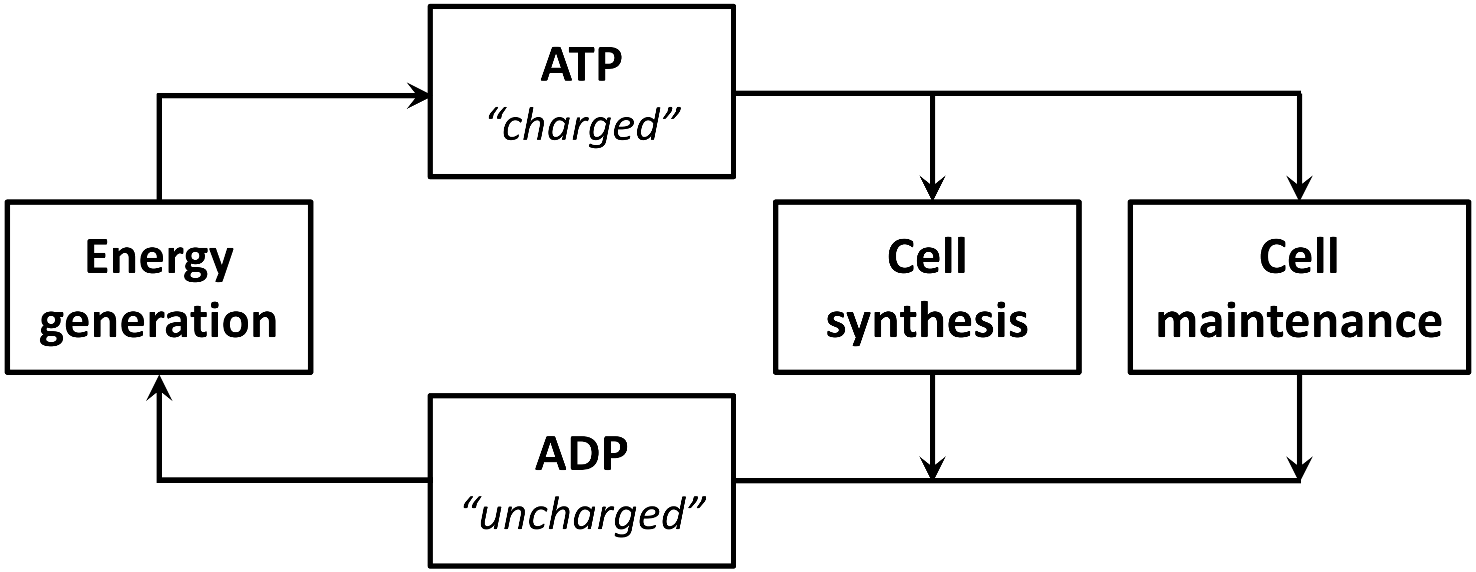
Bacterial energetics

Today's lecture

- Bacterial energetics – overview
- Gibbs free energy of reaction
- Correlation of reaction energetics and yield coefficient

Bacterial energetics

- Microorganisms carry out redox reactions to obtain energy for growth and cell maintenance



Energetics and bacterial growth

- The bacterial cells grow more rapidly when:
  - More energy can be obtained by oxidation of (an e^- equivalent of) e^- donor
  - More energy can be obtained by reduction of (an e^- equivalent of) e^- acceptor
  - When conditions are favorable (abundance of e^- donor, e^- acceptor, nutrients, etc.; low concentration of inhibiting compounds)

    → rapid utilization of substrates

Energetics and bacterial growth

- Consider:

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

  - Larger Y_n when Y >> b: favorable e^- donor and acceptor
  - Larger Y_n when X_a << -dS/dt: favorable conditions for substrate utilization

Gibbs free energy

- "Standard" free energy
  - ΔG^0, free energy at 25°C, 1 atm, and unit activity for any chemicals involved
  - $\Delta G^{0\prime}$, standard free energy adjusted to pH=7

- Free energy of formation (ΔG_f)
  - Gibbs free energy that accompanies the formation of 1 mole of the substance from its component elements

Gibbs free energy

- Free energy change of reaction (ΔG_r)

$$\sum\left[\left(sum\ of\ product\ \Delta G_f\right) - \left(sum\ of\ reactant\ \Delta G_f\right)\right]$$

For a generic reaction written as

$$0 = \sum_{i=1}^{n} v_{ir} A_i$$

v_{ir} = stoichiometric coefficient, (-) for reactants, (+) for products

A_i = reaction constituent, reactants or products

$$\Delta G_r = \sum_{i=1}^{n} v_{ir} \Delta G_f$$

Reaction free energy

Q1: Calculate the standard free energy adjusted pH 7 for the half reaction of 2-chlorobenzoate formation. Use the values of free energy of formation for individual constituents listed in Appendix A.

Q2: Calculate the standard free energy adjusted pH 7 for overall energy reaction with ethanol as an e^- donor and oxygen as an e^- acceptor. Use the half reactions listed in Table 2.2 and 2.3.

Reaction free energy

- For nonstandard conditions,

$$\Delta G_r = \Delta G_r{}^0 + RT\sum_{i=1}^{n} v_{ir} ln a_i$$

a_i = activity of constituent A_i

Caution:
- v_{ir} is negative for reactants and positive for products
- $\Delta G_r{}^0$ is for standard conditions -- pH=0

From $\Delta G_r{}^{0\prime}$, we can calculate $\Delta G_r{}^0$ by:

$$\Delta G_r{}^0 = \Delta G_r{}^{0'} - \mathrm{RT} v_{H^+} ln[10^{-7}]$$

Reaction free energy

Q3: Calculate the free energy of reaction for denitrification of glucose at the following conditions: T = 25°C, pH = 6.0, $[C_6H_{12}O_6] = 10^{-3}$ M, $[NO_3^-] = 10^{-4}$ M, $P_{CO2} = 3 \times 10^{-4}$ atm, $P_{N2} = 0.78$ atm.

Q4: Calculate the free energy of reaction for aerobic ethanol degradation at the following conditions: T = 20°C, pH = 5.0, $[C_2H_5OH] = 2 \times 10^{-3}$ M, $P_{CO2} = 3 \times 10^{-4}$ atm, $P_{O2} = 0.21$ atm.

Yield coefficient and reaction energetics

- The energy generated by energy reactions is spent to make ATP
- ATP is consumed to drive cell synthesis or cell maintenance
- Cell synthesis involves energy loss (bacteria are not 100% efficient engines!) to synthesize C source to an intermediate compound, and then the intermediate compound to cells

Yield coefficient and reaction energetics

- Energy required to convert carbon source to pyruvate, ΔG_p (heterotrophic bacteria, ammonia as N source):

$$\Delta G_p = 35.09 - \Delta G_c{}^{0\prime}$$

(in kJ/e^- eq)

35.09 = reaction free energy for formation of pyruvate from CO_2

$\Delta G_c{}^{0\prime}$ = reaction free energy for formation of carbon source from CO_2

- Energy required to convert pyruvate to cells, ΔG_{pc} = 18.8 kJ/e^- eq

Yield coefficient and reaction energetics

- Energy required for cell synthesis from the carbon source, ΔG_s:

$$\Delta G_s = \frac{\Delta G_p}{\varepsilon^n} + \frac{\Delta G_{pc}}{\varepsilon}$$

ε = energy transfer efficiency

n = -1 for $\Delta G_p < 0$ (C-source is at higher energy state than pyruvate);

+1 for $\Delta G_p > 0$ (C-source is at lower energy state than pyruvate)

- If energy for cell maintenance is neglected (situation for true yield, Y, and f_s^0):

$$A\varepsilon\Delta G_r + \Delta G_s = 0$$

A = e^- equivalent of e^- donor used for energy production per equivalent of cells formed

Yield coefficient and reaction energetics

- Solving for A:

$$A = \frac{\Delta G_p/\varepsilon^n + \Delta G_{pc}/\varepsilon}{\varepsilon \Delta G_r}$$

- From A, we can calculate $f_s^{\,0}$ and $f_e^{\,0}$ as:

$$f_s^{\,0} = \frac{1}{1+A} \qquad f_e^{\,0} = 1 - f_s^{\,0} = \frac{A}{1+A}$$

- Energy transfer efficiency, ε
  - 55-70% under optimal conditions
  - Use 0.6 for ordinary cases

Yield coefficient and reaction energetics

Q5: Estimate f_s^0 and Y for aerobic oxidation of acetate assuming ε=0.4 and 0.6 at standard conditions except for a pH of 7.0. Ammonia is available for cell synthesis.