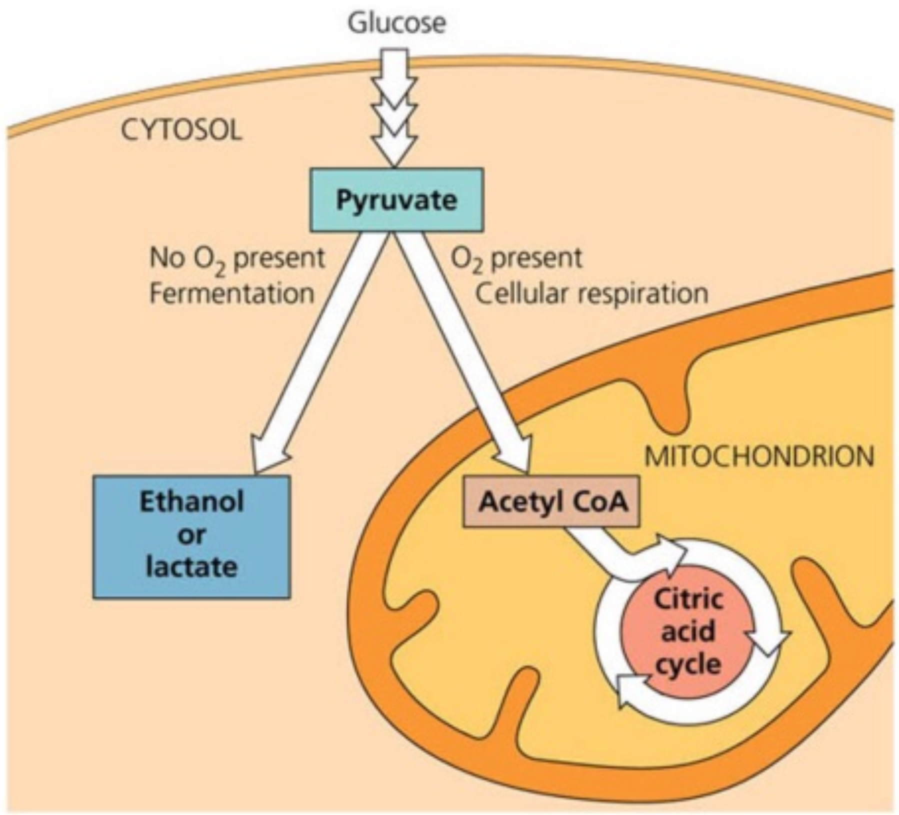
Example 2



Take the reaction where glucose, oxygen, CO_2, ethanol and water are reagents/products.

a) If the oxygen rate is the same as the CO_2 rate but opposite in sign, determine Y_{SE} (S-glucose, E-ethanol)

b) Assume the overall reaction is taking place in a living organism. If the oxygen consumption rate is 2.3 $\frac{mmol}{h}$ and the CO_2 production rate is 7.8 $\frac{mmol}{h}$, what fraction of glucose is used for respiration and what fraction of the total ATP generated is from respiration. Assume a $(P/O)_{NADH}$ of 1.5 and a $(P/O)_{FADH}$ of 1. [12% 59%]

c) In what pathways are CO_2 formed?

d) How does this example relate to the story of the fire where wood is imcompletely burned?

$$C_6H_{12}O_6 + O_2 \rightarrow CO_2 + C_2H_6O + H_2O$$

(Cmol) $CH_2O + Y_{SO}O_2 \rightarrow Y_{SC}CO_2 + Y_{SE}CH_3O_{0,5} + Y_{SW}H_2O$

a)

$$\bar{A} = \begin{array}{c} C \\ H \\ O \\ \text{rate 1} \\ \text{rate 2} \end{array} \begin{bmatrix} 1 & 0 & 1 & 1 & 0 \\ 2 & 0 & 0 & 3 & 2 \\ 1 & 2 & 2 & 0,5 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} Y_S \\ Y_{SO} \\ Y_{SC} \\ Y_{SE} \\ Y_{SW} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1 \\ 1 \end{bmatrix}$$

$Y_S = -1$

$Y_{SO} = -1$

$Y_{SC} = 1$

$\boxed{Y_{SE} = 0}$

$Y_{SW} = 1$

(mol based)

$$b)\ \bar{A} = \begin{array}{c} C \\ H \\ O \\ \text{rate 1} \\ \text{rate 2} \end{array} \begin{bmatrix} 6 & 0 & 1 & 2 & 0 \\ 12 & 0 & 0 & 6 & 2 \\ 6 & 2 & 2 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} Y_S \\ Y_{SO} \\ Y_{SC} \\ Y_{SE} \\ Y_{SW} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -2{,}3 \\ 7{,}8 \end{bmatrix}$$

$Y_S = -3{,}13$
$Y_{SO} = -2{,}3$
$Y_{SC} = 7{,}8$
$Y_{SE} = 5{,}5$
$Y_{SW} = 2{,}3$

$\Rightarrow$ In aerobic respiration, 6 mol O_2 consumed per mol Gluc.

$r_{O_2} = 6\, r_S$

$r_S = \frac{r_{O_2}}{6} = \frac{2{,}3}{6} = 0{,}38$ mmol/h

$\frac{0{,}38 \text{ mmol/h used}}{3{,}13 \text{ mmol/h available}} = 0{,}12 = 12\% \Rightarrow$

Therefore 12% glucose is used for respiration.

Overall equation:

$\Rightarrow C_6H_{12}O_6 + 6H_2O \Rightarrow 6CO_2 + 10\,NADH + 2\,FADH_2 + 4\,ATP$

$NADH + \frac{1}{2}O_2 \Rightarrow (P/O)_{NADH}\, ATP + H_2O \Rightarrow 1{,}5\,ATP + H_2O$
$FADH_2 + \frac{1}{2}O_2 \Rightarrow (P/O)_{FADH_2}\, ATP + H_2O \Rightarrow 1\,ATP + H_2O$

$\Rightarrow$ Total ATP $= 10(1{,}5) + 2(1) + 4 = 21$ ATP/mol Gluc. $\Rightarrow$

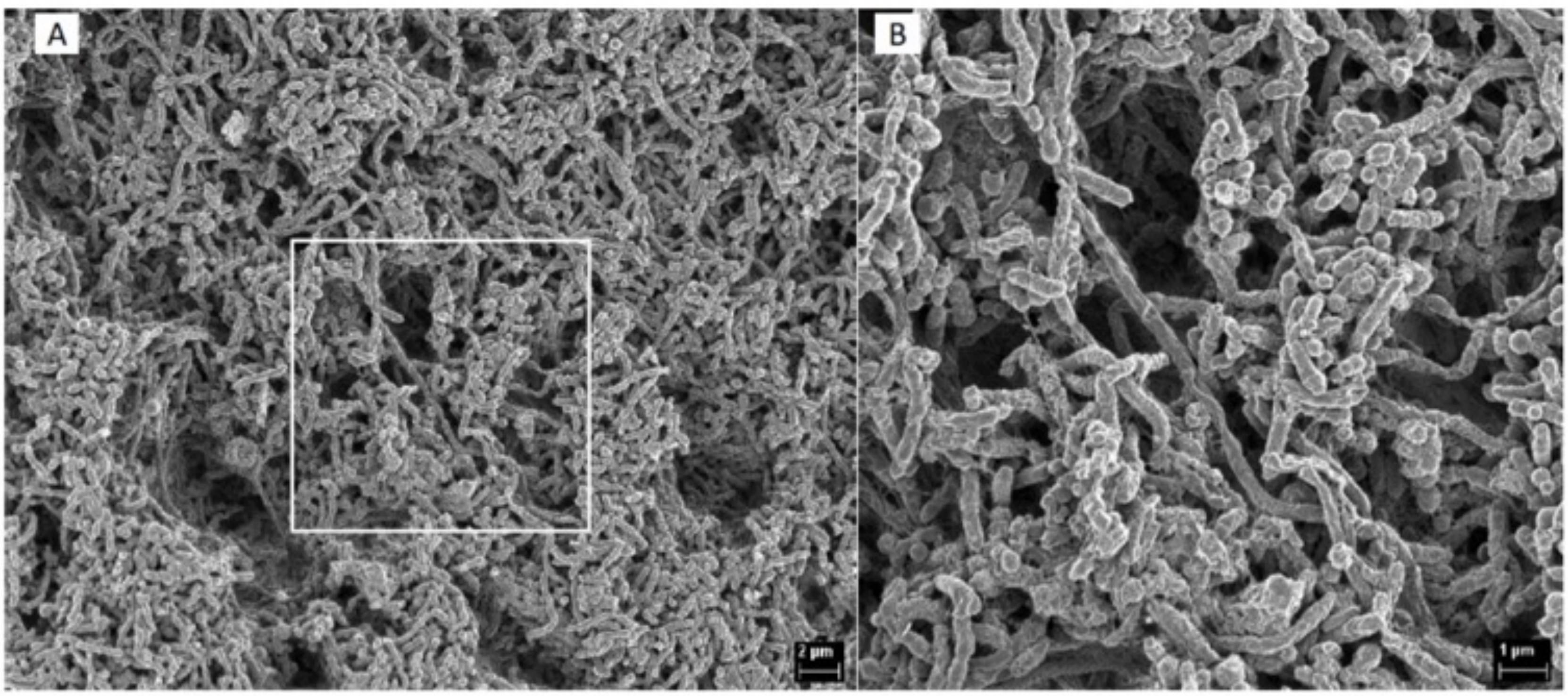
$\frac{21\ ATP}{mol\ C_6H_{12}O_6} \Big|\ 0{,}38$ mol Gluc $= 8{,}05$ ATP from aerobic respiration

$$\frac{2\ ATP}{mol\ Gluc.} \bigg| (3{,}13 - 0{,}38)\ mol\ Glc = 5{,}50\ ATP \text{ from anaerobic respiration}$$

$$\text{Fraction ATP from respiration} = \frac{8{,}05}{8{,}05 + 5{,}50} = 59{,}4\,\% \longrightarrow$$

c) CO_2 is formed in both pathways

Tutorial 1



The rumen bacterium *Actinobacillus succinogenes* consumes glucose anaerobically to produce biomass, succinic and acetic acid when NH_3 is used as nitrogen source. Carbon dioxide can be a reagent or product in this reaction, while water is formed as product. You can assume the standard elemental composition for the biomass.

It was determined from a fermentation run that the acetic acid yield was 0.19 $\frac{g\ AA}{g\ Gluc}$ and the biomass yield 0.0656 $\frac{g\ X}{g\ Gluc}$

a) Determine the mass based yield of succinic acid on glucose. [0.816 $\frac{g}{g}$]

b) Is CO_2 formed as product or used as reagent? Determine the moles of CO_2 formed/used per cmol of glucose used. [0.1 mol/cmol]

c) Repeat the calculation in (a) using the degree of reduction (DOR) method.

d) What will be the mass based succinic acid yield on glucose if zero biomass formed? Acetic acid yield remains the same. [0.91 $\frac{g}{g}$]

$$C_6H_{12}O_6 + NH_3 + CO_2 \rightarrow X + C_4H_6O_4 + C_2H_4O_2 + H_2O$$

$$1/s\ CH_2O + Y_{SN}\ NH_3 + Y_{SC}\ CO_2 \rightarrow Y_{SX}\ CH_{1,8}O_{0,5}N_{0,2} + Y_{SSA}\ CH_{1,5}O + Y_{SAA}\ CH_2O + Y_{SW}\ H_2O$$

$$
\begin{array}{r|c}
 & \begin{array}{ccccccc} S & SN & SC & SX & SSA & SAA & SW \end{array} \\
\begin{array}{r} C: \\ H: \\ O: \\ N: \\ \text{Basis:} \\ \text{rate 1} \\ \text{rate 2} \end{array} &
\begin{bmatrix}
1 & 0 & 1 & 1 & 1 & 1 & 1 \\
2 & 3 & 0 & 1{,}8 & 1{,}5 & 2 & 2 \\
1 & 0 & 2 & 0{,}5 & 1 & 1 & 1 \\
0 & 1 & 0 & 0{,}2 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0
\end{bmatrix}
\end{array}
\times
\begin{bmatrix} y_S \\ y_{SN} \\ y_{SC} \\ y_{SX} \\ y_{SSA} \\ y_{SAA} \\ y_{SW} \end{bmatrix}
=
\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ -1 \\ 0{,}19 \\ 0{,}08 \end{bmatrix}
$$

$$\frac{0{,}19\,g\,C_2H_4O_2}{1\,g\,C_6H_{12}O_6}\left|\frac{gmol\,AA}{60\,g\,AA}\right|\frac{2\,cmol\,AA}{gmol\,AA}\left|\frac{180\,g\,Gluc}{gmol\,Gluc}\right|\frac{gmol\,Gluc}{6\,cmol\,Gluc} = \frac{0{,}19\,cmol\,AA}{cmol\,Glu} = y_{SAA}$$

$$\frac{0{,}0656\,g\,X}{g\,Glu}\left|\frac{180\,g\,Glu}{gmol\,Glu}\right|\frac{gmol\,Glu}{6\,cmol\,Gluc}\left|\frac{gmol\,X}{24{,}6\,g\,X}\right|\frac{cmol\,X}{gmol\,X} = 0{,}08\,\frac{cmol\,X}{cmol\,Gluc} = y_{SX}$$

$y_S = -1$

$y_{SN} = -0{,}016$

$y_{SC} = -0{,}1$

$y_{SX} = 0{,}08$

$y_{SSA} = 0{,}8297$

$y_{SAA} = 0{,}19$

$y_{SW} = 0{,}14$

$$\frac{y_{SSA}}{y_S} = \frac{0{,}8297}{1}\,\frac{cmol\,SA}{cmol\,Glu}\left|\frac{cmol\,Glu}{30\,g\,Glu}\right|\frac{29{,}5\,g\,SA}{cmol\,SA} = 0{,}816\,g\,SA/g\,Gluc$$

b) CO_2 is used as a reagent.

$$\frac{-r_C}{-r_{gluc}} = \frac{0{,}0997}{1}\,\frac{cmol\,CO_2}{cmol\,Gluc}\left|\frac{mol\,CO_2}{cmol\,CO_2}\right. = 0{,}1\,mol\,CO_2/cmol\,Glu$$

c) $(-r_S)CH_2O + (-r_N)NH_3 + (-r_C)CO_2 \rightarrow (r_X)CH_{1,8}O_{0,5}N_{0,2} + (r_{SA})CH_{1,5}O$
$+ (r_{AA})CH_2O + (r_W)H_2O$

DOR:

$CH_2O = 4 + 2(1) - 2 = 4$

$NH_3 = -3 + 3(1) = 0$

$CO_2 = 4 + 2(-2) = 0$

$CH_{1,8}O_{0,5}N_{0,2} = 4 + 1,8(1) + 0,5(-2) + 0,2(-3) = 4,2$

$CH_{1,5}O = 4 + 1,5(1) + (-2) = 3,5$

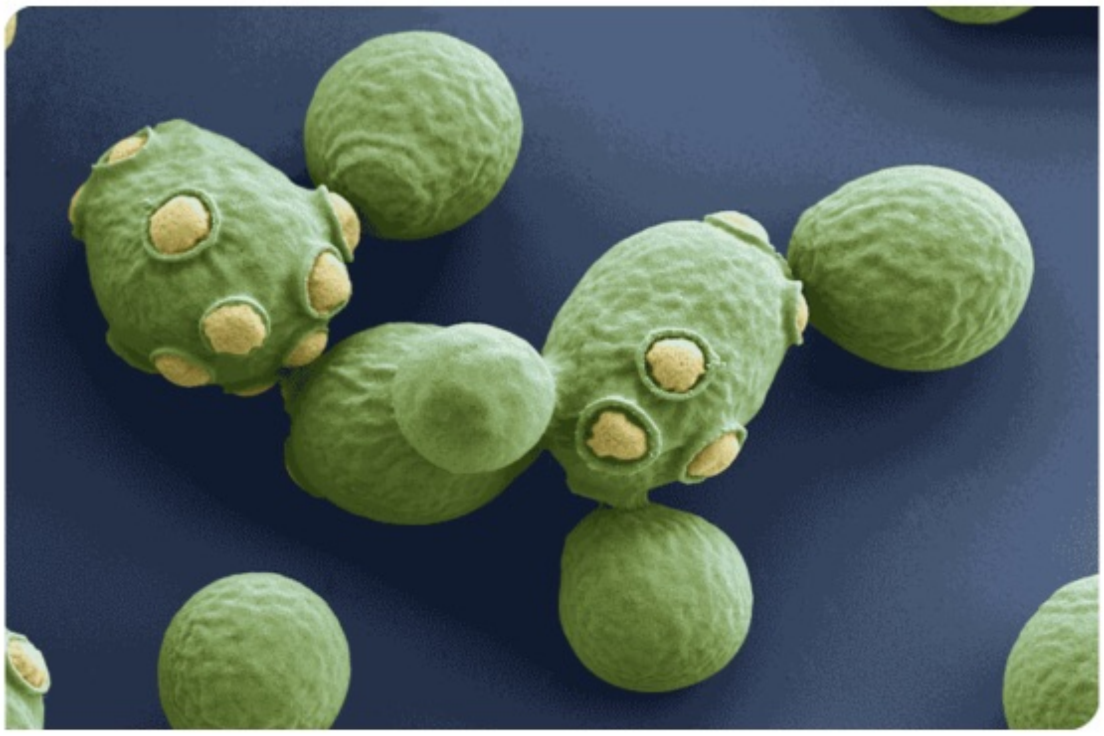
$CH_2O = 4 + 2(1) + (-2) = 4$

$$
\begin{array}{c}
 \\ C \\ DOR \\ N \\ Basis \\ rate1 \\ rate2
\end{array}
\begin{array}{c}
\begin{array}{cccccc} s & sN & sC & sx & sSA & sAA \end{array} \\
\begin{bmatrix}
1 & 0 & 1 & 1 & 1 & 1 \\
4 & 0 & 0 & 4,2 & 3,5 & 4 \\
0 & 1 & 0 & 0,2 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0
\end{bmatrix}
\end{array}
\begin{bmatrix} Y_s \\ Y_{sN} \\ Y_{sc} \\ Y_{sx} \\ Y_{sSA} \\ Y_{sAA} \end{bmatrix}
=
\begin{bmatrix} 0 \\ 0 \\ 0 \\ -1 \\ 0,19 \\ 0,08 \end{bmatrix}
$$

Results are exactly the same as in 5)

d) $\dfrac{0,9257 \text{ cmol SA}}{\text{cmol Glu}} \left| \dfrac{\text{cmol Glu}}{30 \text{ g Glu}} \right| \dfrac{29,5 \text{ g SA}}{30 \text{ g Glu}} = 0,91 \dfrac{\text{g SA}}{\text{g Glu}} \rightarrow$

The yeast *Saccharomyces cerevisiae* is produced commercially on a large scale to provide bakers around the world with the 'magic stuff' that makes dough rise. Using the generic biomass formula for the yeast cells ($CH_{1.8}O_{0.5}N_{0.2}$), write down the overall equation for producing cells from glucose, ammonia and oxygen. Note that CO_2 and H_2O will be products.



a) What is the mass based yield of biomass on glucose if zero oxygen is used? [0.78 g/g]

b) Will the reaction in (a) be feasible, give reasons.

c) If oxygen is introduced into the system (@ 0.38 mol O_2/cmol glucose), what will be the biomass yield and why the change from (a)? [0.48 g/g]

d) All the oxygen is consumed is via the process of oxidative phosphorylation. Use this to determine the moles of ATP generated per cmol of biomass (X) formed for the scenario in (c). Assume a $(P/O)_{NADH}$ of 1.7 and a $(P/O)_{FADH}$ of 1.2. [2.51 $\frac{mol\ ATP}{cmol\ X}$]

$$(-r_s)\,C_6H_{12}O_6 + (-r_N)\,NH_3 + (-r_o)\,O_2 \rightarrow (r_x)\,CH_{1,8}O_{0,5}N_{0,2} + (r_c)\,CO_2 + (r_w)\,H_2O$$

$$\begin{array}{c|cccccc} \text{cmol} & -r_s & -r_N & -r_o & r_x & r_c & r_w \\ \end{array}$$

$$\begin{array}{c} C \\ H \\ O \\ N \\ \text{Basis} \\ \text{rate} \end{array} \begin{bmatrix} 1 & 0 & 0 & 1 & 1 & 0 \\ 2 & 3 & 0 & 1,8 & 0 & 2 \\ 1 & 0 & 1 & 0,5 & 2 & 1 \\ 0 & 1 & 0 & 0,2 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} -r_s \\ -r_N \\ -r_o \\ r_x \\ r_c \\ r_w \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

a) $$\frac{r_x}{-(-r_s)} = \frac{0,952\ \text{cmol}\,x}{1\ \text{cmol Glc}} \left| \frac{\text{cmol Glc}}{30\,g\ \text{Glc}} \right| \frac{24,6\,g\ X}{\text{cmol}\ X} = 0,78\ g\,X/g\,\text{Glc}$$

b) Reaction in (a) is feasible as it is anaerobic.

c) When changing $r_O = 0{,}38 \frac{cmol\ O_2}{cmol\ Glc}$:

$$Y_{Biomass}(mass) = 0{,}59 \frac{cmol\ X}{cmol\ Glc} \left| \frac{24{,}6g\ X}{cmol\ X} \right| \frac{cmol\ Glc}{30g\ Glc} = 0{,}484 \frac{g\ X}{g\ Glc}$$

When O_2 is introduced, the preferred and most efficient pathway to get energy, the less available glucose to make biomass.

d)

$$C_6H_{12}O_6 + 6H_2O \rightarrow 6CO_2 + 10NADH + 2FADH_2 + 4ATP$$

$$NADH + \tfrac{1}{2}O_2 \rightarrow 1{,}7\ ATP + H_2O$$
$$FADH_2 + \tfrac{1}{2}O_2 \rightarrow 1{,}2\ ATP + H_2O$$

$$\text{Total ATPs} = 10(1{,}7) + 2(1{,}2) + 4 = 23{,}4\ ATP/mol\ Glc$$

$$\Rightarrow C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O + 23{,}4\ ATP$$

$$r_{O_2} = 6r_{glc}$$
$$r_{gluc} = \frac{0{,}38}{6} = 0{,}0633 \frac{mol\ Glc}{s}$$

$$r_{ATP} = \frac{0{,}0633\ mol\ Glc}{s} \left| \frac{23{,}4\ ATP}{mol\ Glc} \right. = 1{,}482\ ATP/s$$ from oxidative phosphorylation

$$\frac{1{,}482\ ATP}{s} \times \frac{s}{0{,}5905\ cmol\ X} = 2{,}51\ ATP/cmol\ X$$