Frequently, in papers & scientific literature, other constants that are similar to equilibrium constant are reported.

Most commonly:

Concentration equilibrium ratio:

$$K_c = \prod_i c_i^{\nu_i}$$

Subtly different than

$$K_a \simeq \prod_i (\gamma_i x_i)^{\nu_i}$$

↑ for this class, we automatically assume $\gamma_i = 1$

x_i : mol fraction

c_i : concentration

recall $x_i = \frac{c_i}{C}$ assume $\gamma_i = 1$

$$K_a = \Pi (x_i \gamma_i)^{\nu_i} \rightarrow \Pi (x_i)^{\nu_i}$$

$\gamma_i \rightarrow 1$

$$= \Pi \left(\frac{c_i}{C}\right)^{\nu_i} = C^{-\Sigma \nu_i} K_c$$

$$\boxed{K_a = C^{-\Sigma \nu_i} \cdot K_c}$$

K_a : mol fraction

$C^{-\Sigma \nu_i}$: total concentration of mixture

K_c : concentration equilibrium constant

pervasive in biological literature

$$CH_3COOH + C_2H_5OH \rightarrow$$

$$CH_3COOC_2H_5 + H_2O$$

ethyl acetate → look @ mass balance notes from Jan.

$$\frac{d C_{EA}}{dt} = K C_A C_E - K' C_{EA} C_w$$

what is the K_A?

This is a classical reason why biology pe papers often report K_C

@ S.S.

$$0 = K C_A C_E - K' C_{EA} C_w$$

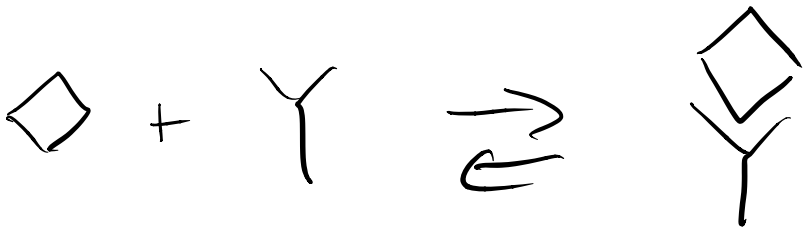
reactants — products

$$\frac{\text{products}}{\text{reactants}} = \frac{C_{EA}\,C_W}{C_A\,C_E} = \frac{k}{k'} \equiv K_C$$

Concentration equilibrium Constant. K_C

For Boochemical complex formation -

e.g. Receptor + Ligand $\rightleftarrows$ R·L



Simple bimolecular interaction

$$R + L \rightleftarrows RL$$

$$\frac{dC_{RL}}{dt} = K_{on} \cdot R \cdot L - K_{off} \cdot RL$$

@ equilibrium

$$\frac{RL}{R \cdot L} = \frac{K_{on}}{K_{off}} \equiv K_C \equiv K_D$$

"Dissociation Constant"

↑

units are always nM → concentration

Chemical Equilibrium in a Liquid Mixture

$CH_2COOH + C_2H_5OH \rightleftharpoons CH_3COOC_2H_5 + H_2O$

acetic acid — ethanol — ethylacetate — water

A — E — EA — W

aqueous solution

100°C

$K_c = 2.92$ (unitless)

→ compute equilibrium concentrations of each component → in aqueous solution w/

250 kg acetic acid in $1 m^3$ V

500 kg ethanol

initial density = $1040 kg/m^3$

recall → N_i → C_i to get concentration extent of RxN, then solve for

$\hat{X}$ → Concentration extent of RxN

This or exact analogy to this

Will be on your Final exam and asked @ 10:30 AM May 2nd. Immediately after "What is balance equation for any conserved quantity?"

$$C_{A0} = \frac{250\ kg/m^3}{60\ g/mol} = 4.17\ kmol/m^3$$

$$C_{E0} = \frac{500\ kg/m^3}{46\ g/mol} \rightarrow 10.9\ kmol/m^3$$

$$C_{w0} = \frac{(1040 - 250 - 500)\ kg/m^3}{18\ g/mol} \rightarrow 16.1\ kmol/m^3$$

$$C_A = 4.17 - \hat{x} \quad kmol/m^3$$

$$C_E = 10.9 - \hat{x} \quad kmol/m^3$$

$$C_W = 16.1 + \hat{x} \quad kmol/m^3$$

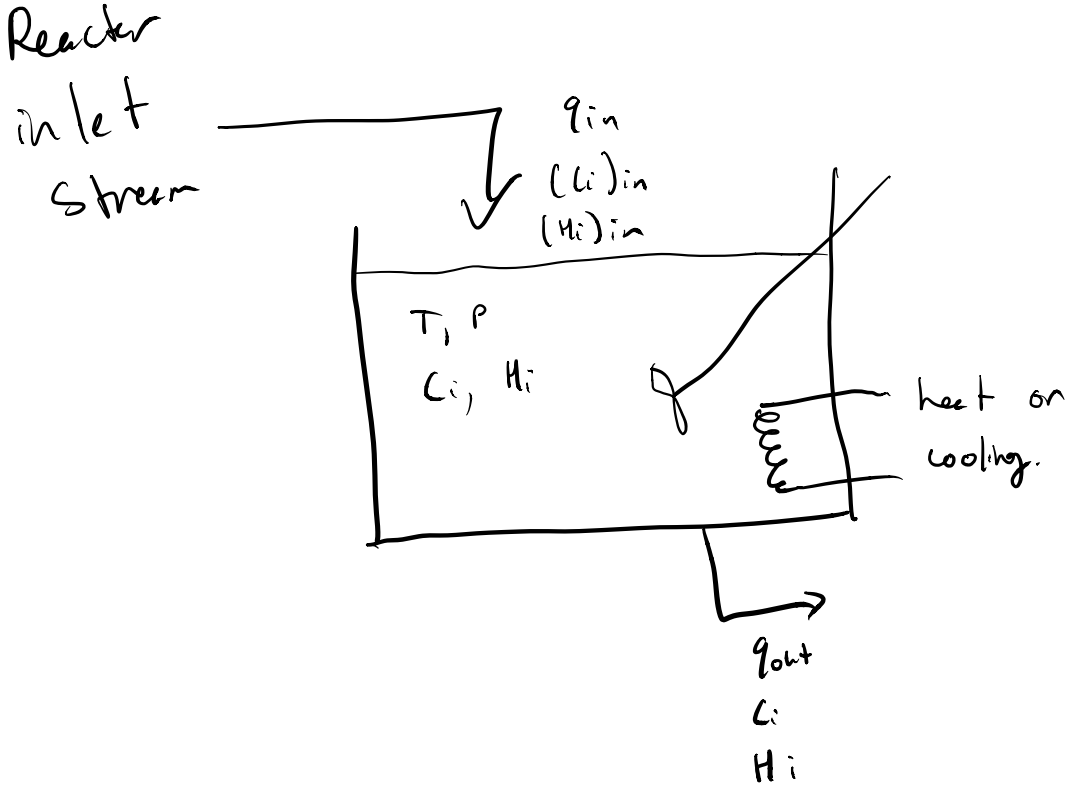
$$C_{EA} = \hat{x} \quad kmol/m^3$$

@ equilibrium

$$K_c(100°C) = 2.92 = \frac{(16.1+\hat{x})(\hat{x})}{(10.9-\hat{x})(4.17-\hat{x})}$$

$$\rightarrow \hat{x} = 2.39 \; kmol/m^3$$

$\sim$ 57.3 % of acetic acid is converted @ equilibrium



$$\frac{dN_i}{dt} = (\dot{N}_i)_{in} - (\dot{N}_i)_{out} + \sum_{j=1}^{M} r_{ij}\,\dot{X}_j$$

mass in — mass out — creation + destruction by Chemical RXNs

$$\frac{dU}{dt} = \sum_{i=1}^{C} (\dot{N}_i \underline{H}_i)_{in} - \sum_{i=1}^{C} (N_i \underline{H}_i)_{out} + \dot{Q}$$

define 2 new quantities:

1) $N_i = C_i \cdot V$

V: volume of vessel/reactor.

2) $r_j = \dot{X}_j / V$ specific reaction rate

$$\frac{d}{dt}(C_i \cdot V) = C_{i_{in}} \cdot q_i - C_i \cdot q_{out} + V \sum_{j=1}^{M} r_{ij} r_j$$

q_i: volumetric flow rate

$$\frac{d}{dt}\left(V \sum_{i=1}^{C} C_i \underline{U}_i\right) = \left(\sum_{i=1}^{C} C_i H_i\right) q_{in} - \left(\sum_{i=1}^{C} C_i \underline{H}_i\right) q_{out} + \dot{Q}$$

V is constant iff $q_{in} = q_{out}$.

$$V \frac{dC_i}{dt} = q\left[(C_i)_{in} - C_i\right] + V \sum_{j=1}^{M} r_{ij} \cdot r_j$$

liquid $\underline{U}_i \equiv \underline{H}_i$

$$V \frac{d}{dt}\left(\sum C_i \underline{H}\right) = q\left(\sum (C_i H_i)_{in} - \sum C_i H_i\right) + \dot{Q}$$

RxNs impact energy balance via $\dot{Q}$

@ steady-state.

$$C_i = (C_i)_{in} + \frac{V}{q} \sum_{j=1}^{M} r_{ij} r_j$$

energy balance @ steady-state. → how does the enthalpy change via RXN? → what Q is needed?

Sub in for C_i in energy balance

Before sub →

$$\dot{Q} = q \sum (C_i)_{in} \left[\underline{H_i} - (\underline{H_i})_{in} \right] + V \sum_j r_j \Delta_{rxn} H$$

$$\Delta_{rxn} \dot{U} = \sum r_{ij} \underline{H_i}$$

i: every component

j: every reaction $j \neq i$