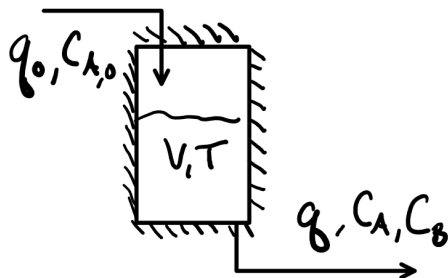


System: Tank with contents and valves



- $A \rightarrow 2B$
- $-r_A = kC_A$
- $\rho, V = \text{const.}$
- $k = k_0 \exp\left(-\frac{E}{RT}\right)$
- Perfect mixing, Adiabatic

Further Assumptions:

- $C_{B,0} = 0$
- Stoichiometry: $-r_A = (1/2)r_B$ (2 B produced per A consumed)
- Kinetic and potential energies are negligible
- No work done by or on the system
- Dilute liquid phase reaction \implies The heat capacity of the solution, $c_{p,s}$, does not depend strongly on the concentrations of A or B, otherwise, the equations get *very* messy. If water is the carrier fluid, then $c_{p,s}$ is approximately the heat capacity of water
- Constant $c_{p,s}$

Variables:

| Inputs | Units |
|------------|-------------------------|
| q | m^3/s |
| $C_{A,0}$ | mol/m^3 |
| Outputs | Units |
| C_A, C_B | mol/m^3 |
| T | K |

Parameters (Constant):

| Var. | Units |
|--------------------|------------------------|
| V | m^3 |
| ρ | kg/m^3 |
| k_0 | s^{-1} |
| E | J/mol |
| R | J/mol · K |
| $c_{p,s}$ | J/kg · K |
| $C_{p,A}, C_{p,B}$ | J/mol · K |
| ΔH_{rxn} | J/mol |

Conservation of Mass:

$$\frac{d(\rho V)}{dt} = \rho(q_0 - q)$$

Since $\rho, V = \text{const.}$,

$$\boxed{q_0 = q}.$$

Component Balances:

$$\frac{d(C_A V)}{dt} = q_0 C_{A,0} - q C_A + r_A V,$$

$$\frac{d(C_B V)}{dt} = q_0 C_{B,0} - q C_B + r_B V.$$

Since $q_0 = q$, $V = \text{const.}$, $-r_A = r_B/2$, and $C_{B,0} = 0$,

$$V \frac{dC_A}{dt} = q(C_{A,0} - C_A) - k C_A V,$$

$$V \frac{dC_B}{dt} = -q C_B + 2k C_A V.$$

By dividing by V and using the Arrhenius equation,

$$\boxed{\frac{dC_A}{dt} = \frac{q}{V} (C_{A,0} - C_A) - \left[k_0 \exp\left(-\frac{E}{RT}\right) \right] C_A},$$

$$\boxed{\frac{dC_B}{dt} = -\frac{q}{V} C_B + 2 \left[k_0 \exp\left(-\frac{E}{RT}\right) \right] C_A}.$$

Energy Balance:

The total energy balance for the system is given by,

$$\frac{d}{dt} (\rho V [U + KE + PE]) = \rho (q_0 H_0 - q H) + r_A V \Delta H_{rxn}(T) + W,$$

Assume $KE = PE = W = 0$, it is also known that $\rho, V = \text{const.}$, $q_0 = q$, and $U \approx H = c_{p,s} T$, where $c_{p,s}$ is the heat capacity per unit mass of the solution. The heat of reaction per mole of A, $\Delta H_{rxn}(T)$, is assumed to be a function of temperature¹, and can be found by thermodynamics,

$$\Delta H_{rxn}(T) = \Delta H_{rxn}(T_{ref}) + \sum_{i=1}^N \nu_i C_{p,i} [T - T_{ref}],$$

where the sum is over all N components, ν_i are stoichiometric coefficients, and T_{ref} is a reference temperature. For convenience, molar heat capacities, $C_{p,i}$, are used instead of mass based heat capacities. For this specific problem,

$$\boxed{\Delta H_{rxn}(T) = \Delta H_{rxn}(T_{ref}) + (-C_{p,A} + 2C_{p,B}) [T - T_{ref}]}.$$

By plugging in these assumptions, the energy balance becomes,

$$\rho V c_{p,s} \frac{dT}{dt} = \rho q c_{p,s} (T_0 - T) - \left[k_0 \exp\left(-\frac{E}{RT}\right) \right] C_A V \Delta H_{rxn}(T),$$

¹For small temperature changes, ΔH_{rxn} could be assumed constant.

or by rearrangement,

$$\boxed{\frac{dT}{dt} = \frac{q}{V} (T_0 - T) - \frac{C_A}{\rho C_{p,s}} \left[k_0 \exp \left(-\frac{E}{RT} \right) \right] \Delta H_{rxn}(T)}.$$

Sanity check: $\Delta H_{rxn}(T) < 0$ since the reaction is exothermic, meaning the generation term is positive when multiplied by $r_A = -kC_A$.

DOF Analysis:

There are 3 differential equations for T , C_A , and C_B and 5 independent variables: T , C_A , C_B , q , $C_{A,0}$. Therefore,

$$\boxed{DOF = 5 - 3 = 2}.$$

Since the differential equations are in T , C_A , and C_B , they are the output variables while q and $C_{A,0}$ are input variables.