Process Design & Development Energy Balance

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Role of Energy Balance Concept

Energy balance is crucial in project engineering for designing systems such as reactors, heat exchangers, and distillation units. It ensures optimal energy utilization, system efficiency, and safety. When chemical reactions are involved, the system's energy balance must account for reaction enthalpies in addition to physical energy changes.

Energy Balance Without Chemical Reaction

This applies to systems where there is no chemical transformation. It primarily deals with heat transfer, work, and changes in sensible or latent heat.

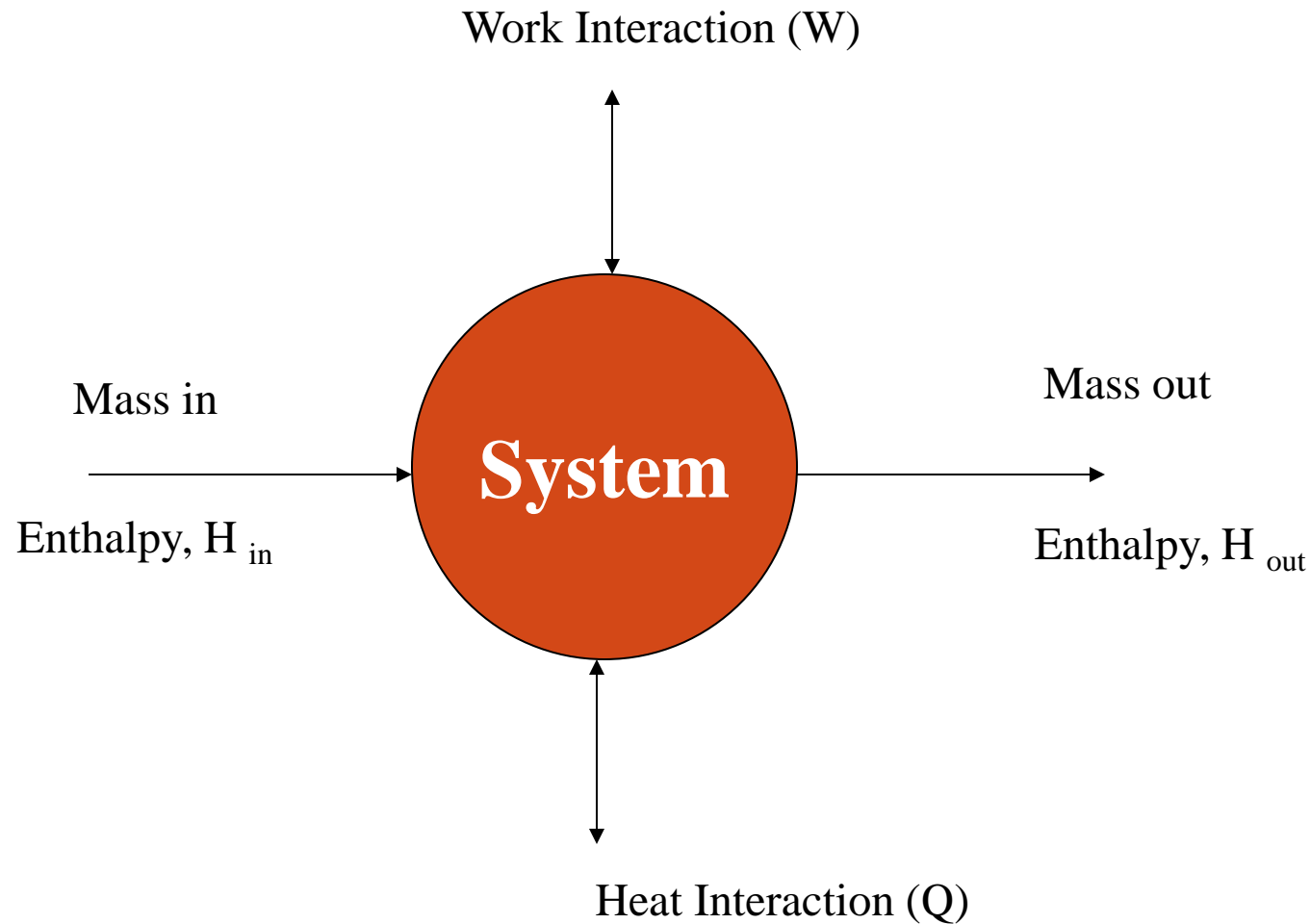**General Energy Balance Equation:**
$$\Delta H + \Delta KE + \Delta PE = Q - W$$

- ΔH: Enthalpy change due to heating/cooling.

- ΔKE: Change in kinetic energy.

- ΔPE: Change in potential energy.

- Q: Heat transfer to/from the system.

- W: Work done by/on the system.

Forms of energy

- Potential energy (P.E) = (mgh)
- Kinetic energy (K.E) = ($1/2\ mv^2$)
- Thermal energy – heat (Q)
  - Q = - ve, removed from a process
  - Q = + ve. supplied to a system
- Work energy – e.g. work done by a pump (W) to transport fluids
  - W = - ve, Work done by the system
  - Q = + ve. Work done on the system
- Internal energy (U) of molecules

Energy balance

Work Interaction (W)

Mass in

Enthalpy, H_{in}

System

Mass out

Enthalpy, H_{out}

Heat Interaction (Q)

Steady state/non-steady state

- Non steady state - accumulation/depletion of energy in system

- **Closed system**

$$\Delta U = Q + W$$

- **Open system**

$$\Delta H + \Delta P.E + \Delta K.E = Q + W$$

$$\Delta H + \frac{\Delta u^2}{2} + g\,\Delta z = Q + W_s$$

Enthalpy balance

- P.E, K.E, W terms = 0

- $Q = H_2 - H_1$ or $Q = \Delta H$

where

H_2 = the total enthalpy of output streams and

H_1 = the total enthalpy of input streams,

Q = the difference in total enthalpy i.e. the enthalpy (heat) transferred to or from the system

Enthalpy changes

- Change of T at constant P
- Change of P at constant T
- Change of phase
- Solution
- Mixing
- Chemical reaction
- Crystallisation

Latent heats (phase changes)

- Vaporization (L to V)
- Melting (S to L)
- Sublimation (S to V)

Mechanical energy balance

- Consider mechanical energy terms only
- Application to flow of liquids
- $\dfrac{\Delta P}{\rho} + \dfrac{\Delta v^2}{2} + \Delta h + h_{fs} = W$

where

W is work done on system by a pump and

h_{fs} is frictional energy loss in system (J/kg)

$\Delta P = P_2 - P_1$; $\Delta v^2 = v_2{}^2 - v_1{}^2$; $\Delta h = h_2 - h_1$

- Bernoulli equation (F=0, W=0)

Sensible heat/enthalpy calculations

- 'Sensible' heat – heat/enthalpy that must be transferred to raise or lower the temperature of a substance or mixture of substances.

- Heat capacities/specific heats (solids, liquids, gases,vapours)

- Heat capacity/specific heat at constant P, $C_p(T) = dH/dT$ or $\Delta H =$ integral $C_p(T)dT$ between limits T_2 and T_1

- Use of mean heat capacities/specific heats over a temperature range

- Use of simple empirical equations to describe the variation of C_p with T

e.g. $Cp = a + bT + cT^2 + dT^3$

,where a, b, c, d are coefficients

$\Delta H = $ integral $CpdT$ between limits T_2, T_1

.

$\Delta H = [aT + \dfrac{bT^2}{2} + \dfrac{cT^3}{3} + \dfrac{dT^4}{4}]$

Calculate values for $T = T_2, T_1$ and subtract

Note: T may be in deg cent or K - check units for Cp!

Example **Heating Water in a Heat Exchanger Problem**:

In a heat exchanger, 500 kg/hr of water is heated from 25°C to 75°C. Calculate the required heat (Q) if the specific heat capacity of water (Cp) is 4.18 kJ/kg·°C.

Solution:

1.$\Delta H = m \cdot Cp \cdot \Delta T$

$\Delta T = T_2 - T_1 = 75 - 25 = 50 \circ C$

$Q = 500 \text{ kg/hr} * 4.18 \text{ kJ/kg°C} * 50 \circ C$

Example 2

Calculate the enthalpy required to heat a stream of nitrogen gas flowing at 100 mole/min., through a gas heater from 20 to 100 deg. cent.

(use mean Cp value 29.1J mol^{-1} K^{-1} **or** Cp = 29 + 0.22 x 10^{-2}T + 0.572 x 10^{-5}T^2 – 2.87 x 10^{-9}T^3, where T is in deg cent)

Energy Balance With Chemical Reaction

When chemical reactions occur, the system must account for the energy released or absorbed during the reaction (ΔHr).

General Energy Balance Equation:

$$\Delta H + \Delta KE + \Delta PE + \Delta Hr = Q - W$$

Where: ΔHr : Enthalpy of reaction, which depends on the extent of the reaction (ξ) and the reaction enthalpy.

• ΔH: Enthalpy change due to heating/cooling.

• ΔKE: Change in kinetic energy.

• ΔPE: Change in potential energy.

• Q: Heat transfer to/from the system. W: Work done by/on the system.
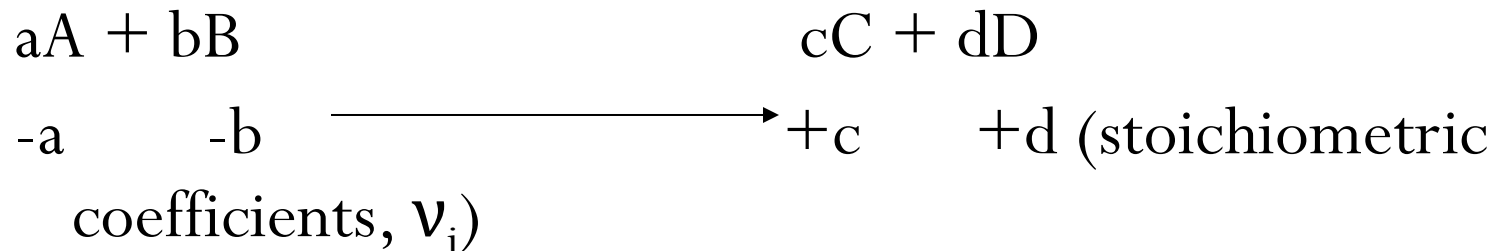
Example – change of phase

A feed stream to a distillation unit contains an equimolar mixture of benzene and toluene at 10 deg cent. The vapour stream from the top of the column contains 68.4 mol % benzene at 50 deg cent. and the liquid stream from the bottom of the column contains 40 mol% benzene at 50 deg cent.

[Need Cp (benzene, liquid), Cp (toluene, liquid), Cp (benzene, vapour), Cp (toluene, vapour), latent heat of vapourisation benzene, latent heat of vapourisation toluene.]

Energy balances on systems involving chemical reaction

- Standard heat of formation (ΔH^o_f) – heat of reaction when product is formed from its elements in their standard states at 298 K, 1 atm. (kJ/mol)

aA + bB   cC + dD

-a   -b   ——————→ +c   +d (stoichiometric coefficients, ν_i)

ΔH^o_{fA}, ΔH^o_{fB}, ΔH^o_{fC}, ΔH^o_{fD} (heats of formation)

$\Delta H^o_R = c\,\Delta H^o_{fC} + d\,\Delta H^o_{fD} - a\,\Delta H^o_{fA} - b\,\Delta H^o_{fB}$

Heat (enthalpy) of reaction

- ΔH^o_R −ve (**exo**thermic reaction)
- ΔH^o_R +ve (**endo**thermic reaction)

Enthalpy balance equation - reactor

$Qp = H_{products} - H_{reactants} + Qr$

Qp – heat transferred to or from process

Qr – reaction heat ($\zeta \, \Delta H^o{}_R$), where ζ is extent of reaction and is equal to [moles component,i, out – moles component i, in]/ ν_i

Example3: Methane Combustion in a Reactor

Methane (CH_4) is combusted with excess air in a reactor. The reaction is:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$
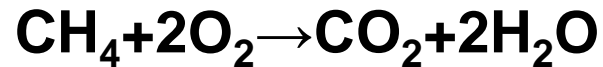
Given: 5 mol of CH_4 reacts; Heat of reaction (ΔHr) = −890 kJ/mol

• Calculate the total heat released.

Solution:

1. Total moles of methane reacting: $\xi = 5$ mol

2. Total heat released: $Q = \xi \cdot \Delta Hr = 5 \cdot (-890) = -4450$ kJ

References

- *The Properties of Gases and Liquids,* R. Reid

- *Elementary Principles of Chemical Processes,* R.M.Felder and R.W.Rousseau

Paul Ashall, 2008

Thank you