Stoichiometry of Biochemical Reactions

Today's lecture

- Biochemical reaction stoichiometry
- Cell yield
- Half reactions to overall reaction

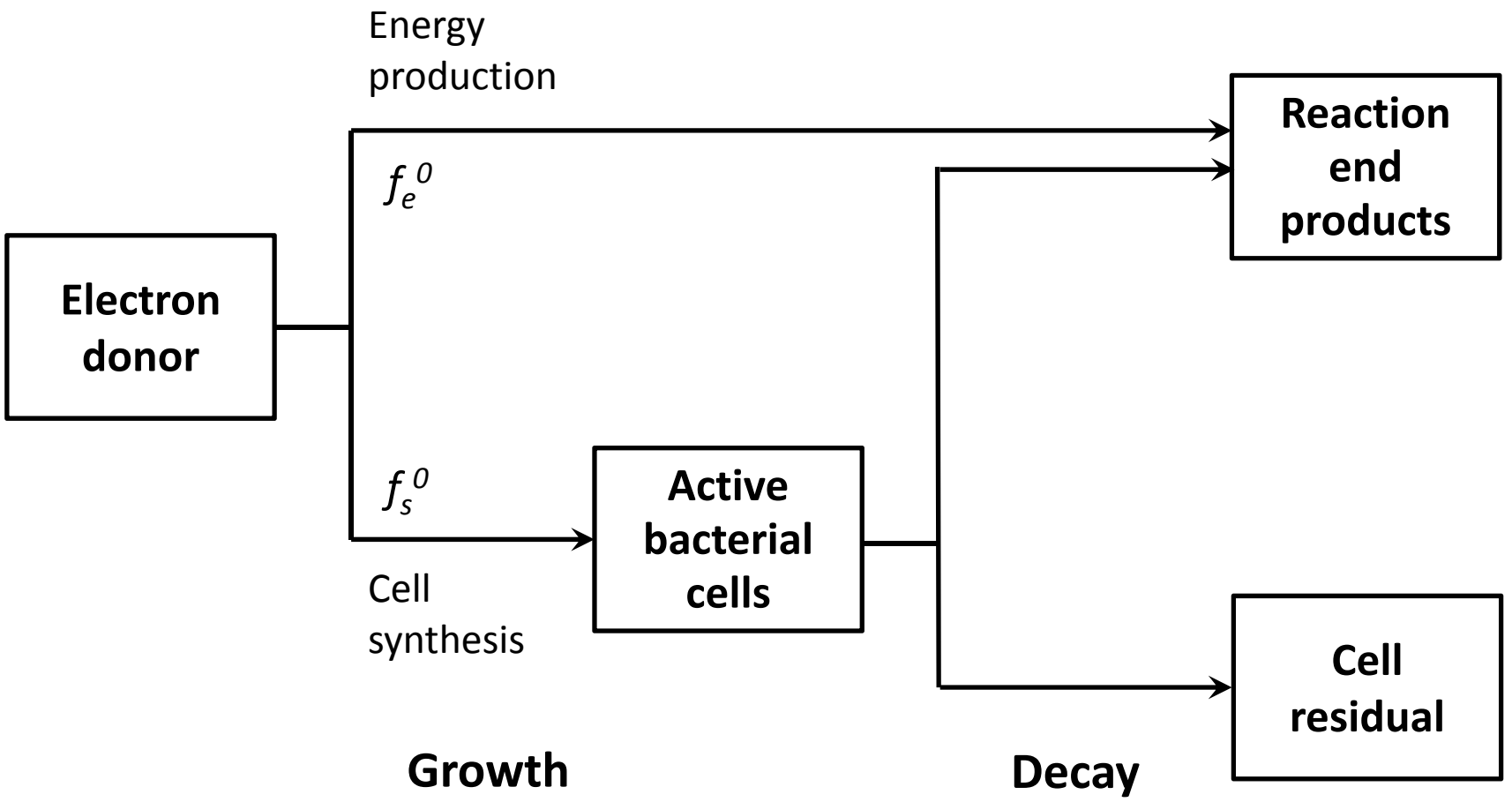
Stoichiometry

- “An aspect of chemistry concerned with mole relationships among reactants and products”
- Based on mass conservation
- Balancing chemical reactions

Cell formula

- Most common: $C_5H_7O_2N$
- COD for a bacterial cell?

Substrate partitioning



Textbook Fig. 2.1

Cell yield

- True yield, *Y*

  Y = (g cells produced) / (g substrate utilized)

- Conversion of f_s^0 to *Y*:

$$Y = f_s^{\,0}\,\frac{\left(M_c\ \text{g cells/mol cells}\right)}{\left(n_e\ \text{e}^-\ \text{eq/mol cells}\right)\left(8\ \text{g COD/e}^-\ \text{eq donor}\right)}$$

Microbial growth rate

$$\frac{dX_a}{dt} = Y\left(\frac{-dS}{dt}\right) - bX_a$$

growth decay

X_a = active biomass concentration [M/L^3]

S = substrate concentration [M/L^3]

Y = true yield [M/M]

b = decay rate [1/T]

Net yield

- Net yield, Y_n

Y_n = (g net cell growth) / (g substrate utilized)

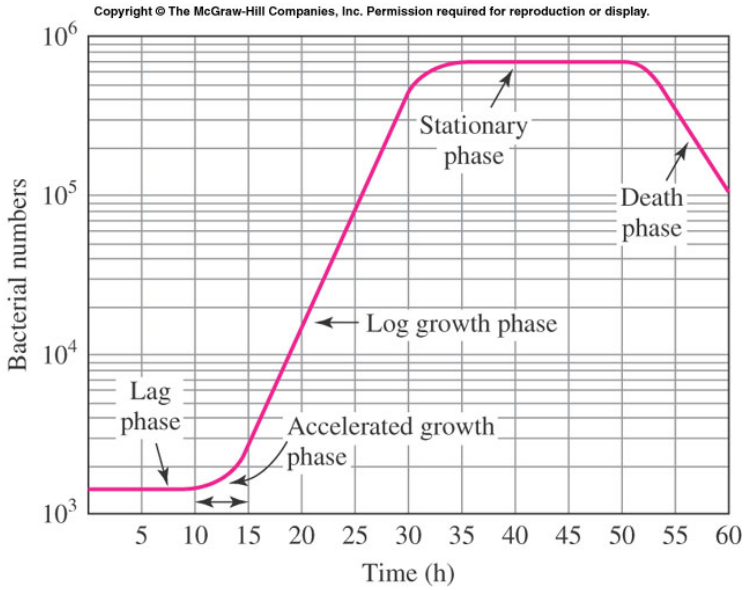
$$= \frac{dX_a / dt}{-dS / dt}$$

$$= Y - b\frac{X_a}{-dS / dt}$$

Log (exponential) growth: $Y_n > 0$

Stationary phase: $Y_n = 0$

Death phase: $Y_n < 0$



Bacterial growth curve for pure culture

Net yield

- Electron partitioning considering net yield, Y_n:

$f_s^0 \rightarrow f_s \qquad (f_s < f_s^0)$

$f_e^0 \rightarrow f_e \qquad (f_e > f_e^0)$

still, $f_s + f_e = 1$

Energy reactions

Aerobic oxidation:

$C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O$, $\Delta G = -2880$ kg/mol

vs.

Sulfate reduction:

$2C_6H_{12}O_6 + 6SO_4^{2-} \rightarrow 12CO_2 + 12H_2O + 3H_2S + 3\ HS^-$,
$\Delta G = -492$ kg/mol

Half reactions

- For complex biochemical redox reactions, it is easier to use half reaction approach
- The oxidation reaction for an electron donor and the reduction reaction for an electron acceptor can be splitted
- Usually written as a reduction reaction

  (see [Table 2.2] & [Table 2.3])

Half reactions

Step 1 Write oxidized form on the left and reduced form on the right

Step 2 Add other species involved in the reaction

Step 3 Balance the reaction for all elements except for oxygen and hydrogen

Step 4 Balance oxygen using water

Step 5 Balance hydrogen using H^+

Step 6 Balance charge using e^-

Step 7 Convert the equation to the e^--equivalent form

Overall reactions

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

   $R_e = R_a - R_d$

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

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

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

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