Textbook example: Nitrification [Ex 2.4]

Step 1)

R_d (Table 2.2, I-1): 0.125NO3- + 1.25H+ + e^- = $0.125NH_4^+ + 0.375H_2O$

R_a (Table 2.2, I-14): $0.25O_2 + H^+ + e^- = 0.5H_2O$

R_c (Table 2.3, O-20): $0.2CO_2 + 0.05NH_4^+ + 0.05HCO_3^- + H^+ + e^- = 0.05\ C_5H_7O_2N + 0.45H_2O$

Step 2)

$f_e = 0.10$, $f_s = 0.90$

Step 3-4)

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

f_sR_c: $0.02CO_2 + 0.005NH_4^+ + 0.005HCO_3^- + 0.1H^+ + 0.1\ e^- \rightarrow 0.005\ C_5H_7O_2N + 0.045H_2O$

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

R: $0.13NH_4^+ + 0.225O_2 + 0.02CO_2 +$ 0.005HCO3- $\rightarrow 0.005C_5H_7O_2N + 0.125NO_3^- + 0.25H^+ + 0.12H_2O$

Textbook example: methanogenesis from wastewater [Ex 2-5]

Wastewater empirical formula given in the example: $C_8H_{17}O_3N$

R_d from [Table 2.3], O-19:

$d = 4 \times 8 + 17 - 2 \times 3 - 3 \times 1 = 40$

R_d: $(1/40)NH_4^+ + (1/40)HCO_3^- + (7/40)CO_2 + H^+ + e^- \rightarrow (1/40)\ C_8H_{17}O_3N + (7/20)H_2O$

R_a from [Table 2.4], O-12

- For methanogenesis, e- donor produces CO2, and CO2 is also acts as an e-acceptor. CO2 is converted to CH4, getting 8 e- eq/mol. This is an energyconsuming process. Why does it happen? – No good electron acceptor (cf: O_2 to H_2O or CO_2: energy producing while accepting electrons)

R_c from Table 2.3, O-20

$f_e = 0.92$, $f_s = 0.08$

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

f_sR_c: $0.0116CO_2 + 0.004NH_4^+ + 0.004HCO_3^- + 0.08H^+ + 0.08e^- \rightarrow 0.004C_5H_7O_2N + 0.036H_2O$

$-R_d$: $0.025\ C_8H_{17}O_3N + 0.35H_2O \rightarrow 0.025NH_4^+ + 0.025HCO_3^- + 0.175CO_2 + H^+ + e^-$

R: $0.025\ C_8H_{17}O_3N + 0.084H_2O \rightarrow 0.004C_5H_7O_2N + 0.115CH_4 + 0.044CO_2 + 0.021NH_4^+ + 0.021HCO_3^-$

Percent methane in the produced gas = 0.115/(0.115+0.044) = 72%

Simple fermentation

Ex) Glucose fermentation to ethanol

First, let's think about energy production (R_e)

Electron donor half reaction (R_d – [Table 2.3] O-7):

$(1/24)C_6H_{12}O_6 + (1/4)H_2O \rightarrow (1/4)CO_2 + H^+ + e^-$

Taking reduction of CO_2 to ethanol for electron acceptor half reaction (R_a – [Table 2.3] O-5):

$(1/6)CO_2 + H^+ + e^- \rightarrow (1/12)CH_3CH_2OH + (1/4)H_2O$

$R_e = R_a - R_d = (1/24)C_6H_{12}O_6 \rightarrow (1/12)CH_3CH_2OH + (1/12)CO_2$

- Note: The reaction actually does not happen in the two steps, but with a complex pathway to partition electrons in glucose to ethanol and CO_2. But with this calculation, we obtain a reaction that will end up with the same reactants and products as the actual fermentation. You can also calculate how much energy is produced by this reaction.

Now, for an overall bacterial growth equation with $f_s = 0.22$,

f_aR_a: $0.13CO_2 + 0.78H^+ + 0.78e^- \rightarrow 0.065CH_3CH_2OH + 0.195H_2O$

f_sR_c: $0.044CO_2 + 0.011NH_4^+ + 0.011HCO_3^- + 0.22H^+ + 0.22e^- \rightarrow 0.011C_5H_7O_2N + 0.099H_2O$

$-R_d$: $0.0417C_6H_{12}O_6 + 0.25H_2O \rightarrow 0.25CO_2 + H^+ + e^-$

R: $0.0417C_6H_{12}O_6 + 0.011NH_4^+ + 0.011HCO_3^- \rightarrow 0.011C_5H_7O_2N + 0.065CH_3CH_2OH + 0.076CO_2 + 0.044H_2O$