Stoichiometry
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**Introduction:**

Stoichiometry is a useful tool in the design and operation of biological processes. The stoichiometric equation can be used to calculate the amount of nutrients needed, the quantity of biosolid produced, the amount of oxygen required in the aerobic processes.

**Half-reaction equation:**

Oxidation-reduction reaction involves the transfer of electrons. In biological treatment processes, the organic pollutant provides electrons as the donor. Both the organism energy requirement and the organism synthesis receive the electrons as the acceptors. In the organism energy requirement, oxygen is the electron acceptor in the aerobic process and carbon dioxide, nitrate, iron, CO2 or sulfate is the electron acceptor in the anaerobic processes. The half reaction equation only expresses either the donor or the electron acceptor part of the stoichiometric equation.

**..the numerical relationship of elements and compounds as reactants and products in chemical reactions**

## Complete reaction (R):

$$R = R_d + f_e R_a + f_s R_c$$

$$f_e = 1 - f_s$$

**...the values for $f_e$ or $f_s$ can be estimated empirically**

**Multiply the electron acceptor half reaction by the appropriate $f_e$, and do the same with the cell synthesis half reaction.**

## Complete reaction (R):

$$R = R_d + f_e R_a + f_s R_c$$

**$R_d$ = Electron donor half reaction**
**$R_a$ = Electron acceptor half reaction**
**$R_c$ = Cell synthesis half reaction**
**$f_e$ = Fraction of electrons used for energy**
**$f_s$ = Fraction of electrons used for synthesis**

## Electron donor half reaction ($R_d$)

Generic organic donors:

$$1/e\,C_aH_bO_cN_d + (2a\text{-}c/e)H_2O = a/e\ CO_2 + d/e\,NH_3 + H^+ + e^-$$

where $e = 4a + b - 2c - 3d$

Inorganic:

$$1/8\,NH_3 + 3/8\,H_2O = 1/8\,NO_3 + 9/8\,H^+ + e^-$$

$$Fe^{+2} = Fe^{+3} + e^-$$

## Electron acceptor half reaction ($R_a$)

Aerobic:

$$1/4O_2 + H^+ + e^- = 1/2H_2O$$

Anaerobic:

$$1/5NO_3 + 6/5H^+ + e^- = 1/10N_2 + 3/5H_2O$$

$$1/8SO_4^{-2} + 5/4H^+ + e^- = 1/8H_2S + 1/2H_2O$$

$$1/8CO_2 + H^+ + e^- = 1/8CH_4 + 1/4H_2O$$

## Cell synthesis half reaction ($R_s$)

Ammonia N source:

$$1/4CO_2 + 1/20NH_3 + H^+ + e^- = 1/20C_5H_7O_2N + 2/5H_2O$$

Nitrate N source:

$$5/28CO_2 + 1/28NO_3 + 29/28H^+ + e^- = 1/28C_5H_7O_2N + 11/28H_2O$$

where $C_5H_7O_2N$ is an empirical description of microbes

# Stoichiometry of Microbial Reactions

**Complete reaction (R)** $R = R_d + f_e R_a + f_s R_c$

**Electron donor half reaction ($R_d$)**

Generic organic donors:

$$\boxed{\frac{1}{e} C_a H_b O_c N_d + \frac{2a-c}{e} H_2O = \frac{a}{e} CO_2 + \frac{d}{e} NH_3 + H^+ + e^-}$$

where **e = 4a + b - 2c - 3d**

Inorganic:

$$\frac{1}{8} NH_3 + \frac{3}{8} H_2O = \frac{1}{8} NO_3 + \frac{1}{8} H^+ + e^-$$

$$Fe^{2+} = Fe^{3+} + e^-$$

**Electron acceptor half reactions ($R_a$)**

Aerobic:

$$\frac{1}{4} O_2 + H^+ + e^- = \frac{1}{2} H_2O$$

Anaerobic:

$$\frac{1}{5} NO_3 + \frac{6}{5} H^+ + e^- = \frac{1}{10} N_2 + \frac{3}{5} H_2O$$

$$\frac{1}{8} SO_4^{-2} + \frac{5}{4} H^+ + e^- = \frac{1}{8} H_2S + \frac{1}{2} H_2O$$

$$\frac{1}{8} CO_2 + H^+ + e^- = \frac{1}{8} CH_4 + \frac{1}{4} H_2O$$

**Cell synthesis half reactions ($R_c$)**

Ammonia N source:

$$\frac{1}{4} CO_2 + \frac{1}{20} NH_3 + H^+ + e^- = \frac{1}{20} C_5H_7O_2N + \frac{2}{5} H_2O$$

Nitrate N source:

$$\frac{5}{28} CO_2 + \frac{1}{28} NO_3^- + \frac{29}{28} H^+ + e^- = \frac{1}{28} C_5H_7O_2N + \frac{11}{28} H_2O$$

## Stoichiometry example: aerobic hydrocarbon utilization

| | |
|---|---|
| Hydrocarbon: | octane |
| Nitrogen source: | ammonia |

**donor reaction:**

$$C_8H_{18} + 16H_2O = 8CO_2 + 50H^+ + 50e^-$$

**acceptor reaction:**

$$\frac{1}{4}O_2 + H^+ + e^- = \frac{1}{2}H_2O$$

**synthesis reaction:**

$$\frac{1}{4}CO_2 + \frac{1}{20}NH_3 + H^+ + e^- = \frac{1}{20}C_5H_7O_2N + \frac{2}{5}H_2O$$

**From $f_s$ values, $f_s = 0.39$ so $f_e = 0.61$**

**$R_d$:** $0.02C_8H_{18} + 0.32H_2O = 0.16CO_2 + H^+ + e^-$

**$f_eR_a$:** $0.15O_2 + 0.61H^+ + 0.61e^- = 0.31H_2O$

**$f_sR_c$:** $0.098CO_2 + 0.02NH_3 + 0.39H^+ + 0.39e^- = 0.02C_5H_7O_2N + 0.16H_2O$

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**Net:** $\underset{(114)}{0.02C_8H_{18}} + \underset{(32)}{0.15O_2} + \underset{(17)}{0.02NH_3} = \underset{(113)}{0.02C_5H_7O_2N} + \underset{(44)}{0.06CO_2} + \underset{(16)}{0.14H_2O}$

**Mass balance on the degradation of 1kg octane:**

**$O_2$ required =** $\frac{(0.15)(32)}{(0.02)(114)}$ **= 2.1 kg**

**$NH_3$ required =** $\frac{(0.02)(17)}{(0.02)(114)}$ **= 0.15 kg**

$$\textbf{Biomass produced} = \frac{(0.02)(113)}{(0.02)(114)} = \textbf{1.0 kg}$$