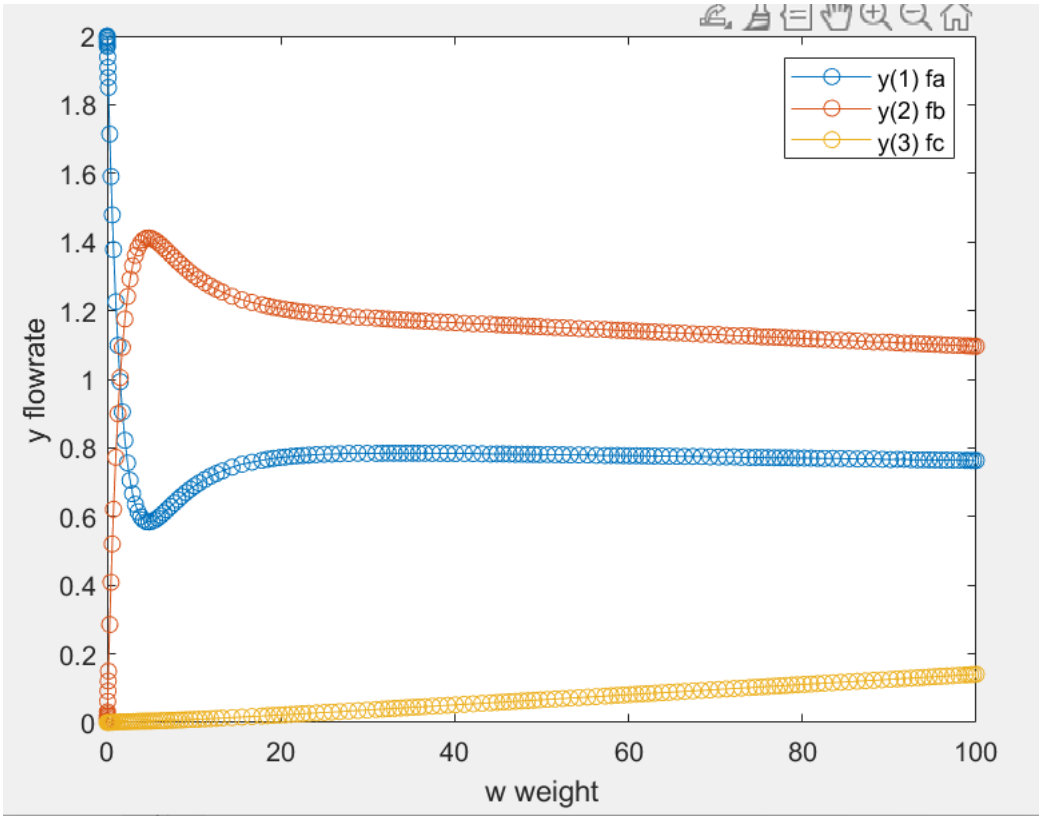
1.9751	0.0249	0.0000	330.0960
1.9689	0.0310	0.0000	330.1203
1.9384	0.0616	0.0001	330.2437
1.9084	0.0915	0.0001	330.3699
1.8790	0.1208	0.0002	330.4989
1.8502	0.1496	0.0002	330.6305
1.7141	0.2854	0.0005	331.3261
1.5908	0.4086	0.0007	332.0784
1.4790	0.5202	0.0008	332.8796
1.3778	0.6212	0.0010	333.7229
1.2260	0.7727	0.0013	335.2495
1.0989	0.8995	0.0016	336.8536
0.9929	1.0052	0.0018	338.5118
0.9050	1.0929	0.0021	340.2029
0.8220	1.1757	0.0023	342.1834
0.7564	1.2410	0.0025	344.1641
0.7055	1.2917	0.0028	346.1284
0.6665	1.3305	0.0030	348.0614
0.6359	1.3609	0.0032	350.0404
0.6141	1.3825	0.0034	351.9645
0.5994	1.3970	0.0036	353.8276
0.5904	1.4058	0.0038	355.6244
0.5854	1.4105	0.0041	357.4296
0.5842	1.4115	0.0043	359.1578
0.5860	1.4095	0.0046	360.8092
0.5898	1.4054	0.0048	362.3837
0.5957	1.3992	0.0051	364.0363
0.6029	1.3918	0.0054	365.5996
0.6110	1.3834	0.0057	367.0771
0.6195	1.3745	0.0060	368.4719
0.6295	1.3641	0.0064	370.0011

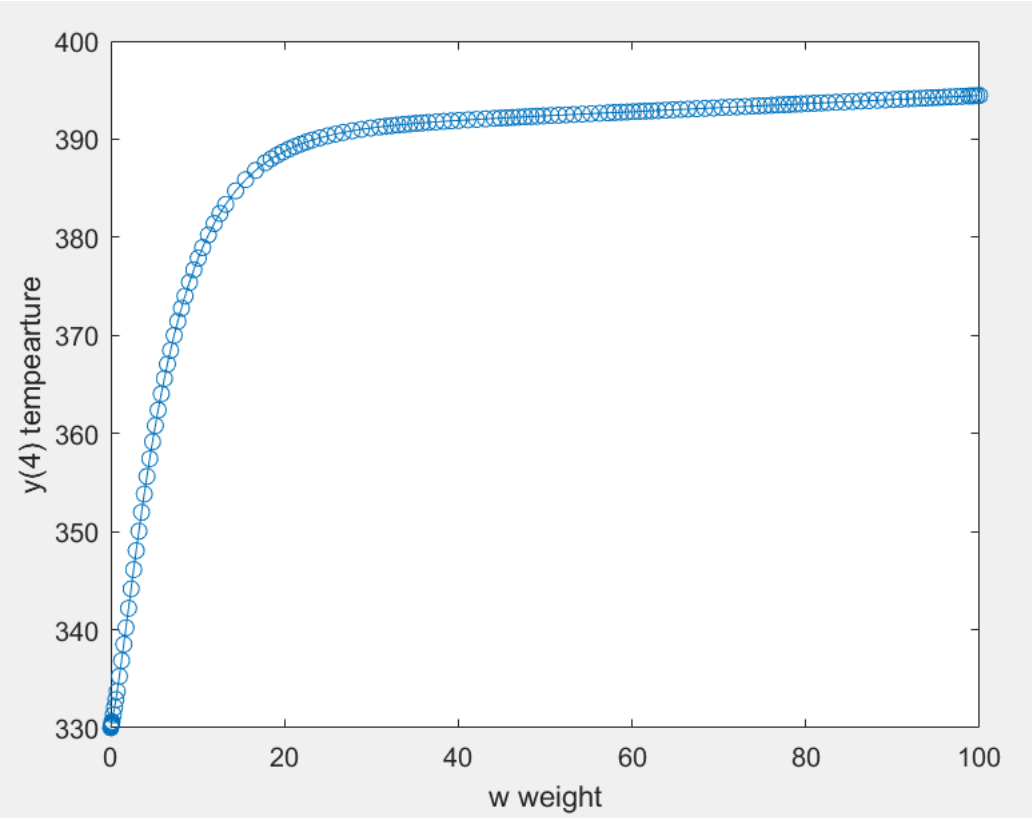
0.6396	1.3537	0.0067	371.4289
0.6495	1.3434	0.0071	372.7617
0.6590	1.3335	0.0076	374.0050
0.6698	1.3221	0.0081	375.4046
0.6799	1.3114	0.0086	376.6904
0.6894	1.3014	0.0092	377.8718
0.6981	1.2922	0.0097	378.9570
0.7083	1.2812	0.0105	380.2449
0.7175	1.2712	0.0113	381.3980
0.7256	1.2623	0.0121	382.4306
0.7328	1.2543	0.0129	383.3559
0.7439	1.2417	0.0144	384.7328
0.7526	1.2315	0.0159	385.8738
0.7586	1.2240	0.0174	386.8175
0.7636	1.2174	0.0190	387.6039
0.7669	1.2132	0.0199	388.0067
0.7696	1.2095	0.0208	388.3686
0.7716	1.2066	0.0218	388.6938
0.7734	1.2038	0.0227	388.9870
0.7752	1.2011	0.0237	389.2522
0.7768	1.1986	0.0247	389.4918
0.7780	1.1964	0.0256	389.7083
0.7791	1.1943	0.0266	389.9045
0.7805	1.1917	0.0279	390.1382
0.7815	1.1893	0.0292	390.3440
0.7822	1.1873	0.0305	390.5255
0.7828	1.1854	0.0318	390.6868
0.7840	1.1827	0.0333	390.8560
0.7846	1.1805	0.0349	391.0039
0.7842	1.1794	0.0364	391.1327
0.7840	1.1780	0.0379	391.2479

0.7846	1.1765	0.0390	391.3193
0.7848	1.1752	0.0400	391.3855
0.7847	1.1743	0.0410	391.4467
0.7845	1.1734	0.0421	391.5043
0.7847	1.1722	0.0431	391.5592
0.7847	1.1712	0.0441	391.6110
0.7845	1.1703	0.0452	391.6599
0.7844	1.1694	0.0462	391.7065
0.7844	1.1681	0.0475	391.7629
0.7843	1.1669	0.0488	391.8162
0.7840	1.1659	0.0501	391.8666
0.7837	1.1649	0.0514	391.9150
0.7839	1.1631	0.0530	391.9701
0.7838	1.1617	0.0545	392.0223
0.7828	1.1612	0.0560	392.0711
0.7822	1.1603	0.0575	392.1191
0.7824	1.1591	0.0585	392.1532
0.7824	1.1580	0.0596	392.1862
0.7820	1.1574	0.0606	392.2180
0.7816	1.1567	0.0617	392.2495
0.7816	1.1557	0.0627	392.2813
0.7814	1.1548	0.0638	392.3125
0.7811	1.1540	0.0648	392.3432
0.7808	1.1533	0.0659	392.3736
0.7807	1.1521	0.0672	392.4114
0.7805	1.1510	0.0685	392.4487
0.7800	1.1502	0.0698	392.4853
0.7796	1.1493	0.0711	392.5218
0.7798	1.1477	0.0726	392.5645
0.7796	1.1464	0.0740	392.6063
0.7786	1.1459	0.0755	392.6464

0.7779	1.1451	0.0770	392.6869
0.7781	1.1438	0.0781	392.7172
0.7780	1.1428	0.0791	392.7470
0.7776	1.1422	0.0802	392.7759
0.7772	1.1416	0.0812	392.8050
0.7772	1.1405	0.0823	392.8347
0.7770	1.1396	0.0834	392.8641
0.7767	1.1389	0.0844	392.8932
0.7763	1.1382	0.0855	392.9223
0.7762	1.1370	0.0868	392.9582
0.7760	1.1360	0.0880	392.9938
0.7755	1.1352	0.0893	393.0290
0.7751	1.1343	0.0906	393.0642
0.7752	1.1327	0.0921	393.1053
0.7750	1.1315	0.0935	393.1456
0.7741	1.1309	0.0950	393.1845
0.7734	1.1302	0.0964	393.2239
0.7740	1.1282	0.0977	393.2622
0.7740	1.1269	0.0991	393.2992
0.7727	1.1269	0.1004	393.3337
0.7718	1.1265	0.1017	393.3689
0.7723	1.1250	0.1028	393.3999
0.7723	1.1238	0.1038	393.4300
0.7717	1.1234	0.1049	393.4588
0.7712	1.1228	0.1060	393.4878
0.7713	1.1218	0.1070	393.5159
0.7712	1.1209	0.1079	393.5436
0.7708	1.1202	0.1089	393.5710
0.7705	1.1195	0.1099	393.5984
0.7704	1.1185	0.1111	393.6308
0.7702	1.1176	0.1122	393.6631

0.7698	1.1168	0.1134	393.6951
0.7695	1.1160	0.1146	393.7272
0.7694	1.1146	0.1160	393.7667
0.7692	1.1135	0.1174	393.8059
0.7685	1.1128	0.1188	393.8443
0.7679	1.1119	0.1202	393.8830
0.7684	1.1100	0.1216	393.9241
0.7683	1.1087	0.1230	393.9643
0.7670	1.1086	0.1244	394.0021
0.7661	1.1081	0.1258	394.0407
0.7668	1.1062	0.1270	394.0753
0.7668	1.1050	0.1282	394.1088
0.7658	1.1048	0.1294	394.1402
0.7651	1.1044	0.1305	394.1721
0.7653	1.1032	0.1315	394.2007
0.7653	1.1022	0.1325	394.2287
0.7649	1.1016	0.1335	394.2561
0.7646	1.1010	0.1345	394.2835
0.7645	1.1000	0.1355	394.3132
0.7643	1.0991	0.1365	394.3427
0.7640	1.0984	0.1376	394.3718
0.7637	1.0977	0.1386	394.4011
0.7636	1.0973	0.1391	394.4147
0.7635	1.0969	0.1396	394.4282
0.7634	1.0965	0.1401	394.4418
0.7633	1.0962	0.1405	394.4554


y(1) fa
y(2) fb
y(3) fc
y flowrate
w weight
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
20
40
60
80
100


y(4) tempearture
w weight
330
340
350
360
370
380
390
400
0
20
40
60
80
100

Solution 2 :

$A \leftrightarrow P + D$

$A \longrightarrow B + C$

$A + D \longrightarrow E + F$

→ $F_{A0} = 3.44$ mol/sec $= 0.00344$ Kmol/sec. $\quad P_{t0} = 2.4$ atm Pressure.

→ $V = 10\ m^3$ [$V = 0 - 10$] → Range of V

→ initial molar Ratio of Inert/Reactant A = 14.5/1

→ $F_{I_0} = F_I = 14.5 \times 3.44 = 49.88$ mol/sec. $= 0.04988$ Kmol/sec.

→ $\Delta H_{RXN1} = 118000 \ \frac{KJ}{Kmol\ of\ A}$

→ $H_{RXN2} = 105200 \ \frac{KJ}{Kmol\ of\ A}$

→ $H_{RXN3} = -53900 \ \frac{KJ}{Kmol\ of\ A}$

Given.

$r_1 = \{r_{1A}\} = r_{1P} = r_{1D} = \rho(1-\phi)\exp\left(-0.08539 - \frac{10925}{T}\right)\left(P_A - \frac{P_P P_D}{K_{P_1}}\right)$ $\left(\frac{Kmol}{m^3 s}\right)$

$r_2 = \{r_{2A}\} = r_{2B} = r_{2C} = \rho(1-\phi)\exp\left(13.2392 - \frac{25000}{T}\right)(P_A)$ $\left(\frac{Kmol}{m^3 s}\right)$

$r_3 = \{r_{3A}\} = \{r_{3D}\} = r_{3E} = r_{3F} = \rho(1-\phi)\exp\left(0.2961 - \frac{11000}{T}\right)(P_A P_D)$ $\left(\frac{Kmol}{m^3 s}\right)$

mole balance :

$\frac{dF_A}{dV} = r_a = -r_{1A} - r_{2A} - r_{3A} = (-r_1) + (-r_2) + (-r_3)$

$\frac{dF_B}{dV} = r_B = r_{2B} = r_2$

$\frac{dF_C}{dV} = r_C = r_{2C} = r_2$

$\frac{dF_D}{dV} = r_D = -r_{3D} + r_{1D} = -r_3 + r_1$

$$\frac{dF_E}{dV} = \gamma_{3E} = \gamma_3$$

$$\frac{dF_F}{dV} = \gamma_{3F} = \gamma_3$$

$$\frac{dF_P}{dV} = \gamma_{1P} = \gamma_1$$

$$P_A = \frac{F_A}{F_T} P_{T_0} \qquad P_D = \frac{F_D}{F_T} P_{T_0} \qquad P_P = \frac{F_P}{F_T} P_{T_0}$$

$$F_T = F_A + F_B + F_C + F_D + F_E + F_F + F_I$$

$\rho = 2137 \text{ kg/m}^3$ $\qquad \phi = 0.4$

$$K_{P_1} = \exp\left[B_1 + \frac{B_2}{T} + B_3 \ln(T) + \left[(B_4 T + B_5)T + B_6\right]T\right] \text{ atm}$$

$B_1 = -17.34$ $\quad B_2 = -1.302 \times 10^4$ $\quad B_3 = -5.051$

$B_4 = -2.314 \times 10^{-10}$ $\quad B_5 = 1.302 \times 10^{-6}$ $\quad B_2 = 4.931 \times 10^{-3}$

$C_{PA} = 299$ [redacted] $\frac{kJ}{kmol\,K}$ $\quad C_{PP} = 273$ [redacted] $\frac{kJ}{kmol\,K}$.

$C_{PB} = 201$ [redacted] $\quad C_{PC} = 90$ [redacted] $\quad C_{PD} = 30$ [redacted]

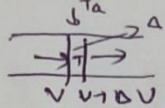
$C_{PE} = 249$ [redacted] $\quad C_{PF} = 68$ [redacted] $\quad C_{pstream} = 40$ [redacted]

⇒ for coding ★★

$F_A = y_1$ $\quad F_B = y_2$ $\quad F_C = y_3$ $\quad F_D = y_4$

$F_E = y_5$ $\quad F_F = y_6$ $\quad F_P = y_7$ $\quad T = y_8$

⊛ Energy balance :



$$\left(\sum F_i h_i\right)\Big|_V - \sum [F_i h_i]\Big|_{V+\Delta V} + UA(T_a - T)\Delta V = 0$$

$$UA(T_a - T) = \frac{d}{dV}\left[\sum F_i h_i\right]$$

$$\sum F_i \frac{dh_i}{dV} + \sum h_i \left(\frac{dF_i}{dV}\right) = 0$$

$$\sum F_i \frac{dh_i}{dV} = \sum F_i \left(\frac{dh_i}{dT}\right)\left(\frac{dT}{dV}\right) = \left(\frac{dT}{dV}\right) \sum F_i C_p$$

$$\sum h_i \frac{dF_i}{dV} = \sum h_i \left(\sum_{j=1}^{r} \gamma_{ij}\right)$$

$$= \sum_{j=1}^{r} \gamma_{Aj}\, \Delta h_{Rxn_j}$$

$$\frac{dT}{dV} = \frac{\sum_{j=1}^{r} \gamma_j \, (\Delta h_{rxn})_j}{\sum_{i=1}^{i} F_i C_{pi}}$$

$$\frac{dT}{dV} = \frac{(-\gamma_{1A})(-h_{Rxn_1}) + (-\gamma_{2A})(-h_{Rxn_2}) + (-\gamma_{3A})(-h_{RxN_n})}{\sum F_i C_{pi}}$$

$$\frac{dT}{dV} = \frac{(\gamma_1)(-h_{Rxn_1}) + (\gamma_2)(-h_{Rxn_2}) + (\gamma_3)(-h_{RxN})}{F_A C_{PA} + F_B C_{PB} + F_C C_{PC} + F_D C_{PD} + F_E C_{PE} + F_F C_{PF} + F_P C_{PP} + F_i C_{pstream}}$$

Assume $\Rightarrow$ $C_{pstream} = C_{pi}$ — Because at inlet it Inert material is stream.

$$\frac{dT}{dV} = \frac{(\gamma_1)(h_{RxN_1}) + (\gamma_2)(h_{Rxn_2}) + (\gamma_3)(h_{RxN})}{F_A C_{PA} + F_B C_{PB} + F_C C_{PC} + F_D C_{PD} + F_E C_{PE} + F_F C_{PF} + C_P C_{PP} + F_i C_{pstream}}$$

then the ODEs

$$\frac{dy_1}{dV} = r_A$$

$$\frac{dy_2}{dV} = r_B$$

$$\frac{dy_3}{dV} = r_C$$

$$\frac{dy_4}{dV} = r_D$$

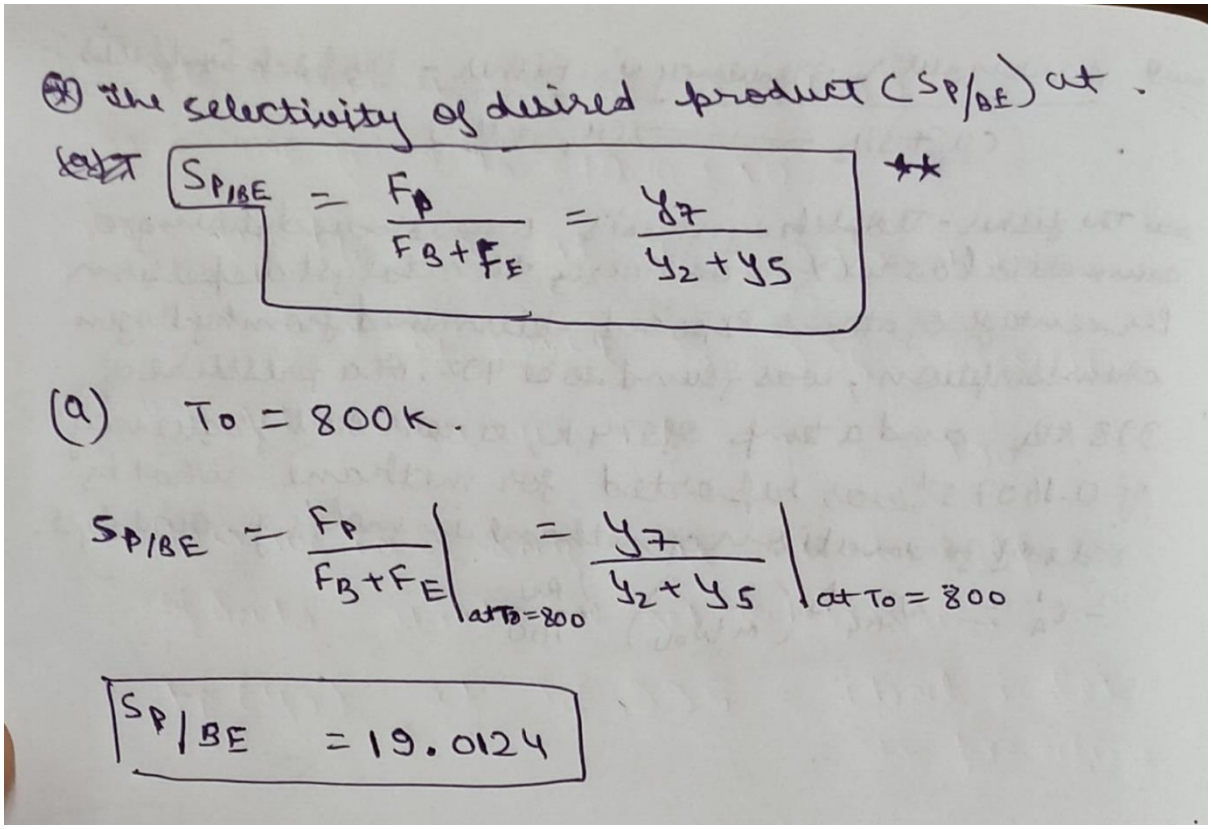
$$\frac{dy_5}{dV} = r_E$$

$$\frac{dy_6}{dV} = r_F$$

$$\frac{dy_7}{dV} = r_P$$

$$\frac{dy_8}{dV} = -\frac{\left((r_1)(h_{Rxn1}) + (r_2)(h_{Rxn2}) + (r_3)(h_{Rxn3})\right)}{F_i C_{pA} + y_2 C_{pB} + y_3 C_{pC} + y_4 C_{pD} + y_5 C_{pE} + y_6 C_{pF} + y_7 C_{pE} + F_i C_{p\,stream}}$$

'−' Because temperature is decreasing as we known ΔH_{Rxn1} and ΔH_{Rxn2} = is (+ve) then endothermic → then we have to put '−' in front of $\left(\frac{dT}{dV}\right)$



Matlab code

```
hrxn1 = 118000.0;
hrxn2 = 105200.0;
hrxn3 = -53900.0;
cpa = 299.0;
cpb = 201.0;
cpc = 90.0;
cpd = 30.0;
cpe = 249.0;
cpf = 68.0;
cpp = 273.0;
cpstream = 40.0;
rho = 2173.0;
fhi = 0.4;
b1 = -17.34;
b2 = -13020.0;
b3 = 5.051;
b4 = -0.0000000002314;
b5 = 0.000001302;
b6 = -0.004931;
fi = 0.04988;
pt = 2.4;
%kp1 = exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8));
%ft = y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi;
%pa = y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi));
%pp = y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi));
%pd = y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi));
%r1 = rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
```

```
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8)));
%r2 = rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)));
%r3 = rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)));
%ra =(-(rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
)+(-(rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))))+(-(rho*(1-
fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))))
%rb =rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))
%rc = rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))
%rd = (rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
+(-(rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))))
%re = rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))
%rf = rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))
%rp = rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8)))))
% ((rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
*(hrxn1)+(rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))*(hrxn2)+(rho*(1
-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))*(hrxn3))/(y(1)*cpa+y(2)*cpb+y(3)*cpc+y(4)*cpd+y
(5)*cpe+y(6)*cpf+y(7)*cpp+fi*cpstream)
f =@(v,y) [(-(rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
)+(-(rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))))+(-(rho*(1-
fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))); rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))); rho*(1-
fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))); (rho*(1-
```

```
fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
+(-(rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))); rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))); rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))); rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8)))));
-((rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
*(hrxn1)+(rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))*(hrxn2)+(rho*(1
-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))*(hrxn3))/(y(1)*cpa+y(2)*cpb+y(3)*cpc+y(4)*cpd+y
(5)*cpe+y(6)*cpf+y(7)*cpp+fi*cpstream)];
[v,y] = ode15s(f,[0 10],[0.00344; 0; 0; 0; 0; 0; 0; 800])
selectivity = y(15,7)/(y(15,2)+y(15,5))
```

Variables - v

v

15x1 double

	1	2	3	4
1	0			
2	0.1608			
3	0.3215			
4	0.4823			
5	1.2086			
6	1.9350			
7	2.6613			
8	3.3876			
9	4.3876			
10	5.3876			
11	6.3876			
12	7.3876			
13	8.3876			
14	9.3876			
15	10			

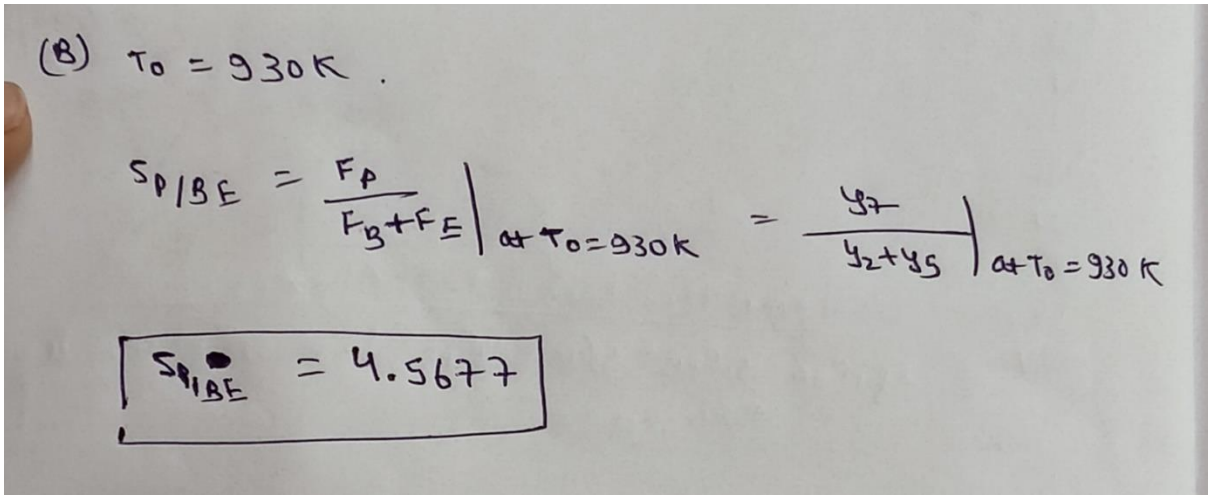
Variables - y

v y

15x8 double

	1	2	3	4	5	6	7	8
1	0.0034	0	0	0	0	0	0	800
2	0.0034	4.6373e-07	4.6373e-07	3.3901e-05	5.7968e-08	5.7968e-08	3.3959e-05	798.6597
3	0.0034	9.0056e-07	9.0056e-07	6.6641e-05	1.7695e-07	1.7695e-07	6.6818e-05	797.3644
4	0.0033	1.3122e-06	1.3122e-06	9.8245e-05	3.5242e-07	3.5242e-07	9.8598e-05	796.1132
5	0.0032	2.9435e-06	2.9435e-06	2.2923e-04	1.6330e-06	1.6330e-06	2.3086e-04	790.9188
6	0.0031	4.2407e-06	4.2407e-06	3.4150e-04	3.6023e-06	3.6023e-06	3.4510e-04	786.4524
7	0.0030	5.2932e-06	5.2932e-06	4.3739e-04	6.0313e-06	6.0313e-06	4.4343e-04	782.6238
8	0.0029	6.1694e-06	6.1694e-06	5.1913e-04	8.7506e-06	8.7506e-06	5.2788e-04	779.3478
9	0.0028	7.1697e-06	7.1697e-06	6.1177e-04	1.2777e-05	1.2777e-05	6.2455e-04	775.6152
10	0.0027	8.0110e-06	8.0110e-06	6.8532e-04	1.6958e-05	1.6958e-05	7.0228e-04	772.6295
11	0.0026	8.7453e-06	8.7453e-06	7.4339e-04	2.1197e-05	2.1197e-05	7.6459e-04	770.2498
12	0.0026	9.4028e-06	9.4028e-06	7.8893e-04	2.5453e-05	2.5453e-05	8.1438e-04	768.3616
13	0.0025	1.0003e-05	1.0003e-05	8.2432e-04	2.9707e-05	2.9707e-05	8.5403e-04	766.8707
14	0.0025	1.0561e-05	1.0561e-05	8.5157e-04	3.3946e-05	3.3946e-05	8.8552e-04	765.6991
15	0.0025	1.0885e-05	1.0885e-05	8.6499e-04	3.6532e-05	3.6532e-05	9.0152e-04	765.1100

selectivity = 19.0124

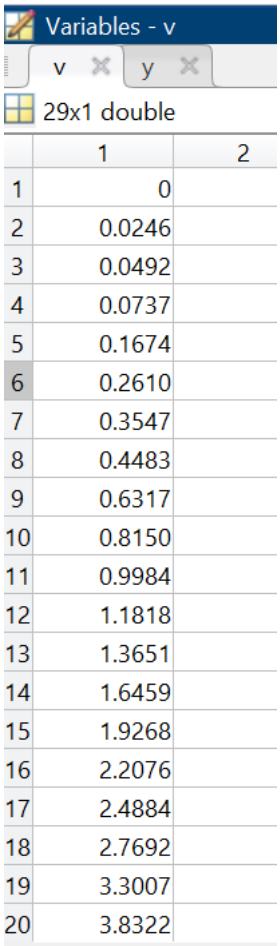


Matlab code

```
hrxn1 = 118000.0;
hrxn2 = 105200.0;
hrxn3 = -53900.0;
cpa = 299.0;
cpb = 201.0;
cpc = 90.0;
cpd = 30.0;
cpe = 249.0;
cpf = 68.0;
cpp = 273.0;
cpstream = 40.0;
rho = 2173.0;
fhi = 0.4;
b1 = -17.34;
b2 = -13020.0;
b3 = 5.051;
b4 = -0.0000000002314;
b5 = 0.000001302;
b6 = -0.004931;
fi = 0.04988;
pt = 2.4;
%kp1 = exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8));
%ft = y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi;
%pa = y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi));
%pp = y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi));
%pd = y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi));
%r1 = rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))));
%r2 = rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)));
%r3 = rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)));
%ra =(-(rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
```

```
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
)+(-(rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))))+(-(rho*(1-
fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))))
%rb =rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))
%rc = rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))
%rd = (rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
+(-(rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))))
%re = rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))
%rf = rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))
%rp = rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8)))))
% ((rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
*(hrxn1)+(rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))*(hrxn2)+(rho*(1
-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))*(hrxn3))/(y(1)*cpa+y(2)*cpb+y(3)*cpc+y(4)*cpd+y
(5)*cpe+y(6)*cpf+y(7)*cpp+fi*cpstream)
f =@(v,y) [(-(rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
)+(-(rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))))+(-(rho*(1-
fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))))); rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))); rho*(1-
fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))); (rho*(1-
fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
+(-(rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))))); rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))); rho*(1-fhi)*exp(0.2961-
```

```
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))); rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8)))));
-((rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
*(hrxn1)+(rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))*(hrxn2)+(rho*(1
-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))*(hrxn3))/(y(1)*cpa+y(2)*cpb+y(3)*cpc+y(4)*cpd+y
(5)*cpe+y(6)*cpf+y(7)*cpp+fi*cpstream)];
[v,y] = ode15s(f,[0 10],[0.00344; 0; 0; 0; 0; 0; 0; 930])
selectivity = y(29,7)/(y(29,2)+y(29,5))
```



	1	2
1	0	
2	0.0246	
3	0.0492	
4	0.0737	
5	0.1674	
6	0.2610	
7	0.3547	
8	0.4483	
9	0.6317	
10	0.8150	
11	0.9984	
12	1.1818	
13	1.3651	
14	1.6459	
15	1.9268	
16	2.2076	
17	2.4884	
18	2.7692	
19	3.3007	
20	3.8322	

21	4.3638
22	4.8953
23	5.4268
24	6.2573
25	7.0879
26	7.9184
27	8.7489
28	9.5795
29	10
30	

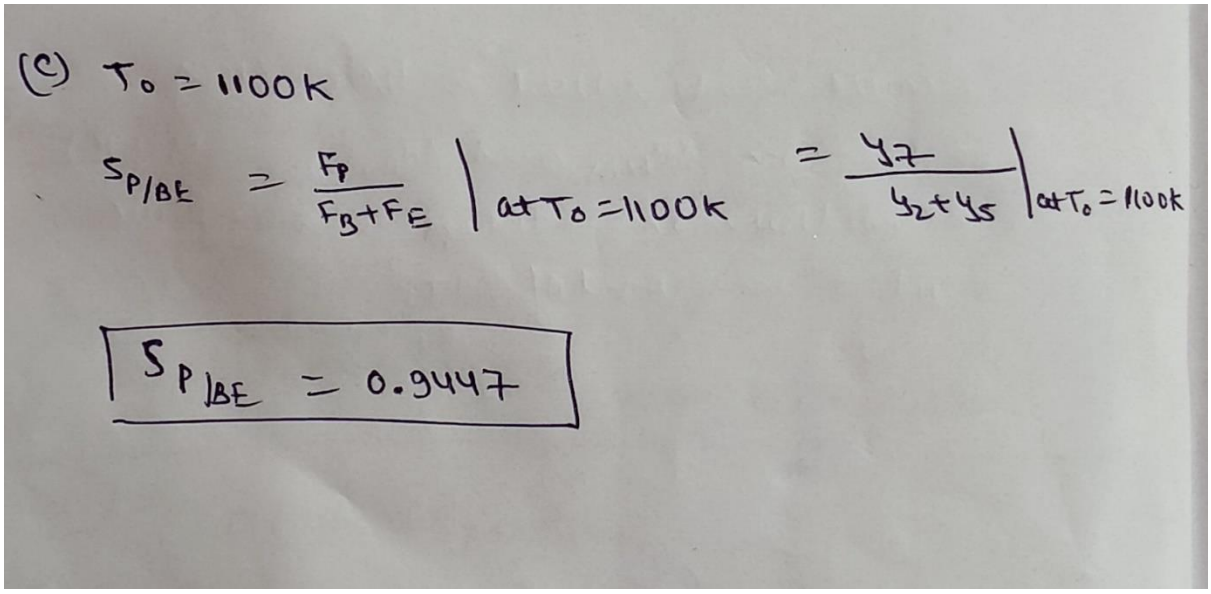
Variables - y

v | y

29x8 double

	1	2	3	4	5	6	7	8
1	0.0034	0	0	0	0	0	0	930
2	0.0034	5.6181e-06	5.6181e-06	3.5000e-05	6.2597e-08	6.2597e-08	3.5062e-05	928.4374
3	0.0034	1.0936e-05	1.0936e-05	6.8866e-05	1.9134e-07	1.9134e-07	6.9058e-05	926.9281
4	0.0033	1.5972e-05	1.5972e-05	1.0164e-04	3.8158e-07	3.8158e-07	1.0202e-04	925.4701
5	0.0032	3.3201e-05	3.3201e-05	2.1844e-04	1.5151e-06	1.5151e-06	2.1996e-04	920.2892
6	0.0031	4.7559e-05	4.7559e-05	3.2298e-04	3.2274e-06	3.2274e-06	3.2621e-04	915.6749
7	0.0030	5.9649e-05	5.9649e-05	4.1706e-04	5.3621e-06	5.3621e-06	4.2242e-04	911.5391
8	0.0029	6.9970e-05	6.9970e-05	5.0229e-04	7.7930e-06	7.7930e-06	5.1009e-04	907.8039
9	0.0027	8.6269e-05	8.6269e-05	6.4800e-04	1.3115e-05	1.3115e-05	6.6111e-04	901.4414
10	0.0025	9.9029e-05	9.9029e-05	7.7187e-04	1.8794e-05	1.8794e-05	7.9066e-04	896.0466
11	0.0024	1.0940e-04	1.0940e-04	8.7889e-04	2.4577e-05	2.4577e-05	9.0347e-04	891.3905
12	0.0023	1.1802e-04	1.1802e-04	9.7229e-04	3.0347e-05	3.0347e-05	0.0010	887.3267
13	0.0022	1.2529e-04	1.2529e-04	0.0011	3.6041e-05	3.6041e-05	0.0011	883.7523
14	0.0021	1.3447e-04	1.3447e-04	0.0012	4.4539e-05	4.4539e-05	0.0012	879.0573
15	0.0019	1.4197e-04	1.4197e-04	0.0013	5.2701e-05	5.2701e-05	0.0013	875.1093
16	0.0018	1.4829e-04	1.4829e-04	0.0013	6.0507e-05	6.0507e-05	0.0014	871.7537
17	0.0018	1.5371e-04	1.5371e-04	0.0014	6.7971e-05	6.7971e-05	0.0015	868.8821
18	0.0017	1.5848e-04	1.5848e-04	0.0014	7.5110e-05	7.5110e-05	0.0015	866.4103
19	0.0016	1.6609e-04	1.6609e-04	0.0015	8.7842e-05	8.7842e-05	0.0016	862.6262
20	0.0015	1.7249e-04	1.7249e-04	0.0016	9.9691e-05	9.9691e-05	0.0017	859.7282
21	0.0014	1.7806e-04	1.7806e-04	0.0016	1.1082e-04	1.1082e-04	0.0018	857.4887
22	0.0013	1.8302e-04	1.8302e-04	0.0017	1.2135e-04	1.2135e-04	0.0018	855.7554
23	0.0013	1.8753e-04	1.8753e-04	0.0017	1.3140e-04	1.3140e-04	0.0018	854.4167
24	0.0012	1.9393e-04	1.9393e-04	0.0017	1.4631e-04	1.4631e-04	0.0019	852.9163
25	0.0012	1.9984e-04	1.9984e-04	0.0017	1.6043e-04	1.6043e-04	0.0019	851.9164
26	0.0011	2.0544e-04	2.0544e-04	0.0017	1.7395e-04	1.7395e-04	0.0019	851.2563
27	0.0011	2.1076e-04	2.1076e-04	0.0017	1.8698e-04	1.8698e-04	0.0019	850.8380
28	0.0011	2.1585e-04	2.1585e-04	0.0017	1.9961e-04	1.9961e-04	0.0019	850.5937
29	0.0011	2.1835e-04	2.1835e-04	0.0017	2.0587e-04	2.0587e-04	0.0019	850.5192

selectivity = 4.5677



Matlab code

```
hrxn1 = 118000.0;
hrxn2 = 105200.0;
hrxn3 = -53900.0;
cpa = 299.0;
cpb = 201.0;
cpc = 90.0;
cpd = 30.0;
cpe = 249.0;
cpf = 68.0;
cpp = 273.0;
cpstream = 40.0;
rho = 2173.0;
fhi = 0.4;
b1 = -17.34;
b2 = -13020.0;
b3 = 5.051;
b4 = -0.0000000002314;
b5 = 0.000001302;
b6 = -0.004931;
fi = 0.04988;
pt = 2.4;
%kp1 = exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8));
%ft = y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi;
%pa = y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi));
%pp = y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi));
%pd = y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi));
%r1 = rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8)));
%r2 = rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)));
```

```
%r3 = rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)));
%ra =(-(rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
)+(-(rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))))+(-(rho*(1-
fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))))
%rb =rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))
%rc = rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))
%rd = (rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
+(-(rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))))
%re = rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))
%rf = rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))
%rp = rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8)))))
% ((rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
*(hrxn1)+(rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))*(hrxn2)+(rho*(1
-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))*(hrxn3))/(y(1)*cpa+y(2)*cpb+y(3)*cpc+y(4)*cpd+y
(5)*cpe+y(6)*cpf+y(7)*cpp+fi*cpstream)
f =@(v,y) [(-(rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
)+(-(rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))))+(-(rho*(1-
fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))); rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))); rho*(1-
fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))); (rho*(1-
fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
```

```
+(-(rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))); rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))); rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))); rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))));
-((rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
*(hrxn1)+(rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))*(hrxn2)+(rho*(1
-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))*(hrxn3))/(y(1)*cpa+y(2)*cpb+y(3)*cpc+y(4)*cpd+y
(5)*cpe+y(6)*cpf+y(7)*cpp+fi*cpstream)];
[v,y] = ode15s(f,[0 10],[0.00344; 0; 0; 0; 0; 0; 0; 1100])
selectivity = y(52,7)/(y(52,2)+y(52,5))
```

Variables - v

v

52x1 double

	1
1	0
2	0.0018
3	0.0036
4	0.0054
5	0.0116
6	0.0179
7	0.0241
8	0.0303
9	0.0425
10	0.0547
11	0.0668
12	0.0790
13	0.0911
14	0.1105
15	0.1299
16	0.1492
17	0.1686
18	0.1880
19	0.2226
20	0.2571
21	0.2917
22	0.3263
23	0.3609
24	0.4191
25	0.4774
26	0.5356
27	0.5939
28	0.6522
29	0.7488
30	0.8454
31	0.9420
32	1.0386
33	1.1352
34	1.2946
35	1.4541
36	1.6135
37	1.7730
38	1.9325
39	2.2369
40	2.5414

41	2.8459
42	3.1503
43	3.4548
44	4.0551
45	4.6554
46	5.2557
47	5.8560
48	6.4563
49	7.4563
50	8.4563
51	9.4563
52	10

Variables - y

y

52x8 double

	1	2	3	4	5	6	7	8
1	0.0034	0	0	0	0	0	0	1100
2	0.0034	2.6531e-05	2.6531e-05	1.5854e-05	1.3004e-08	1.3004e-08	1.5867e-05	1.0985e+03
3	0.0034	5.1954e-05	5.1954e-05	3.1291e-05	3.9965e-08	3.9965e-08	3.1331e-05	1.0970e+03
4	0.0033	7.6320e-05	7.6320e-05	4.6323e-05	8.0122e-08	8.0122e-08	4.6403e-05	1.0955e+03
5	0.0032	1.5423e-04	1.5423e-04	9.5781e-05	2.9694e-07	2.9694e-07	9.6078e-05	1.0909e+03
6	0.0031	2.2273e-04	2.2273e-04	1.4139e-04	6.2645e-07	6.2645e-07	1.4202e-04	1.0867e+03
7	0.0030	2.8339e-04	2.8339e-04	1.8364e-04	1.0464e-06	1.0464e-06	1.8469e-04	1.0829e+03
8	0.0029	3.3757e-04	3.3757e-04	2.2297e-04	1.5375e-06	1.5375e-06	2.2450e-04	1.0795e+03
9	0.0027	4.2821e-04	4.2821e-04	2.9254e-04	2.6490e-06	2.6490e-06	2.9519e-04	1.0736e+03
10	0.0026	5.0403e-04	5.0403e-04	3.5454e-04	3.8948e-06	3.8948e-06	3.5844e-04	1.0685e+03
11	0.0025	5.6890e-04	5.6890e-04	4.1052e-04	5.2222e-06	5.2222e-06	4.1574e-04	1.0641e+03
12	0.0023	6.2524e-04	6.2524e-04	4.6151e-04	6.5992e-06	6.5992e-06	4.6811e-04	1.0601e+03
13	0.0022	6.7471e-04	6.7471e-04	5.0829e-04	8.0050e-06	8.0050e-06	5.1629e-04	1.0565e+03
14	0.0021	7.4221e-04	7.4221e-04	5.7554e-04	1.0272e-05	1.0272e-05	5.8581e-04	1.0515e+03
15	0.0020	7.9915e-04	7.9915e-04	6.3548e-04	1.2533e-05	1.2533e-05	6.4802e-04	1.0471e+03
16	0.0019	8.4807e-04	8.4807e-04	6.8950e-04	1.4764e-05	1.4764e-05	7.0426e-04	1.0432e+03
17	0.0018	8.9065e-04	8.9065e-04	7.3856e-04	1.6950e-05	1.6950e-05	7.5551e-04	1.0398e+03
18	0.0017	9.2810e-04	9.2810e-04	7.8342e-04	1.9085e-05	1.9085e-05	8.0250e-04	1.0367e+03
19	0.0016	9.8481e-04	9.8481e-04	8.5472e-04	2.2753e-05	2.2753e-05	8.7748e-04	1.0318e+03
20	0.0014	0.0010	0.0010	9.1704e-04	2.6231e-05	2.6231e-05	9.4327e-04	1.0277e+03

21	0.0013	0.0011	0.0011	9.7219e-04	2.9519e-05	2.9519e-05	0.0010	1.0241e+03
22	0.0012	0.0011	0.0011	0.0010	3.2626e-05	3.2626e-05	0.0011	1.0209e+03
23	0.0012	0.0011	0.0011	0.0011	3.5563e-05	3.5563e-05	0.0011	1.0181e+03
24	0.0011	0.0012	0.0012	0.0011	4.0155e-05	4.0155e-05	0.0012	1.0140e+03
25	9.5198e-04	0.0012	0.0012	0.0012	4.4338e-05	4.4338e-05	0.0012	1.0105e+03
26	8.6643e-04	0.0012	0.0012	0.0012	4.8156e-05	4.8156e-05	0.0013	1.0075e+03
27	7.9195e-04	0.0013	0.0013	0.0013	5.1653e-05	5.1653e-05	0.0013	1.0049e+03
28	7.2672e-04	0.0013	0.0013	0.0013	5.4864e-05	5.4864e-05	0.0014	1.0026e+03
29	6.3486e-04	0.0013	0.0013	0.0014	5.9638e-05	5.9638e-05	0.0014	999.3860
30	5.5842e-04	0.0013	0.0013	0.0014	6.3820e-05	6.3820e-05	0.0015	996.7386
31	4.9400e-04	0.0014	0.0014	0.0014	6.7507e-05	6.7507e-05	0.0015	994.5164
32	4.3930e-04	0.0014	0.0014	0.0015	7.0773e-05	7.0773e-05	0.0016	992.6366
33	3.9264e-04	0.0014	0.0014	0.0015	7.3680e-05	7.3680e-05	0.0016	991.0401
34	3.2953e-04	0.0014	0.0014	0.0015	7.7821e-05	7.7821e-05	0.0016	988.8926
35	2.7966e-04	0.0014	0.0014	0.0016	8.1303e-05	8.1303e-05	0.0016	987.2087
36	2.3931e-04	0.0014	0.0014	0.0016	8.4258e-05	8.4258e-05	0.0017	985.8569
37	2.0674e-04	0.0015	0.0015	0.0016	8.6792e-05	8.6792e-05	0.0017	984.7755
38	1.8052e-04	0.0015	0.0015	0.0016	8.8988e-05	8.8988e-05	0.0017	983.9157
39	1.4346e-04	0.0015	0.0015	0.0016	9.2443e-05	9.2443e-05	0.0017	982.7250
40	1.1690e-04	0.0015	0.0015	0.0016	9.5188e-05	9.5188e-05	0.0017	981.8958
41	9.8736e-05	0.0015	0.0015	0.0016	9.7466e-05	9.7466e-05	0.0017	981.3575
42	8.6745e-05	0.0015	0.0015	0.0016	9.9434e-05	9.9434e-05	0.0017	981.0340
43	7.8640e-05	0.0015	0.0015	0.0016	1.0119e-04	1.0119e-04	0.0017	980.8451
44	6.9377e-05	0.0015	0.0015	0.0016	1.0423e-04	1.0423e-04	0.0017	980.7030
45	6.3929e-05	0.0015	0.0015	0.0016	1.0696e-04	1.0696e-04	0.0017	980.6889
46	6.0241e-05	0.0015	0.0015	0.0016	1.0951e-04	1.0951e-04	0.0017	980.7318
47	5.7789e-05	0.0016	0.0016	0.0016	1.1193e-04	1.1193e-04	0.0017	980.8141
48	5.6206e-05	0.0016	0.0016	0.0016	1.1426e-04	1.1426e-04	0.0017	980.9233
49	5.4453e-05	0.0016	0.0016	0.0016	1.1797e-04	1.1797e-04	0.0017	981.1287
50	5.2982e-05	0.0016	0.0016	0.0015	1.2154e-04	1.2154e-04	0.0017	981.3353
51	5.1529e-05	0.0016	0.0016	0.0015	1.2498e-04	1.2498e-04	0.0017	981.5344
52	5.0769e-05	0.0016	0.0016	0.0015	1.2680e-04	1.2680e-04	0.0016	981.6403

selectivity = 0.9447

Part D (d)

Here we find ideal inlet temperature for the production of P

Given $\frac{\text{steam}}{F_{A0}} = \frac{58}{1}$

then $F_i = 58 \times 0.00344 = 0.19952$.

And other values are same.

then we find $F_P(y_7)$ at the outlet of the Reactor at Different T_0 (inlet temperature)

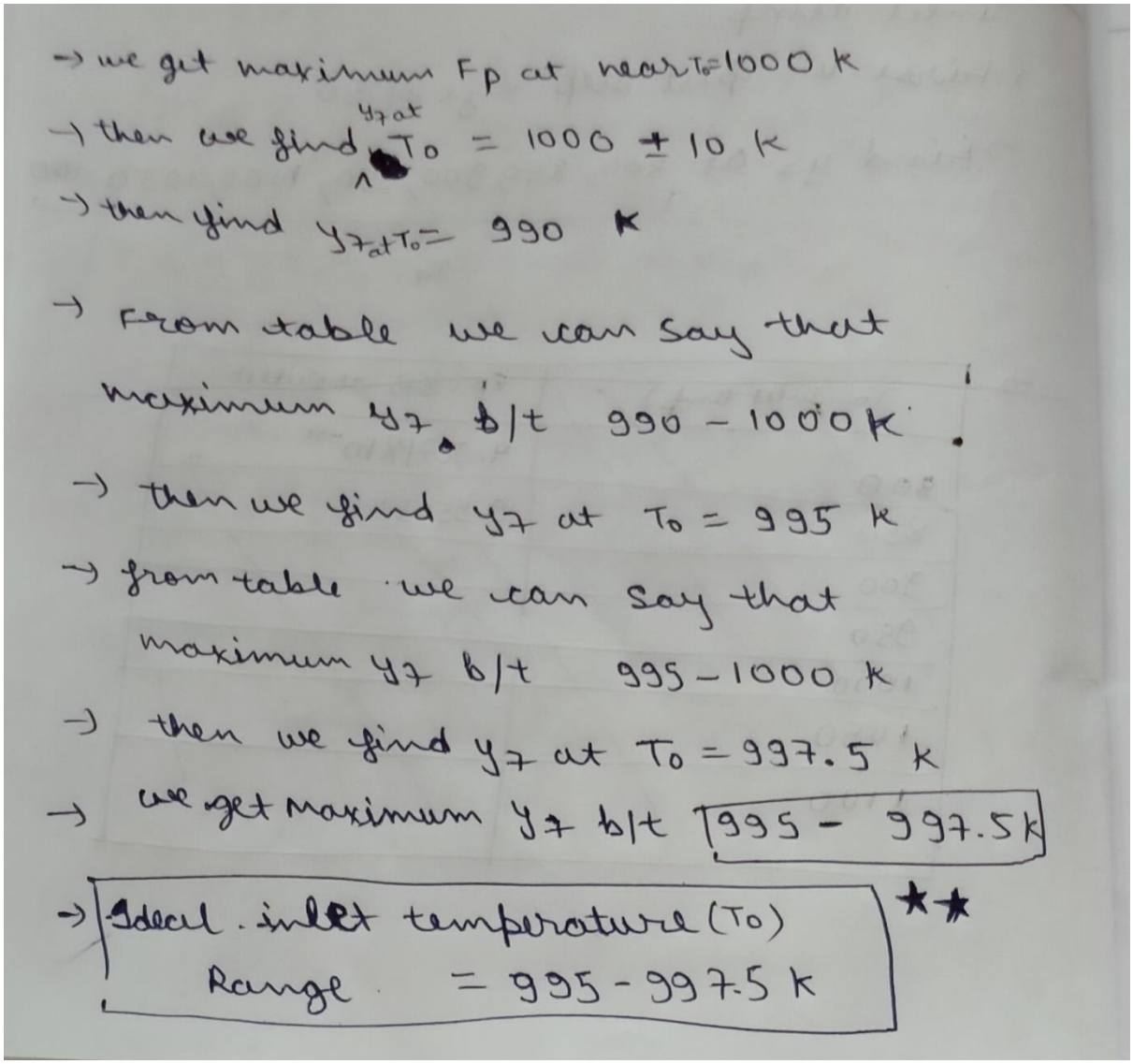
→ those temp which we get highest $F_P(y_7)$ at that point of inlet we get ours ideal inlet temp.

→ First we put step size of 50.

→ Find y_7 at 800, 850, 900, 950, 1000, 1050, 1100

↓

T_0



Ideal inlet temperature = **295 kelvin**

	A	B
1	To (inlet temperature)	fp (y7)
2	800	0.000493
3	850	0.000955
4	900	0.001551
5	950	0.002079
6	980	0.002243
7	990	0.00226
8	995	0.002261
9	997.5	0.002259
10	1000	0.002256
11	1050	0.001964
12	1100	0.001462
13		

Sample calculation for to = 800 and y7 (fp)

Matlab code:

```
hrxn1 = 118000.0;
hrxn2 = 105200.0;
hrxn3 = -53900.0;
cpa = 299.0;
cpb = 201.0;
cpc = 90.0;
cpd = 30.0;
cpe = 249.0;
cpf = 68.0;
cpp = 273.0;
cpstream = 40.0;
rho = 2173.0;
fhi = 0.4;
b1 = -17.34;
b2 = -13020.0;
b3 = 5.051;
b4 = -0.0000000002314;
b5 = 0.000001302;
b6 = -0.004931;
fi = 0.19952;
pt = 2.4;
%kp1 = exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8));
%ft = y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi;
%pa = y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi));
%pp = y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi));
%pd = y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi));
```

```
%r1 = rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8)))));
%r2 = rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)));
%r3 = rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)));
%ra =(-(rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
)+(-(rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))))+(-(rho*(1-
fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))))
%rb =rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))
%rc = rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))
%rd = (rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
+(-(rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))))
%re = rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))
%rf = rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))
%rp = rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8)))))
% ((rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
*(hrxn1)+(rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))*(hrxn2)+(rho*(1
-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))*(hrxn3))/(y(1)*cpa+y(2)*cpb+y(3)*cpc+y(4)*cpd+y
(5)*cpe+y(6)*cpf+y(7)*cpp+fi*cpstream)
f =@(v,y) [(-(rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
)+(-(rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))))+(-(rho*(1-
fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))); rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))); rho*(1-
```

```
fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))); (rho*(1-
fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
+(-(rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))); rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))); rho*(1-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))); rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))));
-((rho*(1-fhi)*exp(-0.08539-
(10925/y(8)))*((y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi)))-
(y(7)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(2)+y(3)+y(4)+y
(5)+y(6)+y(7)+fi))/(exp(b1+(b2/y(8))+b3*log(y(8))+((b4*y(8)+b5)*y(8)+b6)*y(8))))))
*(hrxn1)+(rho*(1-fhi)*exp(13.2392-
(25000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))*(hrxn2)+(rho*(1
-fhi)*exp(0.2961-
(11000/y(8)))*(y(1)*(pt/(y(1)+y(2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))*y(4)*(pt/(y(1)+y(
2)+y(3)+y(4)+y(5)+y(6)+y(7)+fi))))*(hrxn3))/(y(1)*cpa+y(2)*cpb+y(3)*cpc+y(4)*cpd+y
(5)*cpe+y(6)*cpf+y(7)*cpp+fi*cpstream)];
[v,y] = ode15s(f,[0 10],[0.00344; 0; 0; 0; 0; 0; 0; 800])
```

Matlab table for v and y

Variables - v

v

12x1 double

	1
1	0
2	0.8511
3	1.7022
4	2.5533
5	3.5533
6	4.5533
7	5.5533
8	6.5533
9	7.5533
10	8.5533
11	9.5533
12	10

Variables - y

y

12x8 double

	1	2	3	4	5	6	7	8
1	0.0034	0	0	0	0	0	0	800
2	0.0034	6.5813e-07	6.5813e-07	4.7545e-05	2.9973e-08	2.9973e-08	4.7575e-05	799.3694
3	0.0033	1.2921e-06	1.2921e-06	9.3900e-05	9.2311e-08	9.2311e-08	9.3992e-05	798.7544
4	0.0033	1.9028e-06	1.9028e-06	1.3907e-04	1.8536e-07	1.8536e-07	1.3926e-04	798.1550
5	0.0032	2.5967e-06	2.5967e-06	1.9093e-04	3.2505e-07	3.2505e-07	1.9125e-04	797.4668
6	0.0032	3.2639e-06	3.2639e-06	2.4135e-04	4.9855e-07	4.9855e-07	2.4184e-04	796.7975
7	0.0031	3.9043e-06	3.9043e-06	2.9029e-04	7.0505e-07	7.0505e-07	2.9099e-04	796.1476
8	0.0031	4.5190e-06	4.5190e-06	3.3776e-04	9.4241e-07	9.4241e-07	3.3871e-04	795.5170
9	0.0030	5.1094e-06	5.1094e-06	3.8382e-04	1.2081e-06	1.2081e-06	3.8503e-04	794.9051
10	0.0030	5.6770e-06	5.6770e-06	4.2849e-04	1.4995e-06	1.4995e-06	4.2999e-04	794.3115
11	0.0030	6.2230e-06	6.2230e-06	4.7182e-04	1.8145e-06	1.8145e-06	4.7363e-04	793.7355
12	0.0029	6.4603e-06	6.4603e-06	4.9075e-04	1.9623e-06	1.9623e-06	4.9271e-04	793.4837