# Stoichiometry of Biochemical Reactions I

# Today's class

- Major type of biochemical reactions – redox reactions
- What is and what can be done with stoichiometry
- Substrate electron partitioning and cell yield

# Oxidation-reduction (redox) reactions

- Involves changes in the oxidation state
- If there are oxidizing species, there should be reducing species as well
  - Total # of electrons are conserved
  - Oxidizing species – $e^-$ donor / Reducing species – $e^-$ acceptor
- Essential for life – many important biological processes involve redox reactions
  - Involves large free energy change ($\Delta G$)

# Biological benefit of redox reactions

Examples:

photosynthesis of glucose:

$6CO_2 + 6H_2O + \text{sunlight} \rightarrow C_6H_{12}O_6 + 6O_2$

$\Delta G^0 = +2880$ kJ/mol $C_6H_{12}O_6$

*Sunlight energy is converted to chemical energy (storable)*

respiration using glucose:

$C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O$ $\Delta G^0 = -2880$ kJ/mol $C_6H_{12}O_6$

*Chemical energy is released, enabling cells to work*

# Stoichiometry

- “An aspect of chemistry concerned with mole relationships among reactants and products”
- Simply put, balancing chemical reactions
- Based on mass conservation
  - Conservation of elements
  - Conservation of electrons (for redox reactions)

# What can we do with stoichiometry?

A balanced biochemical reaction example

(ethanol fermentation of glucose at $f_s$=0.22)

$$0.0417C_6H_{12}O_6 + 0.011\ NH_4^+ + 0.011HCO_3^-$$

$$\rightarrow 0.011C_5H_7O_2N + 0.065C_2H_5OH + 0.076CO_2 + 0.044H_2O$$

[Bacterial cells]

Available information:

Using 1 g (or 1 mole) of glucose,

- How much ethanol can be produced?
- How much nutrients ($NH_4$-N) are required?
- How much biomass is produced?
- How much alkalinity is consumed?

# Cell formula

- Most common: $C_5H_7O_2N$

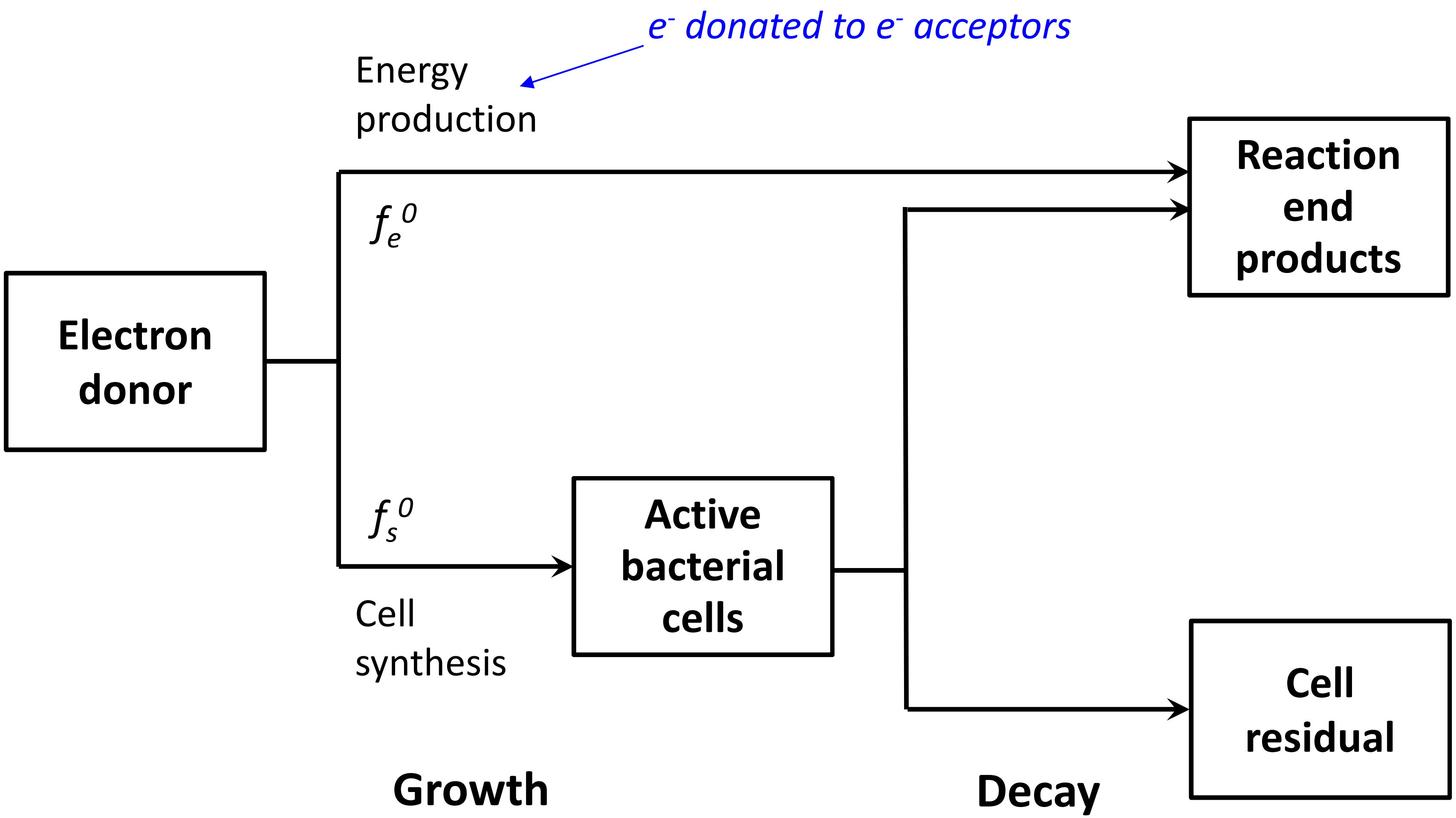
- What is the theoretical COD-per-weight value for a bacterial cell (i.e., g COD / g cells)?
  - Once you get trained with the stoichiometry, you will be able to write the balanced reaction as:

    $$C_5H_7O_2N + 5O_2 \rightarrow 5CO_2 + NH_3 + 2H_2O$$

  - Then you get: 1.42 g COD/g cells

*You will find this value useful in the future!*

# Substrate partitioning



# Cell yield

- True yield, *Y*

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

- Conversion of $f_s^0$ to *Y*:

$$Y = f_s{}^0 \frac{(M_c \;\; g\; cells/mole\; cells)}{(n_e \;\; e^- \; eq\; cells/mole\; cells)(8\; g\; COD/e^- \; eq\; donor)}$$

For $C_5H_7O_2N$, $M_c$ = 113 g/mole;

$n_e$ = 20 $e^-$ eq/mole (see Table 2.3)

then: $Y(in\; g\; cells/g\; COD) = 0.706 f_s{}^0$

# 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]

# Decay

- Generally assumed to be proportional to the amount of cells
- A gross factor for anything that leads to decrease in cell biomass
- Decay = endogenous respiration (+ predation)
  - Endogenous respiration: use of cell matter for maintenance of cell functions (motility, repair, resynthesis, osmotic regulation, transport, compensate heat loss, …)

# Net yield

- Net yield, $Y_n$

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

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

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

# Net yield

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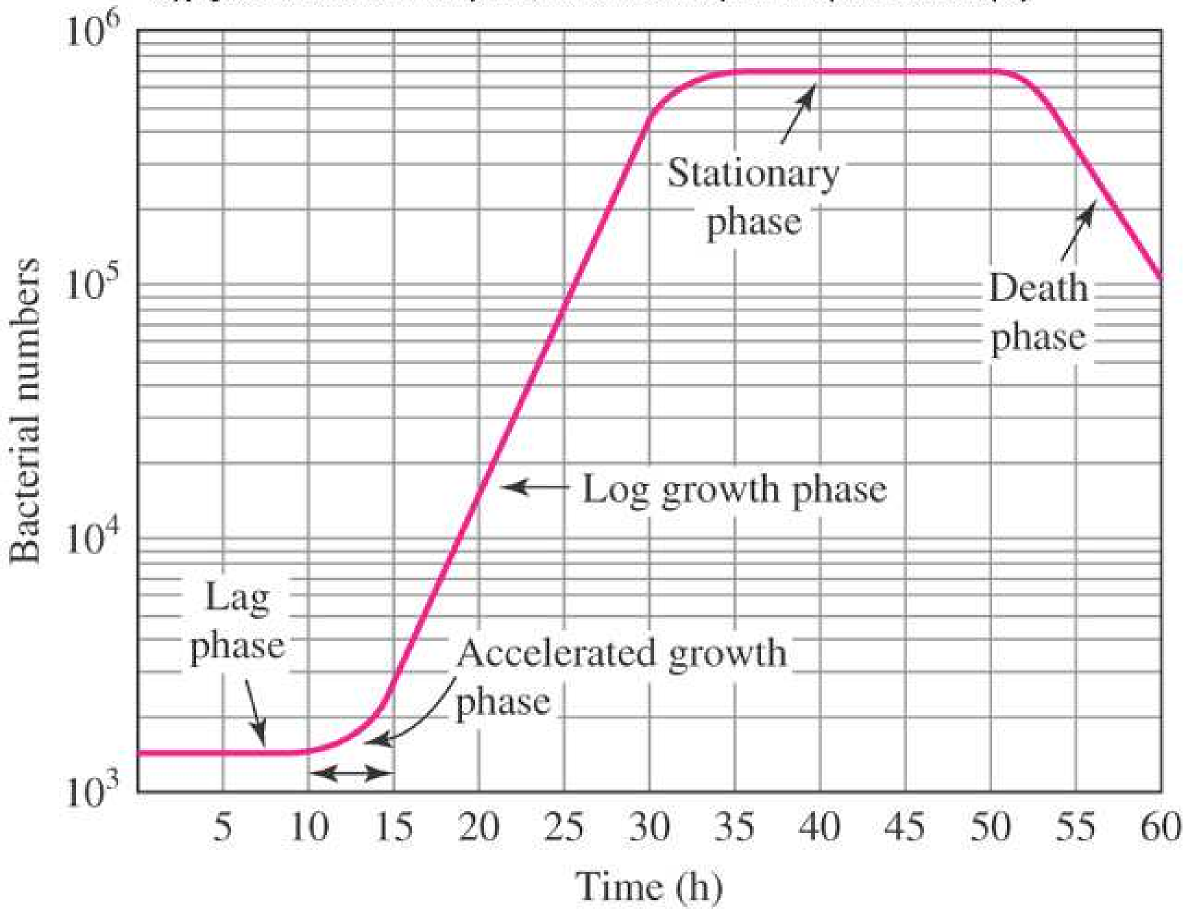


Bacterial growth curve for pure culture

Log (exponential) growth:

Stationary phase:

Death phase:

# Net yield

- Electron partitioning considering net yield, $Y_n$:

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

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

  still, $f_s + f_e = 1$

# Energy reactions

- Microorganisms need energy for growth and maintenance

| | $\Delta G^0$ (in kJ/mole glucose) |
| --- | --- |
| Aerobic oxidation: | |
| $C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O$ | -2,880 |
| Denitrification: | |
| $5C_6H_{12}O_6 + 24NO_3^- + 24H^+ \rightarrow 30CO_2 + 42H_2O + 12N_2$ | -2,720 |
| Sulfate reduction: | |
| $2C_6H_{12}O_6 + 6SO_4^{2-} \rightarrow 12CO_2 + 12H_2O + 3H_2S + 3\,HS^-$ | -492 |
| Methanogenesis: | |
| $C_6H_{12}O_6 \rightarrow 3CO_2 + 3CH_4$ | -428 |
| $(C_6H_{12}O_6 + 3CO_2 \rightarrow 6CO_2 + 3CH_4)$ | |
| Ethanol fermentation: | |
| $C_6H_{12}O_6 \rightarrow 2CO_2 + 2C_2H_5OH$ | -244 |