

**FIGURE 5.1**

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X
30		1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100	N(N2)	Feed
31		0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	300	N(H2)	Feed
32		0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	382.83	N(N2)	Reactor In
33		0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1148.5	N(H2)	Reactor In
34		0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3.8666	N(NH3)	Reactor In
35		0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	287.12	N(N2)	Reactor Out
36		0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	861.37	N(H2)	Reactor Out
37		0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	195.28	N(NH3)	Reactor Out
38		0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1.4356	N(N2)	Product
39		0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	4.3068	N(H2)	Product
40		0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	191.38	N(NH3)	Product
41		0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	285.69	N(N2)	Vapor Out
42		0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	857.06	N(H2)	Vapor Out
43		0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	3.9056	N(NH3)	Vapor Out
44		0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	2.8569	N(N2)	Purge
45		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	8.5706	N(H2)	Purge
46		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0.0391	N(NH3)	Purge
47		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	282.83	N(N2)	Recycle
48		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	848.49	N(H2)	Recycle
49		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	3.8666	N(NH3)	Recycle

**FIGURE 5.11**

	A	B	C	D	E	F	G	H	I	J	K	L	M
5		x(0)	x(1)	x(2)	x(3)	x(4)	x(5)	x(6)	x(7)	x(8)			
6		Reactor Out				Product			Vapor Out				
7		N(N2)	N(H2)	N(NH3)	N(N2)	N(H2)	N(NH3)	N(N2)	N(H2)	N(NH3)	RHS		
8	Feed	1									287.12		
9			1								861.37		
10	Specs			1							195.28		
11	Separator 1	-1			1			1			0		
12			-1			1			1		0		
13	Flash			-1			1			1	0		
14	Separator	0.005			-1						0		
15			0.005			-1					0		
16				0.98			-1				0		
17													
18													
19													
20													
21		1	0	0	0	0	0	0	0	0	287.12	N(N2)	Reactor Out
22		0	1	0	0	0	0	0	0	0	861.37	N(H2)	Reactor Out
23		0	0	1	0	0	0	0	0	0	195.28	N(NH3)	Reactor Out
24		0	0	0	1	0	0	0	0	0	0.67104	N(N2)	Product
25		0	0	0	0	1	0	0	0	0	2.68222	N(H2)	Product
26		0	0	0	0	0	1	0	0	0	178.168	N(NH3)	Product
27		0	0	0	0	0	0	1	0	0	286.449	N(N2)	Vapor Out
28		0	0	0	0	0	0	0	1	0	858.688	N(H2)	Vapor Out
29		0	0	0	0	0	0	0	0	1	17.1117	N(NH3)	Vapor Out
30													
31													
32													
33													
34		1									287.12		
35			1								861.37		
36				1							195.28		
37		-1			1			1			0		
38			-1			1			1		0		
39				-1			1			1	0		
40		-8E-04	-0.0008	0.005	-0.005	-0.005	-0.0048	0	0.0008	0.0008	3.6E-07		
41		0	0	0	-0.366	0.001	0.0014	0	-2E-04	-2E-04	1.1E-10		
42		0	0	0	0.004	-0.271	0.0041	-0	0.0002	-6E-04	-5E-10		

FIGURE 5.13

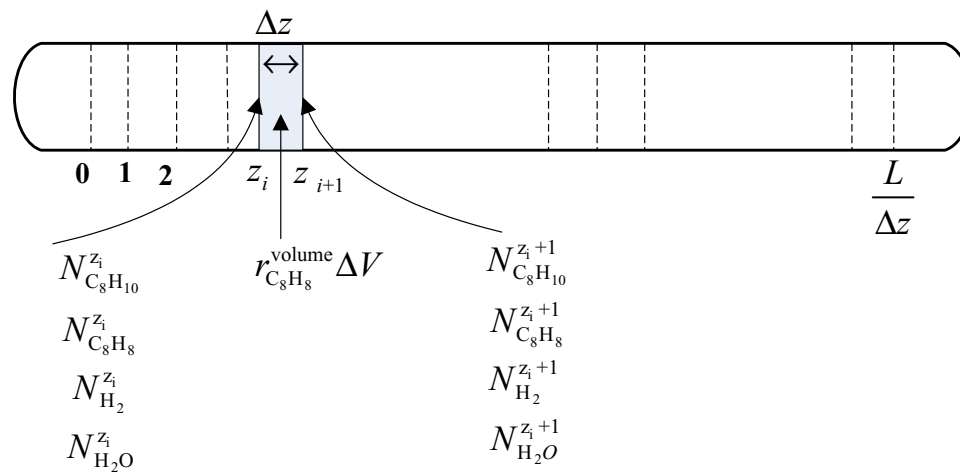
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	
1	Ammonia Material Balance using Gauss Jordan Elimination and Newton Raphson																						
2																							
3	Reaction $N_2 + 3H_2 \rightarrow NH_3$				0.25		conversion																
4																							
5		x(0)	x(1)	x(2)	x(3)	x(4)	x(5)	x(6)	x(7)	x(8)	x(9)	x(10)	x(11)	x(12)	x(13)	x(14)	x(15)	x(16)	x(17)	x(18)	x(19)		
6		Feed	Reactor In		Reactor Out		Product			Vapor Out			Purge			Recycle							
7		N(N2)	N(H2)	N(N2)	N(H2)	N(NH3)	N(N2)	N(H2)	N(NH3)	N(N2)	N(H2)	N(NH3)	N(N2)	N(H2)	N(NH3)	N(N2)	N(H2)	N(NH3)	N(N2)	N(H2)	N(NH3)	RHS	
8	Feed	1																				100	
9	Specs		1																			300	
10	Mixer	1		-1															1			0	
11	Material		1		-1															1		0	
12	Balances					-1															1	0	
13	Reactor			0.75			-1															0	
14	Balances			-0.75	1			-1														0	
15				0.5		1			-1													0	
16	Separator 2											0.01				-1						0	
17													0.01				-1					0	
18														0.01				-1				0	
19												1				-1				-1		0	
20													1				-1				-1	0	
21														1				-1				-1	0
22	Separator 1					1			-1			-1										0	
23							1			-1			-1									0	
24	Flash							1			-1				-1							0	
25	Separator					0.005			-1													0	
26							0.005			-1												0	
27								0.98			-1											0	

(a)

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X
32		1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100	N(N2)	Feed
33		0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	300	N(H2)	Feed
34		0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	385.42	N(N2)	Reactor In
35		0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1100.5	N(H2)	Reactor In
36		0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	16.227	N(NH3)	Reactor In
37		0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	289.07	N(N2)	Reactor Out
38		0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	811.41	N(H2)	Reactor Out
39		0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	208.94	N(NH3)	Reactor Out
40		0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0.762	N(N2)	Product
41		0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	2.8494	N(H2)	Product
42		0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	192.55	N(NH3)	Product
43		0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	288.3	N(N2)	Vapor Out
44		0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	808.56	N(H2)	Vapor Out
45		0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	16.391	N(NH3)	Vapor Out
46		0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	2.883	N(N2)	Purge
47		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	8.0856	N(H2)	Purge
48		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0.1639	N(NH3)	Purge
49		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	285.42	N(N2)	Recycle
50		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	800.47	N(H2)	Recycle
51		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	16.227	N(NH3)	Recycle

(b)

FIGURE 5.14ab



**FIGURE 5.17**

```

Option Explicit
Public Sub Ethylbenzene_Kinetics()

    Dim N_EB(), P_EB(), Conversion_EB() As Double
    Dim N_S(), P_S(), delta_N_S() As Double
    Dim N_H2(), P_H2() As Double
    Dim N_H2O(), P_H2O() As Double

    Dim Temp(), N_Total(), Keq(), r_S(), Q() As Double

    Dim delta_z, Pi, radius, CSA As Double
    Dim rho_catalyst, delta_H_reaction, P_Total As Double
    Dim Cp, MW_EB, MW_S, MW_H2, MW_H2O, F_Total, FCp As Double

    Dim Number_zSteps, i As Integer

    'Set known reactor conditions and constants
    radius = 2.3 ' PFR tube radius
    Pi = 3.14159
    CSA = Pi * (radius) ^ 2 ' cross-sectional area ft^2

    rho_catalyst = 90 ' lbs/ft^3

    P_Total = 1.2 ' Reactor Pressure assumed constant
    delta_H_reaction = 60000.0# ' Heat of Reaction (Btu/lb-mole)
    Cp = 0.52 ' Btu/(lb-R)

    MW_EB = 106.17
    MW_S = 104.15
    MW_H2 = 2.016
    MW_H2O = 18.015

    ' Here we set the step size down the reactor and the number of steps (=length)
    delta_z = 0.1 ' step size z direction [=] ft
    Number_zSteps = 90

    ReDim N_EB(Number_zSteps + 2), P_EB(Number_zSteps + 2), Conversion_EB(Number_zSteps
+ 2)
    ReDim N_S(Number_zSteps + 2), P_S(Number_zSteps + 2), delta_N_S(Number_zSteps + 2)
    ReDim N_H2(Number_zSteps + 2), P_H2(Number_zSteps + 2)
    ReDim N_H2O(Number_zSteps + 2), P_H2O(Number_zSteps + 2)

    ReDim Temp(Number_zSteps + 2), N_Total(Number_zSteps + 2), Keq(Number_zSteps + 2), _
        r_S(Number_zSteps + 2), Q(Number_zSteps + 2)

    ' Establish PFR tube radius initial conditions: moles/s, temperature into PFR, z = 0
    Temp(0) = 1616 ' Temperature z = 0
    N_EB(0) = 18.4615 / 3600 ' Moles Ethylbenzene/hr, z = 0
    N_S(0) = 0.1212 / 3600
    N_H2(0) = 0.0 / 3600
    N_H2O(0) = 353.0745 / 3600
    N_Total(0) = N_EB(0) + N_S(0) + N_H2(0) + N_H2O(0)

    'Calculate the flow rate heat capacity, FCp, of the reacting fluid - assumed
    constant
    F_Total = (N_EB(0) * MW_EB + N_S(0) * MW_S _
        + N_H2(0) * MW_H2 + N_H2O(0) * MW_H2O) ' Total Flow lbs/s
    FCp = F_Total * Cp ' Btu/lb-s

    ' We next set up the numerical integration to find the moles EB reacted
    ' here using a first-order Eulerian difference

    For i = 0 To Number_zSteps

        ' Monitor key values on the Excel sheet

        Sheet1.Cells(6 + i, 4) = delta_z * (i)
        Conversion_EB(i) = ((N_EB(0) - N_EB(i)) / N_EB(0)) * 100
        Sheet1.Cells(6 + i, 5) = Conversion_EB(i)
        Sheet1.Cells(6 + i, 6) = Temp(i) ' R
        Sheet1.Cells(6 + i, 7) = Temp(i) / 1.8 - 273.15 ' C
        Sheet1.Cells(6 + i, 8) = Temp(i) - 459.67 ' F
        Sheet1.Cells(6 + i, 9) = N_EB(i)
        Sheet1.Cells(6 + i, 10) = N_S(i)
        Sheet1.Cells(6 + i, 11) = N_H2(i)
        Sheet1.Cells(6 + i, 12) = N_H2O(i)

        'Calculate species partial pressures

        P_EB(i) = (N_EB(i) / N_Total(i)) * P_Total
        P_S(i) = (N_S(i) / N_Total(i)) * P_Total
        P_H2(i) = (N_H2(i) / N_Total(i)) * P_Total
        P_H2O(i) = (N_H2O(i) / N_Total(i)) * P_Total
    
```

**FIGURE 5.20a**

```

' Calculate Keq

Keq(i) = Exp(15.596 - 26734.68 / Temp(i))

' Calcualte the reaction rate lb-moles Styrene/(ft^3-sec)

r_S(i) = rho_catalyst * 3.5 * Exp(-19800 / Temp(i)) * (P_EB(i) - (P_S(i) *
P_H2(i) / Keq(i)))

delta_N_S(i) = r_S(i) * CSA * delta_z

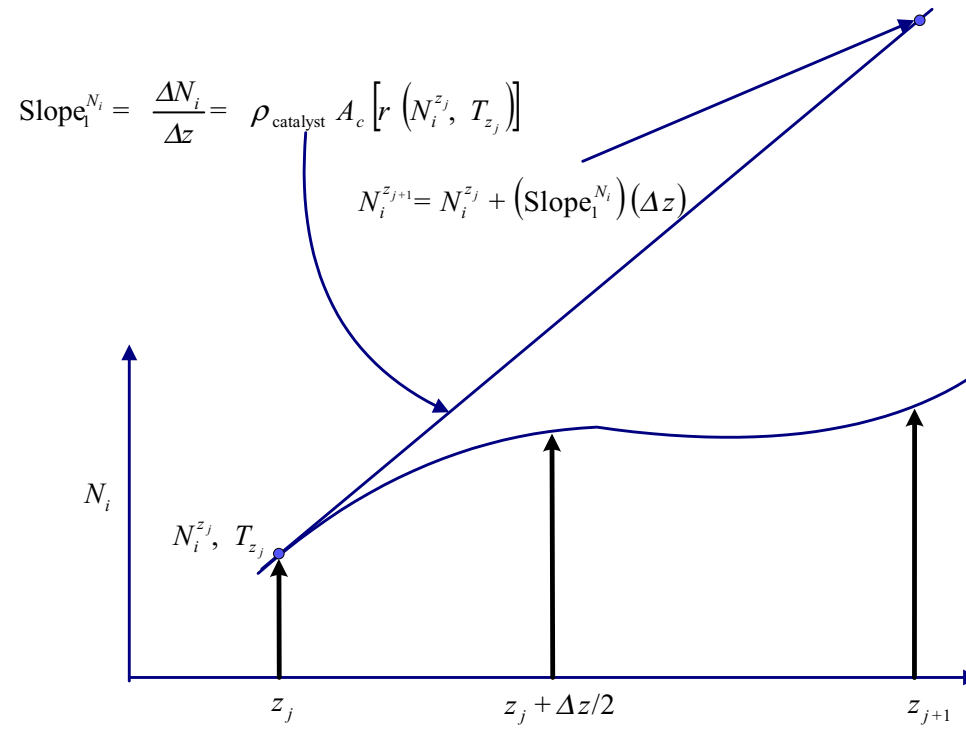
Q(i) = delta_N_S(i) * (-delta_H_reaction)

' Calculate conditions at z + delta_z
Temp(i + 1) = Temp(i) + Q(i) / (FCp)
N_EB(i + 1) = N_EB(i) - delta_N_S(i)
N_S(i + 1) = N_S(i) + delta_N_S(i)
N_H2(i + 1) = N_H2(i) + delta_N_S(i)
N_H2O(i + 1) = N_H2O(i)
N_Total(i + 1) = N_EB(i + 1) + N_S(i + 1) + N_H2(i + 1) + N_H2O(i + 1)
Next i

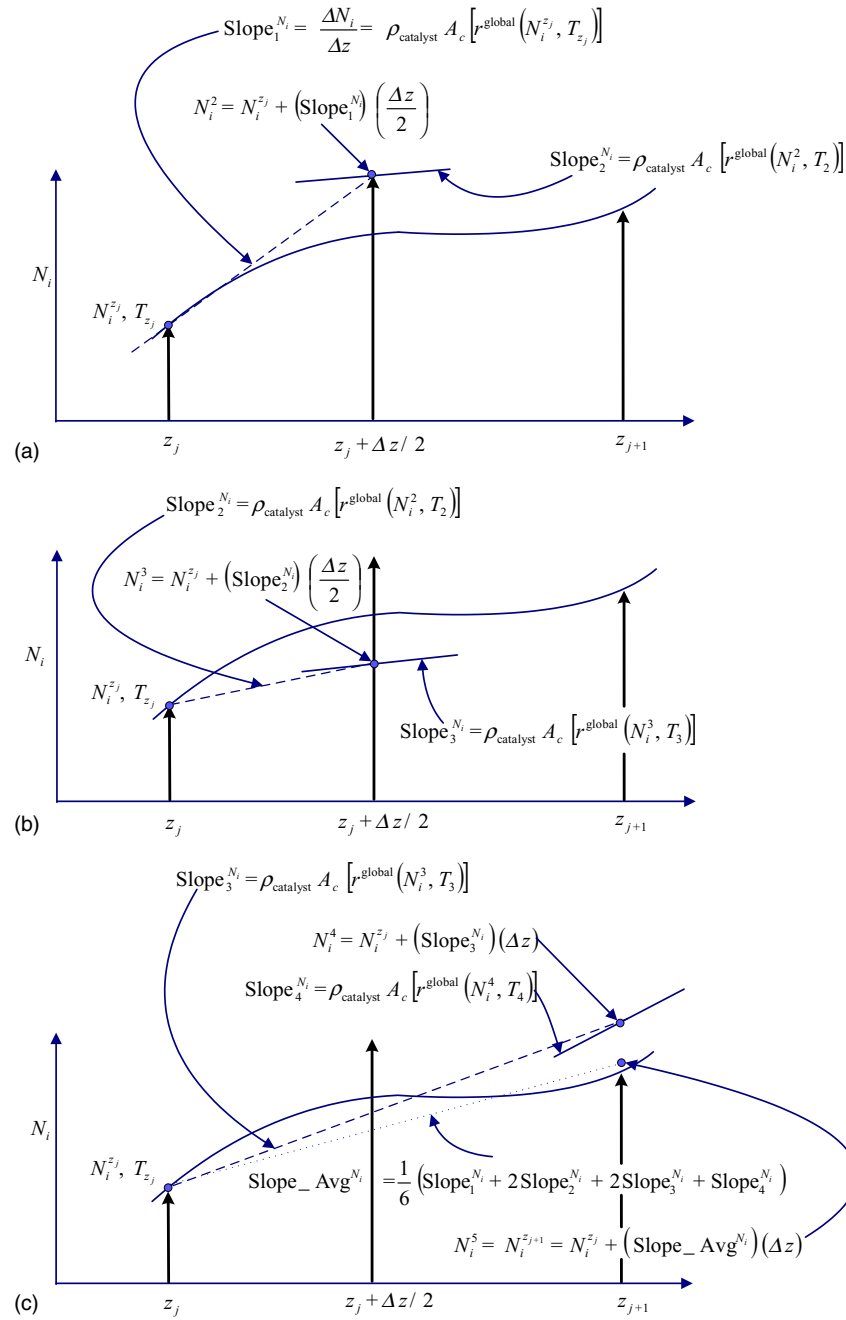
End Sub

```

**FIGURE 5.20b**



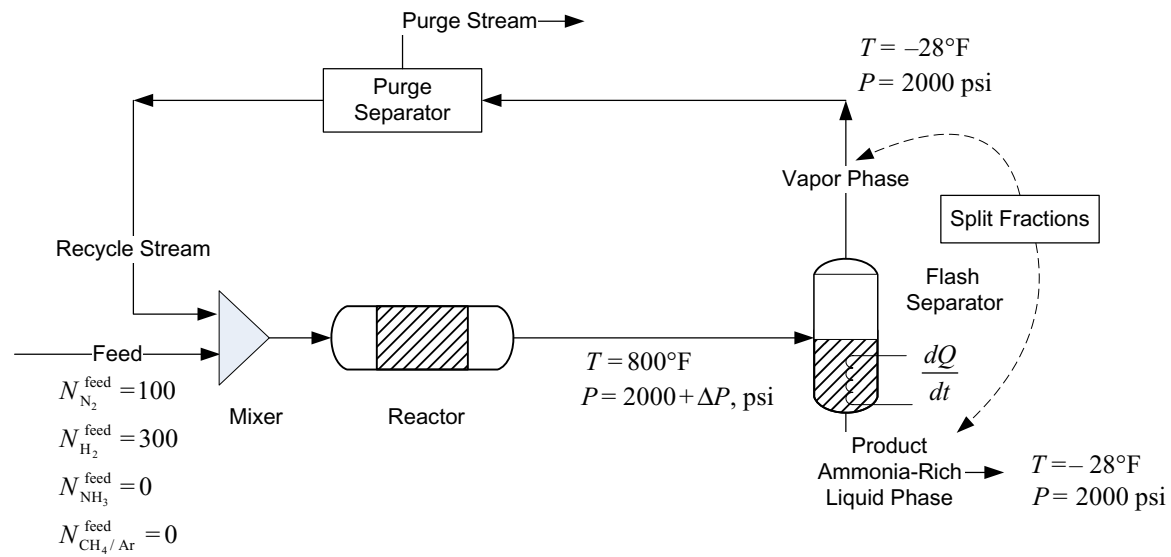
**FIGURE 5.22**



**FIGURE 5.23**

	A	B	C	D	E	F	G	H	I	J	K	L
5				distance z (ft)	% conversion EB	Temperature (R)	Temperature (C)	Temperature (F)	EB mol/s	S mol/s	H2 mol/s	H2O mol/s
6				0	0.00	1616.00	624.63	1156.33	5.13E-03	3.37E-05	0.00E+00	9.81E-02
7				0.1	2.78	1608.88	620.67	1149.21	4.99E-03	1.76E-04	1.43E-04	9.81E-02
8				0.2	5.35	1602.32	617.03	1142.65	4.85E-03	3.08E-04	2.74E-04	9.81E-02
9				0.3	7.73	1596.24	613.65	1136.57	4.73E-03	4.30E-04	3.96E-04	9.81E-02
10				0.4	9.94	1590.59	610.51	1130.92	4.62E-03	5.43E-04	5.10E-04	9.81E-02
11				0.5	12.01	1585.31	607.58	1125.64	4.51E-03	6.49E-04	6.16E-04	9.81E-02
12				0.6	13.94	1580.37	604.83	1120.70	4.41E-03	7.49E-04	7.15E-04	9.81E-02
13				0.7	15.76	1575.72	602.25	1116.05	4.32E-03	8.42E-04	8.08E-04	9.81E-02
14				0.8	17.47	1571.35	599.82	1111.68	4.23E-03	9.29E-04	8.96E-04	9.81E-02
15				0.9	19.08	1567.22	597.53	1107.55	4.15E-03	1.01E-03	9.79E-04	9.81E-02
16				1	20.61	1563.31	595.36	1103.64	4.07E-03	1.09E-03	1.06E-03	9.81E-02
17				1.1	22.06	1559.60	593.30	1099.93	4.00E-03	1.17E-03	1.13E-03	9.81E-02
18				1.2	23.44	1556.09	591.34	1096.42	3.93E-03	1.24E-03	1.20E-03	9.81E-02
19				1.3	24.75	1552.74	589.48	1093.07	3.86E-03	1.30E-03	1.27E-03	9.81E-02
20				1.4	26.00	1549.55	587.71	1089.88	3.80E-03	1.37E-03	1.33E-03	9.81E-02
21				1.5	27.19	1546.50	586.02	1086.83	3.73E-03	1.43E-03	1.39E-03	9.81E-02
22				1.6	28.32	1543.60	584.40	1083.93	3.68E-03	1.49E-03	1.45E-03	9.81E-02
23				1.7	29.41	1540.82	582.86	1081.15	3.62E-03	1.54E-03	1.51E-03	9.81E-02
24				1.8	30.45	1538.15	581.38	1078.48	3.57E-03	1.60E-03	1.56E-03	9.81E-02
25				1.9	31.45	1535.60	579.96	1075.93	3.52E-03	1.65E-03	1.61E-03	9.81E-02
26				2	32.41	1533.16	578.60	1073.49	3.47E-03	1.70E-03	1.66E-03	9.81E-02
27				2.1	33.33	1530.81	577.30	1071.14	3.42E-03	1.74E-03	1.71E-03	9.81E-02
28				2.2	34.21	1528.55	576.04	1068.88	3.37E-03	1.79E-03	1.75E-03	9.81E-02
29				2.3	35.06	1526.37	574.84	1066.70	3.33E-03	1.83E-03	1.80E-03	9.81E-02

**FIGURE 5.24**



**FIGURE 5.4**

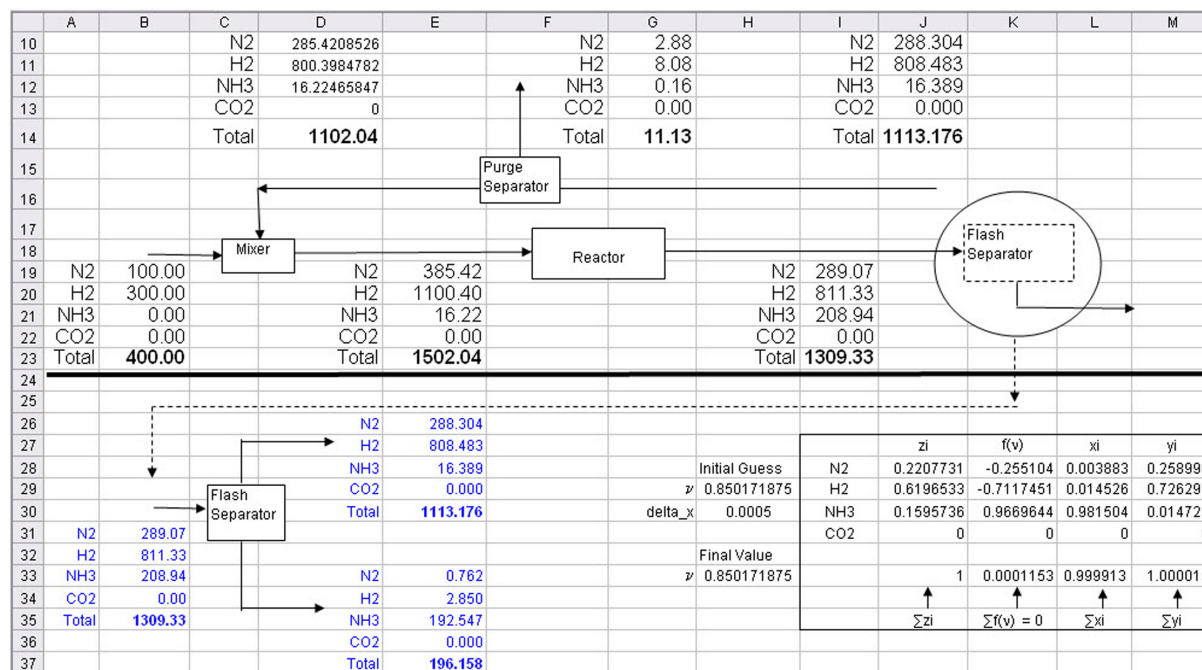
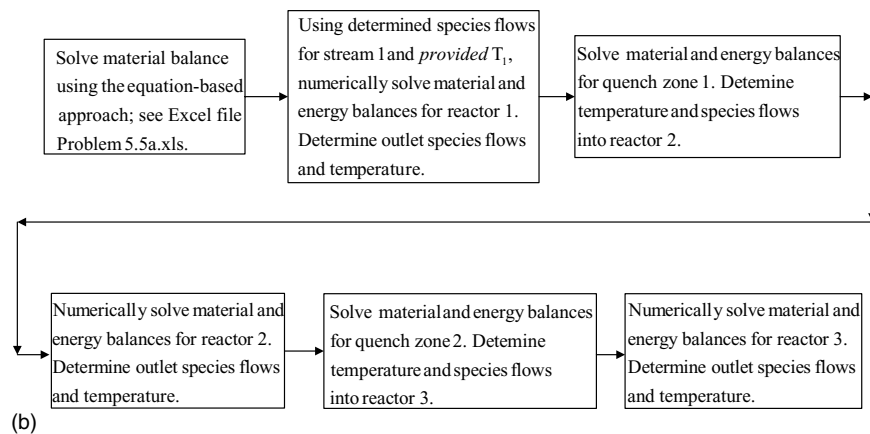


FIGURE 5.9



D	E	F	G	H	I	J	K	L	M	N
		P_Total	225							
distance z (ft)	% conversion N2	Temperature (K)	Temperature (C)	Temperature (F)	N2	H2	NH3	y-NH3	CH4	Ar
0	0.00	602.59	329.44	624.99	4957.32	13131.68	475.47	0.02	2153.99	460.52
0.1	0.23	604.22	331.07	627.92	4945.72	13096.88	498.67	0.02	2153.99	460.52
0.2	0.46	605.82	332.67	630.80	4934.33	13062.72	521.45	0.02	2153.99	460.52
0.3	0.69	607.39	334.24	633.64	4923.13	13029.11	543.85	0.03	2153.99	460.52
0.4	0.91	608.94	335.79	636.43	4912.09	12995.99	565.93	0.03	2153.99	460.52
0.5	1.13	610.48	337.33	639.19	4901.19	12963.29	587.73	0.03	2153.99	460.52
0.6	1.35	611.99	338.84	641.92	4890.41	12930.96	609.28	0.03	2153.99	460.52
0.7	1.56	613.49	340.34	644.62	4879.75	12898.96	630.62	0.03	2153.99	460.52
0.8	1.78	614.98	341.83	647.30	4869.17	12867.24	651.76	0.03	2153.99	460.52
0.9	1.99	616.46	343.31	649.95	4858.68	12835.77	672.74	0.03	2153.99	460.52
1	2.20	617.92	344.77	652.59	4848.27	12804.52	693.58	0.03	2153.99	460.52
6.93	14.94386023	707.7200612	434.5700612	814.2261102	4216.50503	10909.23508	1957.0999	0.099359	2153.99	460.52
6.94	14.96789187	707.8909293	434.7409293	814.5336728	4215.3137	10905.66111	1959.4826	0.099492	2153.99	460.52
6.95	14.99193353	708.0618745	434.9118745	814.8413741	4214.12188	10902.08564	1961.8662	0.099625	2153.99	460.52
6.96	15.01598517	708.2328966	435.0828966	815.1492138	4212.92956	10898.50869	1964.2509	0.099758	2153.99	460.52
6.97	15.04004677	708.4039954	435.2539954	815.4571916	4211.73675	10894.93026	1966.6365	0.099891	2153.99	460.52
18.4	27.82	800.08	526.93	980.47	3578.31	8994.66	3233.48	0.18	2153.99	460.52
18.5	27.82	800.08	526.93	980.48	3578.29	8994.58	3233.54	0.18	2153.99	460.52
18.6	27.82	800.09	526.94	980.49	3578.26	8994.51	3233.58	0.18	2153.99	460.52
18.7	27.82	800.09	526.94	980.49	3578.24	8994.45	3233.63	0.18	2153.99	460.52

(c)

FIGURE p5.5bc

	A	B	C	D	E	F	G	H	I	J	K	L
3	Using average molar heat capacities					7.42 $C_p N_2$						
4						7.02 $C_p H_2$						
5		Tref (K)	273.15			11.86 $C_p NH_3$						
6						14.57 $C_p CH_4$						
7						4.97 $C_p Ar$						
8												
9		323.15	Temp (K)	Feed								
10		2507.98	N(N2)	Feed								
11		7522.93	N(H2)	Feed								
12		0.00	N(NH3)	Feed								
13		96.54	N(CH4)	Feed								
14		34.55	N(Ar)	Feed								
15		3649923.65	$\Sigma N_i h_i$ (Cal)	Feed								
16												
17												
18												
19												
20												
21												
22												
23												
24												
25												
26												
27												

(a)

	A	B	C	D	E	F	G	H
3	Using average molar heat capacities					7.42 $C_p N_2$		
4						7.02 $C_p H_2$		
5		Tref (K)	273.15			11.86 $C_p NH_3$		
6						14.57 $C_p CH_4$		
7						4.97 $C_p Ar$		
8								
9		323.15	Temp (K)	Feed				
10		2507.98	N(N2)	Feed				
11		7522.93	N(H2)	Feed				
12		0.00	N(NH3)	Feed				
13		96.54	N(CH4)	Feed				
14		34.55	N(Ar)	Feed				
15		3649923.65	$\Sigma N_i h_i$ (Cal)	Feed				
16								
17								
18								
19								
20								
21								
22								
23								
24								
25								
26								
27								

(b)

FIGURE p5.6