Energy Balances

One man's magic is another man's engineering. Lazarus Long

Energy Balances

- Temperature and pressure are already fixed in the mass balance calculations of many unit operations due to the assumption of saturated streams.
- An energy balance calculation is necessary to determine the heating and cooling duties in the flowsheet.
- An estimate of the heat content of each stream can be rapidly determined by making the following assumptions:
 - 1. The vapor and liquid streams have ideal properties.
 - 2. Kinetic and potential energies of process streams are neglected and only enthalpy changes are considered.
 - 3. Standard enthalpy reference ($\Delta H = 0$) is at $P_0 = 1 \ atm$, $T_0 = 298 \ K$ and elemental species.

Enthalpies of Vapor Streams



Using the ideal properties assumption, $\Delta H_p = 0$. Thus, $\Delta H_v = \Delta H_f + \Delta H_T$ $\Delta H_f = y_1 H_{f,1}(T_0) + ... + y_n H_{f,n}(T_0) = \sum y_k H_{f,k}(T_0)$ where $H_{f,k}(T_0)$ is the heat of formation of component k at temperature T_0 .

$$\Delta H_T = y_1 \int_{T_0}^T c_{p,1}^0 dT + \dots + y_n \int_{T_0}^T c_{p,n}^0 dT = \sum y_k \int_{T_0}^T c_{p,k}^0 dT$$

where $c_{p,k}^0$ is the temperature dependent heat capacity of _____
component k.

Heat Exchanger Calculation

Consider a heat exchanger with no phase change.



There is temperature change but no composition change. At steady state:

$$(\mu \Delta H)_{in} + Q = (\mu \Delta H)_{out}$$

Since composition does not change, ΔH_f at T_0 is the same on both sides of heat balance and thus cancels out.

$$(\mu \Delta H_f)_{in} + (\mu \Delta H_T)_{in} + Q = (\mu \Delta H_f)_{in} + (\mu \Delta H_T)_{out}$$

This implies:

$$Q = \mu \left(y_1 \int_{T_1}^{T_2} c_{p,1}^0 dT + \dots + y_n \int_{T_1}^{T_2} c_{p,n}^0 dT \right)$$

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Reactor Calculation

Consider a gas phase reactor.



There is temperature change as well as composition change. At steady state:

$$[\mu_1 \Delta H(T_1, y_1)]_{in} + Q_R = [\mu_2 \Delta H(T_2, y_2)]_{out}$$

This implies

$$Q_{R} = \mu_{2} \Delta H(T_{2}, y_{2}) - \mu_{1} \Delta H(T_{1}, y_{1})$$

 $Q_R > 0 \implies$ reaction is endothermic. $Q_R < 0 \implies$ reaction is exothermic.

Enthalpies of Liquid Mixtures

Enthalpies of liquid mixtures are evaluated directly from the ideal vapor enthalpy and subtracting the heat of vaporization at saturation conditions.



Liquid Mixtures and Two Phase Mixtures

The specific stream enthalpy for liquid mixtures is estimated as a weighted sum of respective mole fractions.

 $\Delta H_L(T, x) = x_1 \Delta H_L^1 + x_2 \Delta H_L^2 + \dots + x_n \Delta H_L^n$

• For a vapor-liquid mixture with vapor fraction ϕ , the stream enthalpy is given by the weighted sum of the liquid and vapor enthalpies.

 $\Delta H_L(T, x) = \phi \Delta H_V(T, y) + (1 - \phi) \Delta H_L(T, x)$

Flash Calculations

We considered the following scenarios in flash calculations

 T_V, P_V specified V/F = 1, P_V specified Dew point temperature T_L specified, V/F = 0 T_V specified, V/F = 1 $Q = 0, P_V$ specified Q, P_V specified V/F, P_V specified

Isothermal flash V/F = 0, P_L specified Bubble point temperature Bubble point pressure Dew point pressure Adiabatic flash Nonadiabatic flash Percent vaporization flash

We did not consider the flash calculations that involved energy balance. We will consider the adiabatic flash now.

Nonadiabatic/Adiabatic Flash

<u>Scenario</u>: Heat is added to a liquid mixture stream due to which part of it vaporizes. What is the flash temperature and what are the compositions of the liquid and vapor streams if the pressure is specified? Algorithm:

- For a given enthalpy specification (ΔH_{spec}) and pressure *P*, calculate the bubble point and dew point temperatures and the enthalpies associated with them.
 - If $\Delta H_{spec} > \Delta H_{dew}$, then the mixture is all vapor, and we solve for T from $\Delta H_v(T) = \Delta H_{spec}$.
 - If $\Delta H_{spec} < \Delta H_{dew}$, then the mixture is all liquid, and we solve for *T* from $\Delta H_L(T) = \Delta H_{spec}$.
- If $\Delta H_{dew} \ge \Delta H_{spec} \ge \Delta H_{bub}$, guess ξ_n (or ϕ).

- Perform a flash calculation with ξ_n (or ϕ) and *P* specified to obtain y_k , x_k and *T*. Calculate $\Delta H(T) = \phi \Delta H_v + (1 - \phi) \Delta H_L$
- If $f = \Delta H_{spec} \Delta H(T) = 0$ STOP. Otherwise, if f > 0reguess a higher ξ_n (or ϕ), else guess a lower ξ_n (or ϕ) and go back to previous step.

Illustrative Example

Consider a 50-50 liquid mixture of benzene and toluene flowing at $100 \ gmol/s$ at $300 \ K$ and $1 \ bar$. If heat is added to this stream at the rate of $860.42 \ kcal/s$, what is the temperature of the mixture. Solution

• Compute the enthalpy, ΔH_L , for the incoming liquid stream.

$$\Delta H_L = -847.5 \ kcal/s$$

Heat added to the liquid stream: 860.42 kcal/s. Thus the outlet stream enthalpy is:

$$860.42 - 847.50 = 12.868 \ kcal/s$$

- It can be shown that the outlet stream enthalpy is between the enthalpy of saturated liquid and saturated vapor; thus the mixture has two phases.
- We need to compute the split fractions of benzene and toluene in the vapor stream and the temperature so that the enthalpy of the outlet stream is 12.868 kcal/s
 - Assume toluene to be the key component and guess T = 370 K.

Compute $\alpha_{B/T} = 2.453$ at T = 370 K.

• Guess ξ_T and solve for ξ_B , ϕ and T from:

$$\xi_B = \frac{\alpha_{B/T}\xi_T}{1 + (\alpha_{B/T} - 1)\xi_T}$$

$$\phi = \frac{50(\xi_B + \xi_T)}{100}$$

$$P_T^0(T) = \frac{P}{\bar{\alpha}}$$



$$\Delta H(T) = \phi \Delta H_V(T) + (1 - \phi) \Delta H_L(T)$$

and compare with $\Delta H_{spec} = 12.862$.

• Adjust ξ_T till the computed ΔH converges to the specified value.

ξ_T	ξ_B	T	ϕ	$\Delta H(T)$
0.700	0.851	370.1	0.776	68.439
0.600	0.786	369.5	0.693	20.876
0.570	0.765	369.4	0.667	4.895
0.585	0.776	369.5	0.680	12.993

Thus, the stream is 68% vaporized at a temperature of $_{-369.5 K}$.