Stoichiometry of Biochemical Reactions: Examples

Nitrification, f_s=0.10

Step 1)

R_d (I-1): $0.125NO_3^- + 1.25H^+ + e^- = 0.125NH_4^+ + 0.375H_2O$

R_a (I-14): $0.25O_2 + H^+ + e^- = 0.5H_2O$

R_c (O-20): $0.2CO_2 + 0.05NH_4^+ + 0.05HCO_3^- + H^+ + e^- = 0.05C_5H_7O_2N + 0.45H_2O$

Step 2)

$f_e = 0.90$, $f_s = 0.10$

Nitrification, f_s=0.90

Step 3-4)

f_eR_a: $0.225O_2 + 0.9H^+ + 0.9e^- = 0.45H_2O$

f_sR_c: $0.02CO_2 + 0.005NH_4^+ + 0.005HCO_3^- + 0.1H^+ + 0.1e^-$

$= 0.005C_5H_7O_2N + 0.045H_2O$

$-R_d$: $0.125NH_4^+ + 0.375H_2O = 0.125NO_3^- + 1.25H^+ + e^-$

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

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

Nitrification, f_s=0.90

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 $0.13 \times 14 = 1.82$ 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?

Methanogenesis from wastewater, f_s=0.08

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

Step 1)

R_d (O-19): $0.025NH_4^+ + 0.025HCO_3^- + 0.175CO_2 + H^+ + e^- = 0.025C_8H_{17}O_3N + 0.175H_2O$

R_a (O-12): $0.125CO_2 + H^+ + e^- = 0.125CH_4 + 0.25H_2O$

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)

$f_e = 0.92$, $f_s = 0.08$

Methanogenesis from wastewater, f_s=0.08

Step 3-4)

f_eR_a: $0.115CO_2 + 0.92H^+ + 0.92e^- = 0.115CH_4 + 0.23H_2O$

f_sR_c: $0.0116CO_2 + 0.004NH_4^+ + 0.004HCO_3^- + 0.08H^+ + 0.08e^-$

$= 0.004C_5H_7O_2N + 0.036H_2O$

$-R_d$: $0.025C_8H_{17}O_3N + 0.35H_2O$

$= 0.025NH_4^+ + 0.025HCO_3^- + 0.175CO_2 + H^+ + e^-$

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

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

Methanogenesis from wastewater, f_s=0.08

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,

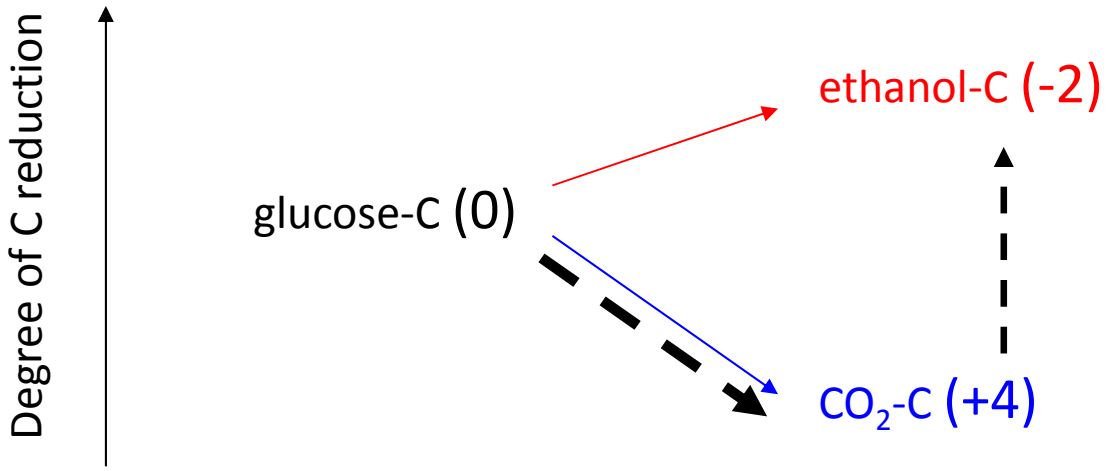
- How much methane is produced?
- What is the composition of the biogas?
- How much biomass is produced?
- How much alkalinity is produced?

Fermentation, 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 **R_e**, the energy production reaction



Fermentation, glucose to ethanol, f_s=0.22

Step 1)

So, we may construct **R_e** by selecting R_d and R_a as:

R_d (O-7): $0.25CO_2 + H^+ + e^- = 0.04167C_6H_{12}O_6 + 0.25H_2O$

R_a (O-5): $0.1667CO_2 + H^+ + e^- = 0.0833C_2H_5OH + 0.25H_2O$

$R_e = R_a - R_d$: $0.04167C_6H_{12}O_6 = 0.0833C_2H_5OH + 0.0833CO_2$

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 determine the reaction free energy change (ΔG)

Fermentation, glucose to ethanol, f_s=0.22

Step 1)

Consequently, we have:

R_d (O-7): $0.25CO_2 + H^+ + e^- = 0.04167C_6H_{12}O_6 + 0.25H_2O$

R_a (O-5): $0.1667CO_2 + H^+ + e^- = 0.0833C_2H_5OH + 0.25H_2O$

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)

$f_e = 0.78$, $f_s = 0.22$

Fermentation, glucose to ethanol, f_s=0.22

Step 3-4)

f_eR_a: $0.13CO_2 + 0.78H^+ + 0.78e^- = 0.065C_2H_5OH + 0.195H_2O$

f_sR_c: $0.044CO_2 + 0.011NH_4^+ + 0.011HCO_3^- + 0.22H^+ + 0.22e^-$

$= 0.011C_5H_7O_2N + 0.099H_2O$

$-R_d$: $0.04167C_6H_{12}O_6 + 0.25H_2O = 0.25CO_2 + H^+ + e^-$

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

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

Methanogenesis from wastewater, f_s=0.08

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?