

2.6. Entropy balance

- Typically calculate temperature change from property function for isentropic process (reversible adiabatic process with $Q = 0$ and $\Delta S_{gen} = 0$).
- Entropy balance for a steady state system exchanging material streams j and duties k :

$$\sum_{j=1}^{out} (wS)_j - \sum_{j=1}^{in} (wS)_j = \sum_{k=1}^{all} \left(\frac{Q}{T} \right)_k + w\Delta S_{gen}$$

S = stream specific entropy (kJ/kg.K)

Q = heat flow into system (kJ/h, + in, - out)

= 0 for adiabatic process

ΔS_{gen} = entropy change due to irreversibilities (kJ/kg.K)

= 0 for reversible process

w = stream mass flow (kg/h)

- Entropy property function (point function).
 - Change in entropy only depends on start and end point, not on path taken.
 - Entropy is a function of temperature and pressure, at constant composition:

$$dS = \left(\frac{C_p}{T} \right) dT - \left(\frac{\partial V}{\partial T} \right)_{P, x_i} dP$$

C_p = fluid heat capacity at constant pressure (kJ/kg.K)

V = fluid specific volume (m³/kg)

T = fluid temperature (K)

P = pressure (kPaa)

- For hand calcs, integration is typically done from inlet to outlet.

$$S_{out} - S_{in} = C_p \ln \left(\frac{T_{out}}{T_{in}} \right) - \frac{R}{M_w} \ln \left(\frac{P_{out}}{P_{in}} \right) \quad \text{ideal gas}$$

$$S_{out} - S_{in} = C_p \ln \left(\frac{T_{out}}{T_{in}} \right) \quad \text{ideal liquid}$$

- For simulators, integration is typically done from a reference state. The reference state is almost always $S_{ref} = 0$ at 1 K/°R and 0 kPaa for pure component (API Databook 7A1.1, with the $x_i \ln x_i$ term in mole fractions):

$$S_{out} = \int_1^{T_{out}} \sum x_i \left(\frac{C_{p,i}^0}{T} \right) dT - \int_0^{P_{out}} \left(\frac{\partial V}{\partial T} \right)_{T_{out}, mix} dP - \frac{R}{M_w} \sum x_i \ln x_i$$

$$S_{in} = \int_1^{T_{in}} \sum x_i \left(\frac{C_{p,i}^0}{T} \right) dT - \int_0^{P_{in}} \left(\frac{\partial V}{\partial T} \right)_{T_{in}, mix} dP - \frac{R}{M_w} \sum x_i \ln x_i$$