

## CHAPTER VI CALCULATIONS

### 6.1 Calculation of Enthalpy Change from % Composition of the products

The thermodynamic equilibrium constant  $K^u$  is related to the standard Gibbs energy change for the process by

$$\Delta G^\circ = -RT \ln K^u \quad (6.1)$$

The thermodynamic equilibrium constant  $K^u$  is a dimensionless quantity. If the standard state for  $\Delta G^\circ$  is 1 atm pressure,  $K^u$  is  $K^u_p$ , which is the dimensionless form of  $K_p$  in which pressures are in atmospheres; if the standard state is 1 mol dm<sup>-3</sup> the  $K^u$  is  $K^u_c$ , which is the dimensionless form of  $K_c$  in which concentrations are expressed in mol dm<sup>-3</sup>.

$$\ln K^u_p = -\Delta G^\circ / RT = -(\Delta H^\circ / RT) + (\Delta S^\circ / R) \quad (6.2)$$

$$\ln K_2 - \ln K_1 = -(\Delta H^\circ / RT_2) + (\Delta H^\circ / RT_1) \quad (6.3)$$

$$\ln (K_2 / K_1) = (\Delta H^\circ / R) [(1/T_1) - (1/T_2)] \quad (6.4)$$

$$= (\Delta H^\circ / R) [(T_2 - T_1) / (T_1 T_2)] \quad (6.5)$$

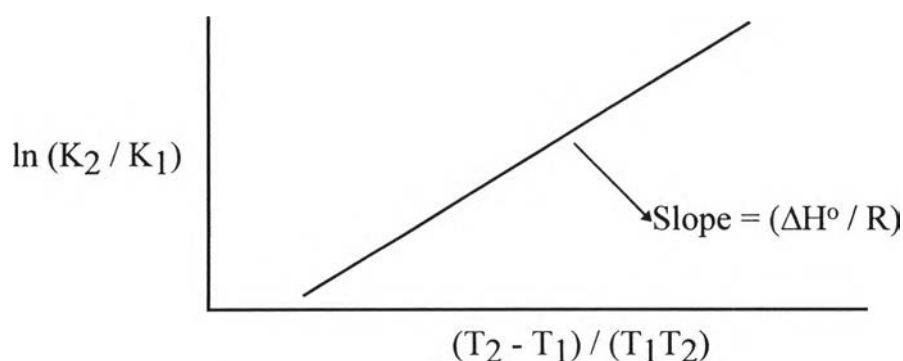


Figure 6.1 Plots of  $\ln (K_2 / K_1)$  against  $(T_2 - T_1) / (T_1 T_2)$ .

### 6.1.1 Enthalpy Change of Rubber Solvent

Table 6.1 Rubber Solvent by GC PIONA Method

Fractions	Temperature ( $^{\circ}\text{C}$ )					Mean Values
	125	130	135	140	150	
C <sub>4</sub>	0.03	0	0	0	0	0.006
C <sub>5</sub>	3.45	2.00	1.81	1.75	2.48	2.298
C <sub>6</sub>	31.76	29.08	34.30	32.90	39.82	33.572
C <sub>7</sub>	53.10	56.65	57.65	59.77	50.71	55.576
C <sub>8</sub>	11.17	11.77	6.01	5.34	6.72	8.202
C <sub>9</sub>	0.23	0.20	0	0	0.05	0.096
C <sub>10</sub>	0.16	0.18	0.18	0.19	0.15	0.172
C <sub>11</sub>	0.04	0.04	0	0	0	0.016
					Total	99.938

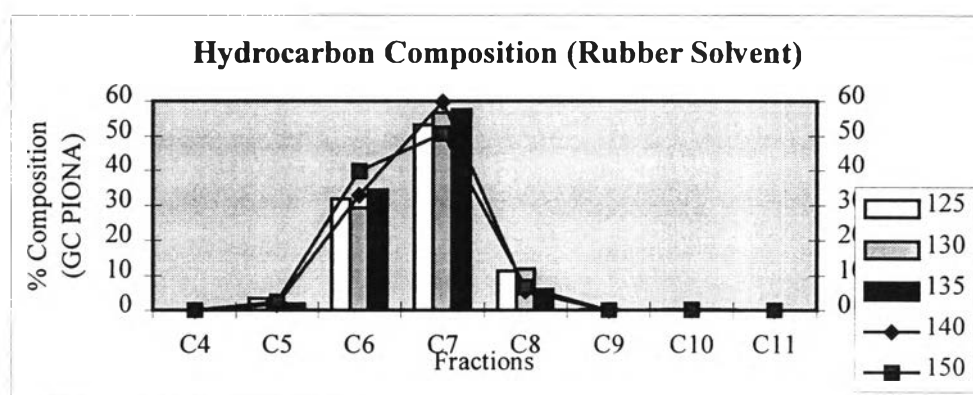


Figure 6.2 Plot of % composition by GC PIONA against temperature.

From the GC PIONA method, we found that Rubber solvent is C<sub>5</sub> to C<sub>8</sub> dominant. Therefore, use the data C<sub>5</sub> to C<sub>8</sub> % composition to calculate the enthalpy of the product.

Table 6.2 Enthalpy change of Rubber solvent (based on C<sub>5</sub> to C<sub>8</sub>)(a) Enthalpy Change Calculation Based on C<sub>5</sub> (K<sub>1,C5</sub>@140°C = 1.75, R = 8.314 J/Mol K)

T2 (°C)	T2 (K)	K <sub>2</sub>	K <sub>2</sub> / K	ln (K <sub>2</sub> / K <sub>1</sub> )	(T <sub>2</sub> - T <sub>1</sub> ) / T <sub>1</sub> T <sub>2</sub>	T <sub>1</sub> T <sub>2</sub> /(T <sub>2</sub> -T <sub>1</sub> )	ln (K <sub>2</sub> /K <sub>1</sub> )*[T <sub>1</sub> T <sub>2</sub> /(T <sub>2</sub> -T <sub>1</sub> )], ΔH <sup>0</sup> /R	ΔH <sup>0</sup> <sub>C5</sub>
125	398	3.45	1.971	0.678758	-9.12553E-05	-10958.27	-7438.016022	-61839.67
130	403	2.00	1.143	0.133531	-6.00821E-05	-16643.90	-2222.483146	-18477.72
135	408	1.81	1.034	0.033711	-2.96729E-05	-33700.80	-1136.089601	-9445.45
150	423	2.48	1.417	0.348643	5.72413E-05	17469.90	6090.754367	50638.53

(b) Enthalpy Change Calculation Based on C<sub>6</sub> (K<sub>1,C6</sub>@140°C = 32.90, R = 8.314 J/Mol K)

T2 (°C)	T2 (K)	K <sub>2</sub>	K <sub>2</sub> / K	ln (K <sub>2</sub> / K <sub>1</sub> )	(T <sub>2</sub> - T <sub>1</sub> ) / T <sub>1</sub> T <sub>2</sub>	T <sub>1</sub> T <sub>2</sub> /(T <sub>2</sub> -T <sub>1</sub> )	ln (K <sub>2</sub> /K <sub>1</sub> )*[T <sub>1</sub> T <sub>2</sub> /(T <sub>2</sub> -T <sub>1</sub> )], ΔH <sup>0</sup> /R	ΔH <sup>0</sup> <sub>C6</sub>
125	398	31.76	0.965	-0.035265	-9.12553E-05	-10958.27	386.4435084	3212.89
130	403	29.08	0.884	-0.123422	-6.00821E-05	-16643.90	2054.223511	17078.81
135	408	34.30	1.043	0.041673	-2.96729E-05	-33700.80	-1404.403207	-11676.21
150	423	39.82	1.210	0.190897	5.72413E-05	17469.90	3334.945226	27726.73

(c) Enthalpy Change Calculation Based on  $C_7(K_{1,C7}@140^\circ\text{C} = 59.77, R = 8.314 \text{ J/Mol K})$

T2 ( $^\circ\text{C}$ )	T2 (K)	$K_2$	$K_2 / K_1$	$\ln(K_2 / K_1)$	$(T_2 - T_1) / T_1 T_2$	$T_1 T_2 / (T_2 - T_1)$	$\ln(K_2/K_1) * [T_1 T_2 / (T_2 - T_1)], \Delta H^0/R$	$\Delta H^0_{C7}$
125	398	53.10	0.888	-0.118327	-9.12553E-05	-10958.27	1296.658103	10780.42
130	403	56.65	0.948	-0.053612	-6.00821E-05	-16643.90	892.3106923	7418.67
135	408	57.65	0.965	-0.036114	-2.96729E-05	-33700.80	1217.057754	10118.62
150	423	50.71	0.848	-0.164381	5.72413E-05	17469.90	-2871.714968	-23875.44

(d) Enthalpy Change Calculation Based on  $C_8(K_{1,C8}@140^\circ\text{C} = 5.34, R = 8.314 \text{ J/Mol K})$

T2 ( $^\circ\text{C}$ )	T2 (K)	$K_2$	$K_2 / K_1$	$\ln(K_2 / K_1)$	$(T_2 - T_1) / T_1 T_2$	$T_1 T_2 / (T_2 - T_1)$	$\ln(K_2/K_1) * [T_1 T_2 / (T_2 - T_1)], \Delta H^0/R$	$\Delta H^0_{C10}$
125	398	11.17	2.092	0.738006	-9.12553E-05	-10958.27	-8087.266112	-67237.53
130	403	11.77	2.204	0.790328	-6.00821E-05	-16643.90	-13154.14466	-109363.56
135	408	6.01	1.125	0.118199	-2.96729E-05	-33700.80	-3983.40408	-33118.02
150	423	6.72	1.258	0.229863	5.72413E-05	17469.90	4015.674916	33386.32

(e) Enthalpy Change Calculation Based on C<sub>5</sub> to C<sub>8</sub>

Temperature, °C	Percent	$\Delta H^{\circ}_{C_5}$	Percent	$\Delta H^{\circ}_{C_6}$	Percent	$\Delta H^{\circ}_{C_7}$	Percent	$\Delta H^{\circ}_{C_8}$	$\Delta H^{\circ}_{Total}$
125	3.45	61839.7	31.76	3212.89	53.10	10780.4	11.17	67237.53	<b>16388.72</b>
130	2.00	18477.7	29.08	17078.8	56.65	7418.67	11.77	109363.56	<b>22410.84</b>
135	1.81	9445.45	34.30	11676.2	57.65	10118.6	6.01	33118.02	<b>11999.68</b>
150	2.48	50638.5	39.82	27726.7	50.71	23875.4	6.72	33386.32	<b>26647.42</b>

### 6.1.2 Enthalpy Change of Straight Run Light Hydrocarbon

Table 6.3 Straight Run Light Hydrocarbon by GC PIONA method

Fractions	Temperature ( $^{\circ}\text{C}$ )					Mean Values
	125	130	135	140	150	
C <sub>4</sub>	0.04	0.04	0.03	0.02	0.04	0.034
C <sub>5</sub>	0.84	0.85	0.65	0.53	0.76	0.726
C <sub>6</sub>	9.12	8.83	8.04	6.92	7.88	8.158
C <sub>7</sub>	30.44	28.68	32.25	31.29	29.17	30.366
C <sub>8</sub>	43.33	42.73	46.48	47.75	47.12	45.482
C <sub>9</sub>	11.49	16.04	9.42	12.00	13.51	12.492
C <sub>10</sub>	4.41	2.49	2.77	1.08	1.18	2.396
C <sub>11</sub>	0.23	0.24	0.29	0.33	0.26	0.270
					Total	99.914

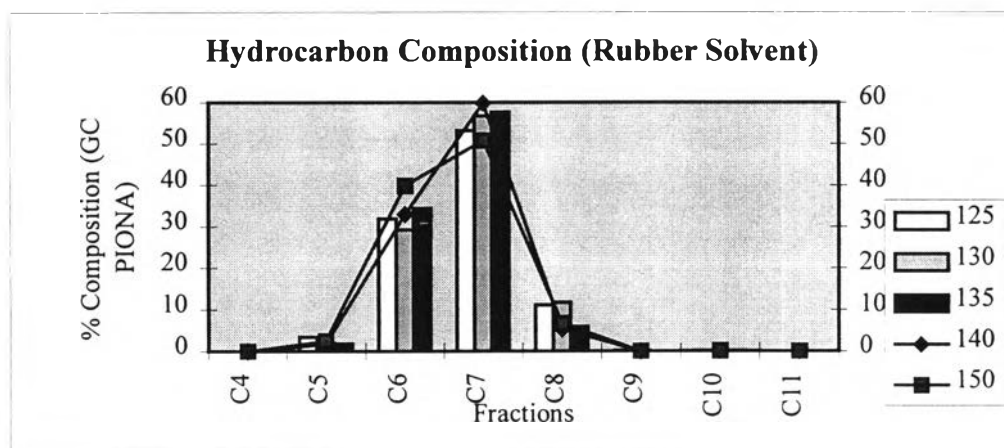


Figure 6.3 Plot of % composition by GC PIONA against temperature.

From the GC PIONA method, we found that Straight Run Light Hydrocarbon is C<sub>6</sub> to C<sub>10</sub> dominant. Therefore, use the data of the C<sub>6</sub> to C<sub>10</sub> % composition to calculate the enthalpy of the product.

Table 6.4 Enthalpy Change Calculation Based on C<sub>6</sub> to C<sub>10</sub>

Temperature, °C	Percent	$\Delta H^{\circ}_{,C6}$	Percent	$\Delta H^{\circ}_{,C7}$	Percent	$\Delta H^{\circ}_{,C8}$	Percent	$\Delta H^{\circ}_{,C9}$	Percent	$\Delta H^{\circ}_{,C10}$	$\Delta H^{\circ}_{,Total}$
125	9.12	25150.5	30.44	2509.18	43.33	8849.57	11.49	3956.74	4.41	128179.72	7346.66
130	8.83	33728.00	28.68	12052.5	42.73	15370.7	16.04	40154.20	2.49	115589.63	19443.45
135	8.04	42032.00	32.25	8467.15	46.48	7553.03	9.42	67825.66	2.77	263905.66	16009.85
150	7.88	18869.1	29.17	10190.1	47.12	1929.07	13.51	17214.92	1.18	12861.92	7694.03

### 6.1.3 Enthalpy Change of Spirit

Table 6.5 Spirit by GC PIONA method

Fractions	Temperature ( $^{\circ}\text{C}$ )					Mean Values
	125	130	135	140	150	
C <sub>4</sub>	0	0	0	0	0	0
C <sub>5</sub>	0	0	0	0	0	0
C <sub>6</sub>	0.05	0.06	0.18	0.04	0.16	0.098
C <sub>7</sub>	2.17	2.02	3.31	2.21	2.55	2.452
C <sub>8</sub>	22.90	18.58	40.76	25.98	28.99	27.442
C <sub>9</sub>	42.20	37.23	41.95	42.14	42.85	41.274
C <sub>10</sub>	25.20	29.73	11.96	22.89	19.96	21.948
C <sub>11</sub>	3.86	6.63	0.89	3.48	2.64	3.500
					Total	96.714

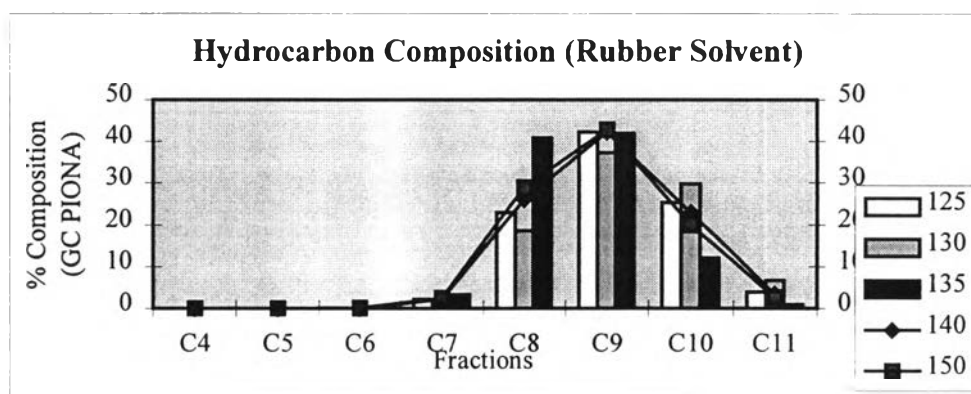


Figure 6.4 Plot of % composition by GC PIONA against temperature.

From the GC PIONA method, we found that Spirit is C7 to C11 dominant. Therefore, use the data of the C7 to C11 % composition to calculate the enthalpy of the product.



Table 6.6 Enthalpy Change Calculation Based on C<sub>7</sub> to C<sub>11</sub>

Temperature, °C	Percent	$\Delta H^{\circ}_{C7}$	Percent	$\Delta H^{\circ}_{C8}$	Percent	$\Delta H^{\circ}_{C9}$	Percent	$\Delta H^{\circ}_{C10}$	Percent	$\Delta H^{\circ}_{C11}$	$\Delta H^{\circ}_{Total}$
125	2.17	1664.10	22.9	11496.81	42.20	129.63	25.2	8759.38	3.86	9441.87	4930.95
130	2.02	12439.44	18.58	46389.81	37.23	17142.5	29.73	36179.67	6.63	89194.26	26008.89
135	3.31	113183.71	40.76	126189.65	41.95	1266.16	11.96	181879.40	0.89	382055.48	77465.21
150	2.55	20784.65	28.99	15922.3	42.85	2426.78	19.96	19894.15	2.64	40124.35	10156.63

### 6.1.4 Enthalpy Change of Distillate

Table 6.7 Distillate by GC PIONA method

Fractions	Temperature ( $^{\circ}\text{C}$ )					Mean Values
	125	130	135	140	150	
C <sub>4</sub>	0	0	0	0	0	0
C <sub>5</sub>	0	0	0	0	0	0
C <sub>6</sub>	1.31	1.38	1.07	1.18	1.34	1.256
C <sub>7</sub>	1.38	1.39	1.98	1.25	0.71	1.342
C <sub>8</sub>	7.32	6.43	11.55	6.89	4.91	7.420
C <sub>9</sub>	13.25	11.97	21.49	13.17	11.83	14.342
C <sub>10</sub>	18.22	16.33	20.19	17.88	17.03	17.930
C <sub>11</sub>	12.63	13.21	10.33	12.93	12.92	12.404
					Total	54.694

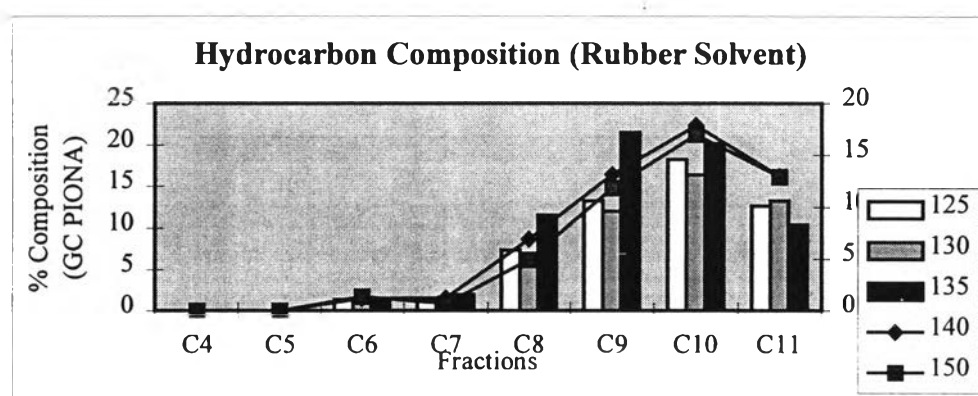


Figure 6.5 Plot of % composition by GC PIONA against temperature.

From the GC PIONA method, we found that Spirit is C<sub>6</sub> to C<sub>11</sub> dominant, use the data of the C<sub>6</sub> to C<sub>11</sub> % composition to calculate the enthalpy of the product.

Table 6.8 Enthalpy Change Calculation Based on C<sub>6</sub> to C<sub>11</sub>

Temperature, °C	%	$\Delta H^{\circ}_{C6}$	%	$\Delta H^{\circ}_{C7}$	%	$\Delta H^{\circ}_{C8}$	%	$\Delta H^{\circ}_{C9}$	%	$\Delta H^{\circ}_{C10}$	%	$\Delta H^{\circ}_{C11}$	$\Delta H^{\circ}_{Total}$
125	1.31	9521.84	1.38	9014.12	7.3	5515.55	13.3	551.75	18.2	1716.19	12.6	2138.76	<b>725.98</b>
130	1.38	21665.62	1.39	14690.17	6.4	9561.40	12.0	13220.30	16.3	12547.90	13.2	2964.59	<b>2700.45</b>
135	1.07	27418.06	1.98	128873.6	11.6	144749	21.5	137193.2	20.2	34044.2	10.3	62901.72	<b>49046.44</b>
150	1.34	18468.62	0.71	82155.35	4.9	49208.5	11.8	15585.17	17.0	9074.33	12.9	112.38	<b>5090.65</b>

## 6.2 Calculation of Enthalpy Change from the First Law of Thermodynamics

The first law of a steady-flow process is expressed by;

$$\Delta H = Q - W_s \quad (6.6)$$

In this experiment, no shaft work is accomplished between state1 (140°C) and state2 (125, 130, 135, 150 °C). Hence equation 6.6 reduces to

$$\Delta H = H_2 - H_1 = Q \quad (6.7)$$

### $\Delta H$ of Raw Material Calculation

From experiment;    Raw material feed rate        = 45 GPM  
                                   Steady - state time                        = 120 minutes  
                                    $C_p / R$     =  $A + BT + CT^2 + DT^2$   
                                    $R$     = 8.314 J/mol K

Table 6.9 Percent Composition of Raw Material

PIONA Analysis	% Volume	Percent Composition
C <sub>4</sub>	0.07	0.0192
C <sub>5</sub>	4.29	1.177
C <sub>6</sub>	36.35	9.973
C <sub>7</sub>	87.09	23.890
C <sub>8</sub>	84.72	23.244
C <sub>9</sub>	67.21	18.439
C <sub>10</sub>	67.99	18.654
C <sub>11</sub>	16.76	4.598

Note : All carbon compositions in raw material are paraffin dominant.

$$C_p(\text{Total}) = 0.0002C_{p,C4} + 0.0117C_{p,C5} + 0.099C_{p,C6} + 0.238C_{p,C7} \\ + 0.2324C_{p,C8} + 0.184C_{p,C9} + 0.186C_{p,C10} + 0.045C_{p,C11} \quad (6.8)$$

Table 6.10 Heat Capacities Calculation

Composition	$C_p$ (Ideal Gas, 60°F, 14.696 psia)	$C_p$	
		<u>Btu</u> lbmol F	<u>J</u> mol K
C <sub>4</sub>	0.3970	0.0000794	0.000084
C <sub>5</sub>	0.3972	0.0046472	0.004903
C <sub>6</sub>	0.3984	0.0394416	0.041614
C <sub>7</sub>	0.3992	0.0950096	0.100244
C <sub>8</sub>	0.3998	0.0929135	0.098033
C <sub>9</sub>	0.3850	0.0708400	0.074743
C <sub>10</sub>	0.3870	0.0719820	0.075948
C <sub>11</sub>	-	-	-
	Total	0.3749133	0.395569

Note : 1 Btu = 1055.1 Joules

1 lbmol F = 1000 mol K

Table 6.11 Heat of Vaporization Calculation

Composition	Heat of Vaporization (Cal./g)	Heat of Vaporization (Cal./g)
C <sub>4</sub>	86.63	0.0173
C <sub>5</sub>	87.54	1.024
C <sub>6</sub>	87.50	8.662
C <sub>7</sub>	87.18	20.748
C <sub>8</sub>	86.80	20.172
C <sub>9</sub>	94.90	17.462
C <sub>10</sub>	56.14	10.442
C <sub>11</sub>	58.05	2.612
	Total	81.1393

**Raw Material (Feed) :**

Heat capacities	=	C <sub>p</sub>	=	0.395569	J/mol K
Heat of vaporization	=	L	=	81.1393	Cal./g
			=	339.714	J/g
			=	339.714 $\frac{\text{J}}{\text{g}}$ * 116.642 $\frac{\text{g}}{\text{mol}}$	
			=	39,624.92	J/mol
Specific Gravity	=	0.7535	=	$\frac{\text{Density of oil (Kg/Gal.)}}{\text{Density of water (Kg/Gal.)}}$	
Density of feed	=	0.7535			
Flow rate	=	45	Gal./min		
Steady state time	=	120	min.		
Volume	=	45	Gal.	=	0.170325 m <sup>3</sup>
Mass	=	m	=	0.7535*0.170325	Kg

$$\begin{aligned}
 &= 0.12833 \quad \text{Kg} \\
 &= 128.33 \quad \text{g} \\
 \text{Molecular Weight of feed} &= (0.0002M.W._{C_4H_{10}})+(0.0117M.W._{C_5H_{12}}) \\
 &+ (0.099M.W._{C_6H_{14}})+(0.238M.W._{C_7H_{16}}) \\
 &+ (0.2324M.W._{C_8H_{18}})+(0.184M.W._{C_9H_{20}}) \\
 &+ (0.186M.W._{C_{10}H_{22}})+(0.045M.W._{C_{11}H_{24}}) \\
 &= (0.0002*58)+(0.0117*72)+(0.099*86) \\
 &+ (0.238*100)+(0.2324*114)+(0.184*128) \\
 &+ (0.186*142)+(0.045*156) \\
 &= 0.0116+0.8424+8.514+23.8+26.49+23.552 \\
 &+ 26.412+7.02 \\
 &= 116.642 \quad \text{g/mol} \\
 \text{Mass} &= \frac{128.33}{116.642} = 1.1002 \quad \text{mol}
 \end{aligned}$$

### 6.2.1 At Feed Inlet Temperature @ 125°C

Raw material is not completely evaporated. There are 2 fractions: one is a liquid with boiling point lower than 125°C, and is assumed to be totally evaporated in the first distillation tower. The other fraction is a liquid with boiling point higher than 125°C, and is not evaporated.

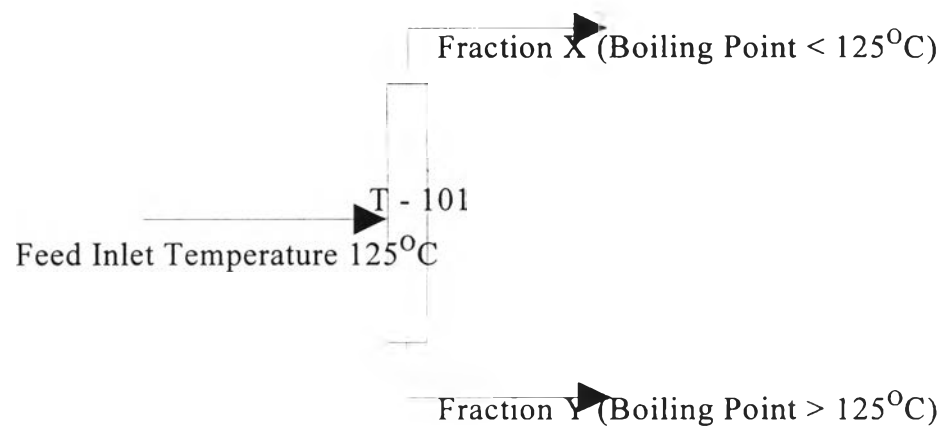


Figure 6.6 Drawing of T-101 on mass balance.

Table 6.12 Boiling range of raw material (ASTM D86)

IBP	30
10%	63
20%	75
30%	93
40%	109
50%	125
60%	147
70%	179
80%	236
90.00%	313.5
EP	348



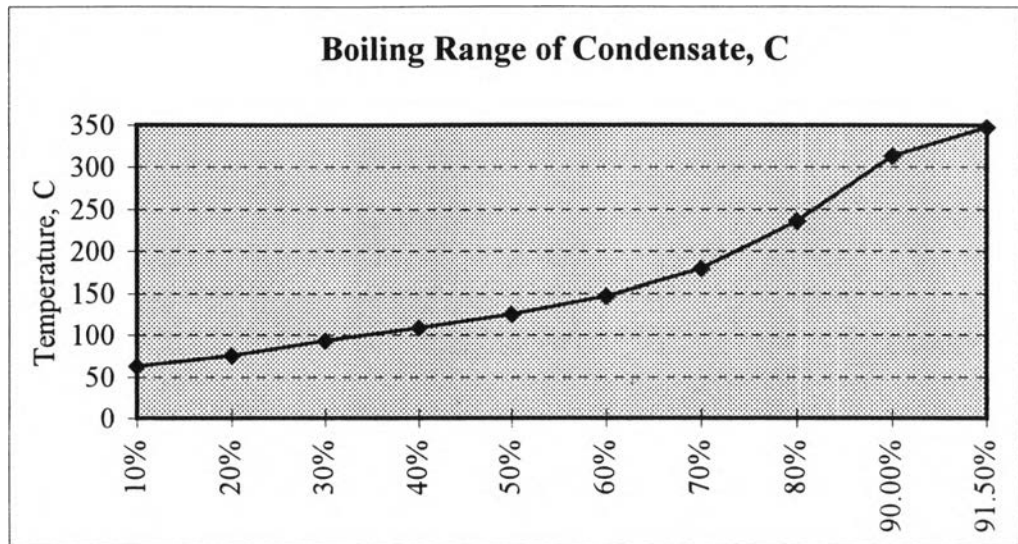


Figure 6.6 Equilibrium Flash Vaporization curve of raw material.

From Figure 6.6 at 125°C, fraction X = 0.5 and fraction Y = 0.415

$$Q = \Delta H = [X(mC_p\Delta T + mL)] + [Y(mC_p\Delta T)] \quad (6.9)$$

$$\begin{aligned} \Delta H_{\text{feed}} &= [0.5(1.1002 \cdot 0.39556 \cdot (125-25) + 1.1002 \cdot 39624.92 \cdot 10^5)] \\ &\quad + [0.415(1.1002 \cdot 0.39556 \cdot (125-25))] \\ &= 21819.43 + 18.061 \end{aligned}$$

$$\begin{aligned} &[(\text{mol})(\text{J}/\text{molK})(\text{K}) + (\text{mol})(\text{J}/\text{mol})] + [(\text{mol})(\text{J}/\text{molK})(\text{K})] \\ &= 21837.49 \text{ J} \end{aligned}$$

Therefore,  $\Delta H$  of feed inlet (raw material) @ 125°C = 21,837.49 J

Table 6.13 Product Specification

Products	Boiling Range, °C	% from EFV Curve
Rubber	68 - 112	25.458
Straight Run Lt. HC	87 - 145	30.910
Spirit	137 - 178	13.641
Distillate	152.5 - 276	23.636

Table 6.14  $\Delta H$  of products

Products	$\Delta H @ 125^\circ\text{C}$
Rubber	5,559.38
Straight Run Light HC	6,747.78
Spirit	2,978.85
Distillate	5,161.51

### 6.2.2 At Feed Inlet Temperature @ $130^\circ\text{C}$

Raw material is not completely evaporated. There are 2 fractions, one is a liquid with boiling point lower than  $130^\circ\text{C}$  and is assumed to be totally evaporated in the first distillation tower. The other fraction is a liquid with boiling point higher than  $130^\circ\text{C}$  and is not evaporated.

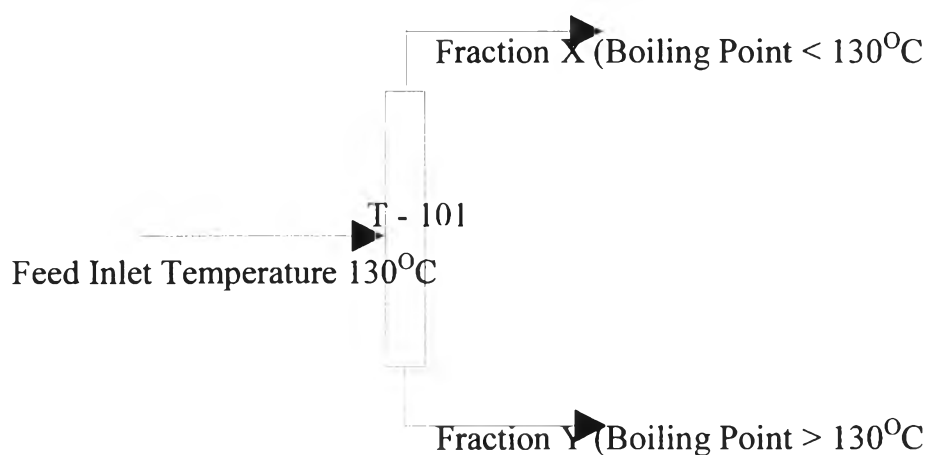


Figure 6.7 Drawing of T-101 on mass balance.

From Figure 6.6 at 130°C, fraction X = 0.52 and fraction Y = 0.395

$$Q = \Delta H = [X(mC_p\Delta T + mL)] + [Y(mC_p\Delta T)] \quad (6.9)$$

$$\begin{aligned} \Delta H_{\text{feed}} &= [0.52(1.1002 \cdot 0.39556 \cdot (130-25) + 1.1002 \cdot 39624.92) \\ &\quad + [0.395(1.1002 \cdot 0.39556 \cdot (130-25))] \\ &= 22693.34 + 18.049 \\ &= 22711.39 \text{ J} \end{aligned}$$

Therefore  $\Delta H$  of feed inlet (raw material) @ 130°C = 22,711.39 J

Table 6.15 Product specification

Products	Boiling Range, °C	% from EFV Curve
Rubber	69 - 111	26.25
Straight Run Lt. HC	83 - 155	38.06
Spirit	141 - 187	14.13
Distillate	149 - 271	23.89

Table 6.16  $\Delta H$  of products

Products	$\Delta H$ @ 130°C (J)
Rubber	5,961.74
Straight Run Lt. HC	8,643.96
Spirit	3,209.12
Distillate	5,425.75

### 6.2.3 At Feed Inlet Temperature @ 135 °C

Raw material is not completely evaporated. There are 2 fractions, one is a liquid with boiling point lower than 135°C and is assumed to be totally evaporated in the first distillation tower. The other fraction is a liquid with boiling point higher than 135°C and is not evaporated.

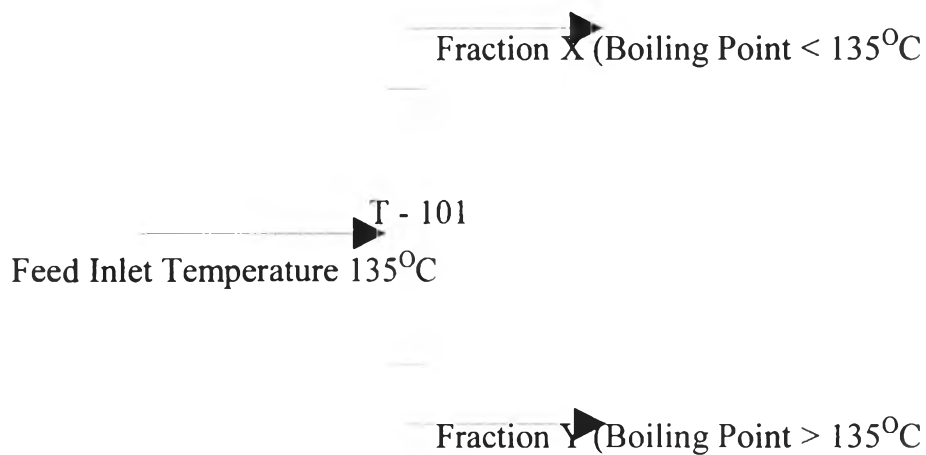


Figure 6.8 Drawing of T-101 on mass balance.

From Figure 6.8 at 135°C, fraction X = 0.545 and fraction Y = 0.

$$\begin{aligned}
 Q = \Delta H &= [X(mC_p\Delta T + mL)] + [Y(mC_p\Delta T)] \\
 \Delta H_{\text{feed}} &= [0.545(1.1002 \cdot 0.39556 \cdot (135-25) + 1.1002 \cdot 39624.92)] \\
 &\quad + [0.37(1.1002 \cdot 0.39556 \cdot (135-25))] \\
 &= 23785.55 + 17.712 \\
 &= 23803.26 \text{ J}
 \end{aligned}$$

Therefore  $\Delta H$  of feed inlet (raw material) @ 135°C = 23,803.26 J

Table 6.17 Product specification

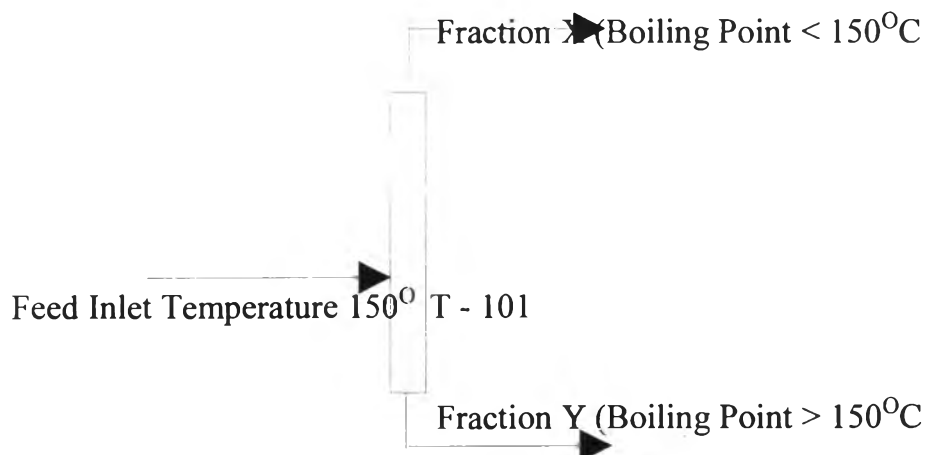
Products	Boiling Range, °C	% from EFV Curve
Rubber	73 - 105.5	19.48
Straight Run Lt. HC	89 - 141	29.49
Spirit	130 - 171	15.23
Distillate	140 - 266	27.05

Table 6.18  $\Delta H$  of products

Products	$\Delta H @ 135^\circ\text{C}$ (J)
Rubber	4,636.88
Straight Run Lt. HC	7,019.58
Spirit	3,625.24
Distillate	6,438.78

#### 6.2.4 At Feed Inlet Temperature @ 150°C

Raw material is not completely evaporated. There are 2 fractions, one is a liquid with boiling point lower than 150°C and is assumed to be totally evaporated in the first distillation tower. The other fraction is a liquid with boiling point higher than 150°C and is not evaporated.



From Figure 6.8 at 150°C, fraction X = 0.61 and fraction Y = 0.305

$$Q = \Delta H = [X(mCp\Delta T + mL)] + [Y(mCp\Delta T)] \quad (6.9)$$

$$\begin{aligned} \Delta H_{\text{feed}} &= [0.61(1.1002*0.39556*(150-25) + 1.1002*39624.92) \\ &\quad + [0.305(1.1002*0.39556*(150-25))] \\ &= 26626.33 + 16.59 \\ &= 26642.92 \text{ J} \end{aligned}$$

Therefore  $\Delta H$  of feed inlet (raw material) @ 150°C = 26,642.92 J

Table 6.19 Product specification

Products	Boiling Range, °C	% from EFV Curve
Rubber	72 - 106	20.62
Straight Run Lt. HC	92 - 154	32.74
Spirit	140 - 183	13.88
Distillate	151 - 286	25.20

Table 6.20  $\Delta H$  of products

Products	$\Delta H$ @ 150°C (J)
Rubber	5,493.77
Straight Run Lt. HC	8,722.89
Spirit	3,698.04
Distillate	6,714.02

### 6.3 Comparison of $\Delta H$ from GC PIONA Analysis and Theory

Enthalpy change from 6.1 (PIONA Analysis) in unit of J/mol. But for enthalpy change from theory, the unit is J. For comparison, we have to convert J/mol to J by the following:

$$\begin{aligned} \text{For Rubber Solvent : } & [(\text{feed inlet, Gal.})(\% \text{Yield of Rubber})(\text{Sp.Gr.of Rubber}) \\ & (\text{conversion factor from Gal. to m}^3) \\ & (\text{conversion factor from Kg to g})/\text{MW.of Rubber C}_7\text{H}_{16} \\ & = [(45)(0.25)(0.74)(0.003785)(1000)]/100 \\ & = 0.315 \text{ mol} \end{aligned}$$

For Straight Run Lt. HC :

$$\begin{aligned} & [(\text{feed inlet, Gal.})(\% \text{Yield of SRLHC})(\text{Sp.Gr.of SRLHC}) \\ & (\text{conversion factor from Gal. to m}^3) \\ & (\text{conversion factor from Kg to g})/\text{MW.of SRLHC C}_8\text{H}_{18} \\ & = [(45)(0.31)(0.77)(0.003785)(1000)]/114 \\ & = 0.357 \text{ mol} \end{aligned}$$

For Spirit :

$$\begin{aligned} & [(\text{feed inlet, Gal.})(\% \text{Yield of Spirit})(\text{Sp.Gr.of Spirit}) \\ & (\text{conversion factor from Gal. to m}^3) \\ & (\text{conversion factor from Kg to g})/\text{MW.of Spirit C}_9\text{H}_{20} \\ & = [(45)(0.14)(0.79)(0.003785)(1000)]/128 \\ & = 0.147 \text{ mol} \end{aligned}$$

For Distillate :

$$\begin{aligned} & [(\text{feed inlet, Gal.})(\% \text{Yield of Distillate})(\text{Sp.Gr.of Distillate}) \\ & (\text{conversion factor from Gal. to m}^3) \\ & (\text{conversion factor from Kg to g})/\text{MW.of Dist. C}_{10}\text{H}_{22} \\ & = [(45)(0.24)(0.81)(0.003785)(1000)]/142 \\ & = 0.233 \text{ mol} \end{aligned}$$

Table 6.21  $\Delta H$  from GC PIONA Analysis

Feed Inlet Temp., °C	Rubber	Straight Run Lt. HC	Spirit	Distillate
	$\Delta H$ (J/mol)			
125	16,388.72	7,346.66	4,930.95	725.98
130	22,410.84	19,443.45	26,008.89	2,700.45
135	11,999.68	16,009.85	77,465.21	49,046.44
150	26,647.42	7,694.03	10,156.63	5,090.65

Table 6.22  $\Delta H$  from GC PIONA Analysis

Feed Inlet Temp., °C	Rubber	Straight Run Lt. HC	Spirit	Distillate
	$\Delta H$ (J)			
125	5,162.45	2,622.76	724.85	169.15
130	7,059.41	6,941.31	3,823.31	629.20
135	3,779.90	5,715.52	11,387.39	11,427.82
150	8,393.94	2,746.77	1,493.02	1,186.12

Table 6.23  $\Delta H$  from Theory

Feed Inlet Temp., °C	Rubber	Straight Run Lt. HC	Spirit	Distillate
	$\Delta H$ (J)			
125	5,559.38	6,747.78	2,978.85	5,161.51
130	5,961.74	8,643.96	3,209.12	5,425.75
135	4,636.88	7,019.58	3,625.24	6,438.78
150	5,493.77	8,722.89	3,698.04	6,714.02