

PROTON BALANCE

THE AUTHOR

1. PROTONATED ACETATE

We use this notation:

- A_T is total concentration of acetate;
- A_H is protonated acetate which inhibits growth;
- $A^- := A_T - A_H$
- $f_1 := \frac{A^-}{A_T}$ fraction of hydrogen atoms H^+ that is disassociated from acetic acid.
- $pKa_1 = 4.75$,

We now that the following ratio depends on current concentration of H^+

$$\frac{A^-}{A_H} = 10^{(-\log H^+ - pKa_1)} =: f_1^*.$$

Therefore we compute

$$A^- = f_1^* A_H = f_1^* (A_T - A^-)$$

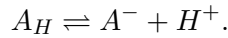
and therefore

$$(1) \quad A^- = \frac{f_1^*}{1 + f_1^*} A_T$$

and

$$(2) \quad f_1 = \frac{f_1^*}{1 + f_1^*}.$$

The protonation and de-protonation reaction of acetate is



with forward rate k_f^A , reverse rate k_r^A and equilibrium constant $K_{eq}^A = \frac{k_f^A}{k_r^A} = 10^{-4.75}$. **Is this correct?**

Then at the equilibrium we have

$$r_2^A = k_f^A A_H = k_{eq}^A k_r^A A_H$$

and since

$$A_H = A_T \frac{1}{1 + f_1^*}$$

we arrive at

$$r_2^A = k_{eq}^A k_r^A \frac{A_T}{1 + f_1^*}.$$

Similarly

$$r_3^A = k_3^A H^+ A^- = k_3^A H^+ \frac{f_1^*}{1 + f_1^*} A^T.$$

where the second part follows from (4).

2. PROTON CONCENTRATION

Protons are produced by growth rate, protonation of acetate and by protonation (flux r_2) and de-protonation (flux r_3) of phosphatase (?) This gives the following balance of fluxes in that order

$$(3) \quad \frac{dH^+}{dt} = (r_p + r_s)Y_{H/p+s} + r_{AT}f_1 + r_2 - r_3$$

Protonation and de-protonation of phosphatase will be analogous to the same process for acetate. Let

- P_T is total concentration of phosphate;
- P_H is protonated acetate which inhibits growth;
- $P^- := P_T - P_H$
- $f_2 := \frac{P^-}{P_T}$ fraction of hydrogen atoms H^+ that is disassociated from phosphate.
- $pK_{a2} = 7.03$.

We now that the following ratio depends on current concentration of H^+

$$\frac{P^-}{P_H} = 10^{(-\log H^+ - pK_{a2})} =: f_2^*.$$

Therefore we compute

$$P^- = f_2^* P_H = f_2^* (P_T - P^-)$$

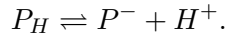
and therefore

$$(4) \quad P^- = \frac{f_2^*}{1 + f_2^*} P_T.$$

Since $P^- + P_H = P_T$ we have

$$P_H = P_T - P^- = P_T - \frac{f_2^*}{1 + f_2^*} P_T = (1 - \frac{f_2^*}{1 + f_2^*}) P_T = \frac{P_T}{1 + f_2^*}.$$

The protonation and de-protonation reaction that we want to track is



with forward rate k_f , reverse rate k_r and equilibrium constant $K_{eq} = \frac{k_f}{k_r}$. Then at the equilibrium we have

$$r_2 = k_f P_H = k_{eq} k_r P_H$$

and since

$$P_H = P_T \frac{1}{1 + f_2^*}$$

we arrive at

$$r_2 = k_{eq}k_r \frac{P_T}{1 + f_2^*}.$$

Similarly

$$r_3 = k_3 H^+ P^- = k_3 H^+ \frac{f_2^*}{1 + f_2^*} P^T.$$

where the second part follows from (4).

3. NEW H EQUATION

We analyze equation

$$\dot{H} = -P_0 \dot{f}_2 + r_p Y_{H/p+s} + A \dot{f}_1,$$

where

$$f_1 = \frac{f_1^*}{1 + f_1^*}$$

$$f_2 = \frac{1}{1 + f_2^*}.$$

We rewrite

$$f_1^* = \frac{C}{H} \quad C = 10^{-4.75}$$

$$f_2^* = \frac{D}{H} \quad D = 10^{-7.03}$$

which then gives

$$f_1 = \frac{C}{C + H}$$

$$f_2 = \frac{H}{D + H}.$$

We differentiate to get

$$\dot{f}_1 = - \frac{C}{(C + H)^2} \dot{H}$$

$$\dot{f}_2 = \frac{D}{(D + H)^2} \dot{H}.$$

Therefore we have

$$\begin{aligned}\dot{H} &= -P_0 \frac{D}{(D+H)^2} \dot{H} + r_p Y_{H/p+s} - A \frac{C}{(C+H)^2} \dot{H} \\ \dot{H} + P_0 \frac{D}{(D+H)^2} \dot{H} + A \frac{C}{(C+H)^2} \dot{H} &= r_p Y_{H/p+s} \\ \dot{H} \left(1 + \frac{DP_0}{(D+H)^2} + \frac{CA}{(C+H)^2}\right) &= r_p Y_{H/p+s} \\ \dot{H} &= \frac{r_p Y_{H/p+s}}{\left(1 + \frac{DP_0}{(D+H)^2} + \frac{CA}{(C+H)^2}\right)}\end{aligned}$$