(E30C!)

1,3 Propanediol, $C_3H_8O_2$

X : $CH_{1,91}O_{0,48}N_{0,22}$

$$Glu + NH_3 + O_2 \rightarrow X + CO_2 + H_2O + PDO$$

$$Y_S\, C_6H_{12}O_6 + Y_{SN}NH_3 + Y_{SO}\,O_2 \rightarrow Y_{SX}\,CH_{1,91}O_{0,48}N_{0,22} + Y_{SC}\,CO_2 + Y_{SW}\,H_2O + Y_{SP}\,C_3H_8O_2$$

$$Y_S\,CH_2O + Y_{SN}NH_3 + Y_{SO}O_2 \rightarrow Y_{SX}\,CH_{1,91}O_{0,48}N_{0,22} + Y_{SC}\,CO_2 + Y_{SW}H_2O + Y_{SP}\,CH_{8/3}O_{2/3}$$

a) $Y_{SX} = 0,0822\ \frac{g\,X}{g\,Glu} \left| \frac{Cmol\,X}{24,67\,g\,X} \right| \frac{30\,g\,Glu}{Cmol\,Glu} = 0,09996\ \frac{Cmol\,X}{Cmol\,Glu}$

$Y_{SO} = 0,00267\ \frac{mol\,O_2}{g\,Glu} \left| \frac{30\,g\,Glu}{Cmol\,Glu} \right| \frac{Cmol\,O_2}{mol\,O_2} = 0,0801\ \frac{Cmol\,O_2}{Cmol\,Gluc}$

$$\begin{array}{c} \\ C \\ H \\ O \\ N \\ Deg's \\ r_1 \\ r_2 \end{array}
\begin{array}{c} \begin{array}{ccccccc} S & N & O & X & C & W & P \end{array} \\
\begin{bmatrix} 1 & 0 & 0 & 1 & 1 & 0 & 1 \\ 2 & 3 & 0 & 1,91 & 0 & 2 & 8/3 \\ 1 & 0 & 2 & 0,48 & 2 & 1 & 2/3 \\ 0 & 1 & 0 & 0,22 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix} \end{array}
\begin{array}{c} \underline{b} \\ \begin{bmatrix} Y_S \\ Y_{SN} \\ Y_{SO} \\ Y_{SX} \\ Y_{SC} \\ Y_{SW} \\ Y_{SP} \end{bmatrix} \end{array}
= \begin{array}{c} \overline{C} \\ \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0,09996 \\ -0,0801 \end{bmatrix} \end{array}$$

Results from excel: $Y_S = 1$, $Y_{SX} = 0,09996$, $Y_{SW} = 0,1248$

$Y_{SN} = -0,022$, $Y_{SC} = 0,291$

$Y_{SO} = -0,0801$, $Y_{SP} = 0,60952$

$Y_{SP} = 0,60952\ \frac{Cmol\,P}{Cmol\,Glu} \left| \frac{Cmol\,Glu}{30\,g\,Glu} \right| \frac{25,33\,g\,P}{Cmol\,P} = 0,51\ g\,P/g\,Gluc$

b) $GL \rightarrow PDO + x\ NADH$

$$CH_2O \rightarrow 0{,}61\ CH_{8/3}O_{2/3} + x\ NADH$$

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

$CH_{\frac{8}{3}}O_{2/3} = 4 + \frac{8}{3}(1) - 2\left(\frac{2}{3}\right) = 5{,}333$.

$$\begin{array}{c c} & \begin{array}{ccc} S & P & NADH \end{array} \\ \begin{array}{c} C \\ DoR \\ rate \end{array} & \begin{bmatrix} 1 & 1 & 0 \\ 4 & 5{,}333 & 2 \\ 1 & 0 & 0 \end{bmatrix} \end{array} \begin{bmatrix} Y_s \\ Y_p \\ Y_{NADH} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ -1 \end{bmatrix}$$

results: $x_N = -0{,}67$ (NADH is consumed)

$$\frac{0{,}67\ H}{Cmol\ GL} \left| \frac{6\ Cmol\ GL}{mol\ Glu} \right| \frac{NADH}{2H} = 2\ NADH \text{ consumed (confirms map)}$$

c) $\frac{1}{3}$ ATP/Cmol Gluc consumed (according to metabolic map)

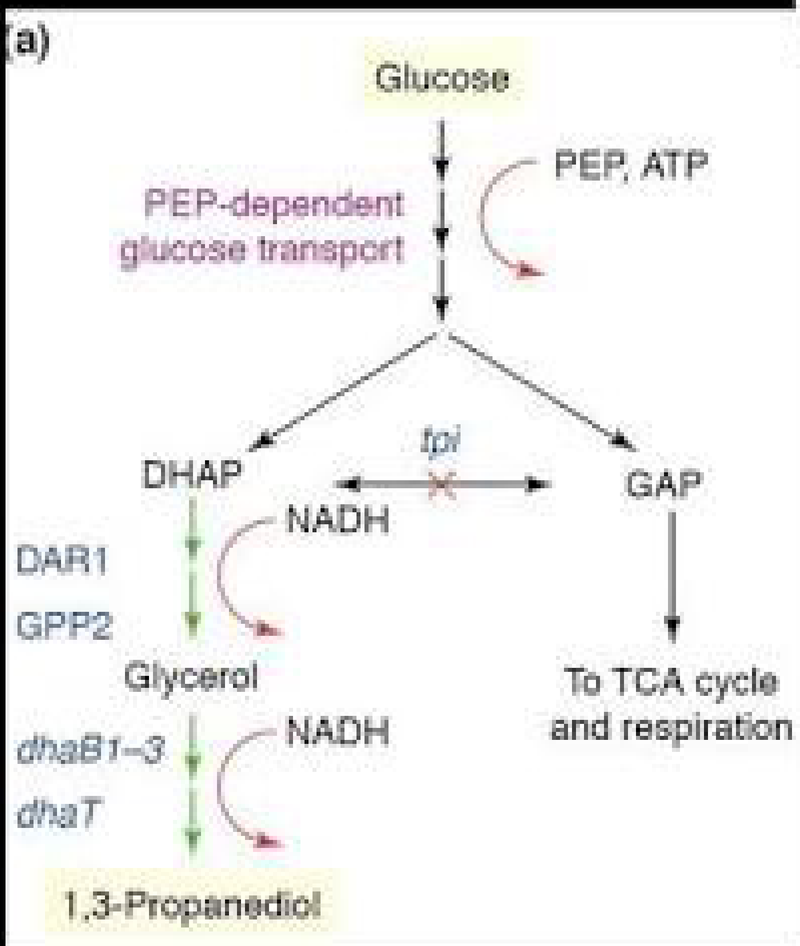
↳ from 1 mol Glucose, 2 ATP are consumed to DHAP (1^{st} 5 steps). Then from DHAP to PDO, only 2 NADH are consumed.

$\therefore \frac{2\ ATP}{6\ Cmol\ GL} = \frac{1}{3}$ ATP/Cmol GL.

d) From DHAP to PDO, O_2 is consumed in the consumption of NADH, i.e. oxidative phosphorylation.

e) Yes. The bacteria in the sorona blocks with its enzymes other paths from DHAP and favours PDO.

Metabolic engineering



- nature of synthesizing of 1,3PD
- *tpi* gene
- *dhaT* and *dhaB*, gene encoding glycerol dehydratase and PDOR
- DAR1, GPP2 encoding phosphate dehydrogenase and glycerol 3-phosphate phosphatase

f) From oxidative phosphorylation:

$$\frac{ATP}{mol\ Gluc} = 10(1,5) + 2(1,5) + 4 = 22\ \frac{ATP}{mol\ Gluc}\left|\frac{mol\ Gluc}{6\ mol\ O_2}\right.$$

$$= 3\tfrac{2}{3}\ \frac{ATP}{mol\ O_2}$$

* We use O_2 to determine the ATP because all the O_2 is used in oxidative phosphorylation where a fraction Glucose is used for PDO and the rest towards biomass.

Therefore:

$$Y_{XO} = \frac{Y_{SO}}{Y_{SX}} = \frac{0{,}0806 \text{ mol } O_2}{0{,}0996 \text{ cmol } X} = 0{,}806 \frac{\text{mol } O_2}{\text{mol } X}$$

$$\Rightarrow \text{Energy consumption} = \frac{0{,}806 \text{ mol } O_2}{\text{cmol } X} \left| \frac{3\frac{2}{3} \text{ ATP}}{\text{mol } O_2} \right.$$

$$= 2{,}955 \text{ ATP} / \text{cmol } X$$

g) → Production of more DHAP

→ Production of Biomass

→ Cell maintenance