Stoichiometry of Biochemical Reactions III

Today's lecture

- How to write overall reactions from half reactions
- Overall stoichiometry – exercise!
  - Types of biochemical reactions
  - What can be known from reaction stoichiometry

Overall reactions

1. Obtain half-reactions for an electron donor (R_d), electron acceptor (R_a), and cell formation (R_c)
2. Obtain f_s and f_e
3. Write energy and cell synthesis reactions (R_e & R_s):

$$R_e = R_a - R_d$$

$$R_s = R_c - R_d$$

4. Calculate overall reaction: $R = f_e R_e + f_s R_s$

Or, instead of Step 3 & 4, $R = f_e R_a + f_s R_c - R_d$

Oxidation of benzoate w/ nitrate as e^- acceptor, f_s=0.40

Step 1)

Step 2)

f_e = 0.60, f_s = 0.40

Step 3)

Step 4)

Or, by combining steps 3) & 4)

Nitrification, f_s=0.10

Step 1)

Step 2)

f_e = 0.90, f_s = 0.10

Step 3-4)

R: $0.13NH_4^+ + 0.225O_2 + 0.02CO_2 + 0.005HCO_3^-$

$$= 0.005C_5H_7O_2N + 0.125NO_3^- + 0.25H^+ + 0.12H_2O$$

Information available from the stoichiometry:

when 0.13 mole of NH_4^+ (or $0.13\times14=1.82$ g NH_4-N) is consumed,

- How much oxygen is consumed (should be supplied)?
- How much biomass is produced?
- How much nitrate is produced?
- How much alkalinity is consumed?

Nitrification: perspective on alkalinity

R: $0.13NH_4^+ + 0.225O_2 + 0.02CO_2 + 0.005HCO_3^-$

$= 0.005C_5H_7O_2N + 0.125NO_3^- + 0.25H^+ + 0.12H_2O$

***Alkalinity** = $[HCO_3^-] + 2[CO_3^{2-}] + \ldots + [OH^-] - [H^+]$*
***Carbonate alkalinity** = $[HCO_3^-] + 2[CO_3^{2-}]$*

If a solution does not contain any carbonate alkalinity, we may write ***R*** as

$0.13NH_4^+ + 0.225O_2 + 0.025CO_2 = 0.005C_5H_7O_2N + 0.125NO_3^- + \mathbf{0.255H^+} + 0.115H_2O$

⇨ 0.255 eq of acidity is produced per 0.13 mole of NH_4^+ (solution pH ↓)

If a solution contains sufficient carbonate alkalinity, we may write ***R*** as

$0.13NH_4^+ + 0.225O_2 + 0.255HCO_3^- = 0.005C_5H_7O_2N + 0.125NO_3^- + 0.25CO_2 + 0.37H_2O$

⇨ 0.255 eq of carbonate alkalinity is consumed per 0.13 mole of NH_4^+ (negligible change in solution pH)

Methanogenesis from wastewater, f_s=0.08

** Assume "waste" in water is represented as $C_8H_{17}O_3N$*

Step 1)

Step 2)

f_e = 0.92, f_s = 0.08

Step 3-4)

R: $0.025C_8H_{17}O_3N + 0.084H_2O$

$$= 0.004C_5H_7O_2N + 0.115CH_4 + 0.044CO_2 + 0.021NH_4^+ + 0.021HCO_3^-$$

Information available from the stoichiometry:

when 0.025×175=4.375 g waste is consumed,

- How much methane is produced?
- What is the composition of the biogas?
- How much biomass is produced?
- How much alkalinity is produced?

Fermentation

- Organic compound serves as both e^- donor and e^- acceptor
- In the absence of oxygen
- Sugar is converted to acid, gases, and/or alcohol

ex1) ethanol fermentation

$$C_6H_{12}O_6 \rightarrow 2C_2H_5OH + 2CO_2$$

ex2) lactic acid fermentation

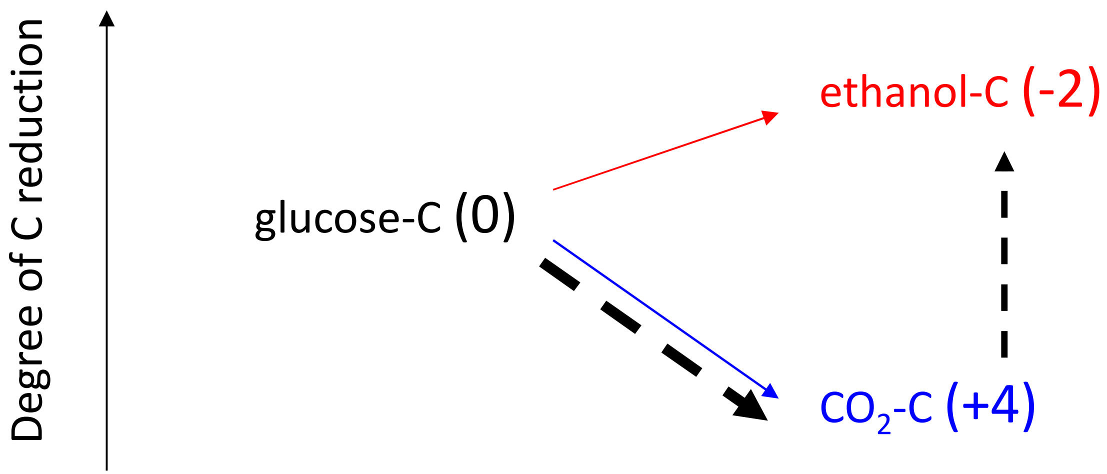
$$C_6H_{12}O_6 \rightarrow 2CH_3CH(OH)COOH$$

Fermentation, glucose to ethanol, f_s=0.22

Step 1)

We want to fit fermentation, the “special case” of biochemical reaction, to our framework

Let’s think about $\boldsymbol{R_e}$, the energy production reaction



So, we may construct $\boldsymbol{R_e}$ by selecting R_d and R_a as:

Note the actual fermentation does not occur this way, but by a complex pathway to partition electrons in glucose to ethanol and CO_2. But we can use this procedure to write up the reaction stoichiometry and also to determine the reaction free energy change (ΔG_r)

We may use the typical form of R_c

R_c (O-20): $0.02CO_2 + 0.05NH_4^+ + 0.05HCO_3^- + H^+ + e^- = 0.05C_5H_7O_2N + 0.45H_2O$

Step 2)

$f_e = 0.78$, $f_s = 0.22$

Step 3-4)

R: $0.04167C_6H_{12}O_6 + 0.011NH_4^+ + 0.011HCO_3^-$

$= 0.011C_5H_7O_2N + 0.065C_2H_5OH + 0.076CO_2 + 0.044H_2O$

Information available from the stoichiometry:

when $0.04167 \times 180 = 7.506$ g glucose is consumed,

- How much ethanol is produced?
- How much biomass is produced?
- How much alkalinity is consumed?