IB01x - 3.1 - The process reaction

Welcome again. As you have understood, during this course we focus on a case for making propanediol using microorganisms. Let us now have a look at how this production will look like.

Propanediol is a molecule which has the composition of $C_3H_8O_2$. You would like to use microorganisms to make PDO from sustainable substrate, for example glucose.

For understanding the production process of any biotech product it is useful to write down a theoretical product reaction, which is a reaction for making 1 mol product. When writing down this product reaction you want to find the best possible stoichiometry where the lowest amount of substrate is consumed. Therefore this reaction is written in absence of oxygen. O_2 consumption relates to substrate oxidation and is therefore unwanted in the theoretical product reaction because it increases the amount of substrate consumed to create one mol of PDO. However other compounds, like H^+, H_2O, CO_2, are always involved in the theoretical product reaction. We can calculate this reaction by using propanediol as an example. The theoretical product reaction starts with 1 mol propanediol on the right side. Then you have to make a choice for a feedstock which will supply the carbon atoms for the product. In this case, let us assume this is glucose. From this we can complete the reaction by adding carbon dioxide, water and protons. The stoichiometric coefficients a, b, c and d are unknown values for our theoretical product reaction at this point. Note that in this reactions all the consumed compounds such as glucose have a negative sign, in this case only glucose, and therefore a will be negative, and the produced compounds do have positive sign, therefore b, c, and d are positive.

But we know that all the elements and charge going into the reaction need to come out. Therefore finding a,b,c and d requires to write down the element and charge conservation relations. Let us take carbon conservation as a example. The glucose carbon equals 6a, the PDO carbon equals 3*1 and the CO_2 carbon equals 1b, al which add to 0 We now have 4 linear equations with 4 unknowns which means that we can solve this to find the values for a, b, c and d.

This calculation leads to the theoretical PDO reaction. From this reaction we learn 2 important things: First of all we now know the absolute minimum glucose requirement, which is 0.67 mol glucose/mol PDO. This is an important value to judge variable costs of your fermentation process. Secondly you can see whether the product could supply energy for the organism. From glucose this is indeed the case, because the Gibbs energy of the reaction tells you that 1 mol PDO produces 110 kJ Gibbs energy. This thermodynamic calculation shows that the energy is there but we cannot decide whether organisms can convert this energy into biological useful energy such as ATP.

Following this energy consideration it is now important to distinguish 2 product classes: energy producing and energy consuming products. The first class of products generates energy in the form of biological energy. If this is the case, then you have an anaerobic process which means that no oxygen is needed for the organism to grow and to produce.

The theoretical product reaction of PDO, which we just derived, shows that in principle it is an energy producing product reaction. Thus it would be possible to perform this production anaerobically. Unfortunately research has not succeeded in this yet. The second product class consumes energy. Therefore the microorganism needs a source of biological energy which comes most efficiently from the oxidation of substrate. For this product class the fermentation process needs to be done aerobically and we need to supply O2 as nutrient. Most microbial production processes are at this moment aerobic.

Besides the theoretical product reaction there is another reaction which is central in the design of our PDO process. This is called the process reaction. In this process reaction you quantify the uptake and secretion rates of all important nutrients but also all the products and by-products that are being made. As shown in the figure this involves many q-rates not only for growth, substrate and PDO but also oxygen, carbon dioxide, ammonium, water, protons and even heat.

By combining all these q-rates together into one reaction you can get the process reaction, which is the basis for process design. It is convenient to normalize this process reaction to the production of 1mol PDO.

This process reaction has important properties. Its stoichiometric coefficients are qi/qp ratio's, either positive in mol i produced per mol PDO produced or negative in mol i consumed per mol PDO produced. The coefficients represent the process stoichiometry, which depends on the q-rates and which are not constant. In absence of growth or O2 consumption the process reaction reduces to the theoretical product reaction. The process reaction is the basis of process design.

I showed you that you can calculate the theoretical product reaction from only knowing the product and substrate composition. The remaining obvious question is how to obtain the process reaction. Here we need the values of the q-rates for which we will need the black box kinetic model, to be discussed in the next unit.

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