Tut 3

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0.0.1 Tutorial 3

The production of 1,3 propanediol (PDO) by the company DuPont is one of the success stories of bioproduction of polymer intermediates on a bulk scale. Read on the polymer SORONA for some background on the process and final product.

PDO is a natural metabolic product when *Klebsiella pneumonica* grows on glycerol as substrate. DuPont opted for glucose as feedstock and engineered *Escherichia coli* to aerobically convert glucose into PDO.

Write out the overall stoichiometry of the reaction using glucose, ammonia and oxygen as feed. Assume that apart from PDO and biomass, no by-products are formed except water and CO_2 . It is further given that biomass can be described by $CH_{1.91}O_{0.48}N_{0.22}$. The following yields are specified:

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Y_{SX} = 0.0822 \text{ g/g}

Y_{SO} = 0.00267 \text{ mol } O_2/\text{g [reagent]}
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- a) Determine the mass based yield of PDO on glucose(YSP). [0.51~g/g]
- b) PDO synthesis is a two step reaction from Dihydroxyacetone Phosphate (DHAP) in glycolysis. In order to calculate the amount of **NADH** required/generated in the pathway from glucose to PDO, we can consider the following reaction within the cell:

$$Gluc \rightarrow PDO + xNADH$$

Determine the NADH amount with a DOR balance and confirm your answer by googling the metabolic pathway map.

- c) What is the ATP requirements in the pathway from glucose to PDO?
- d) Why is oxygen used in the overall stoichiometry?
- e) Will all the DHAP that form proceed to produce PDO?
- f) Determine the moles of ATP formed in oxidative phosphorylation. Express the answer using a cmol of boimass as basis. Assume a $(P/O)_{NADH}$ and $(P/O)_{FADH}$ of 1.5. [2.9 $\frac{mol\ ATP}{cmol\ X}$]
- g) What is the ATP in (f) used for. Identify 3 separate targets.

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