IB01x - 4.4 - Gas transport

Welcome in this unit about gas transport! As we observe from the process reaction, in most fermentation processes oxygen is required and CO_2 is produced. These are important gasses. On large scale, the supply of oxygen and the removal of CO_2 may very well limit the overall reaction rate.

You can estimate the relative transfer requirements based on simple stoichiometry. Taking glucose catabolism as an example, you can calculate that one gram of oxygen is required for every gram of glucose consumed. A problem with oxygen is that the solubility in water is very low, with about 7 mg/l, making it difficult to transfer the oxygen from the gas bubbles to the liquid.

Solubility is dependent on the partial pressure of the oxygen in the gas phase, which is determined by the overall pressure and the composition of the gas phase. According to the film-theory, the bubbles are surrounded by a thin liquid film interface, through which the oxygen is transferred first to the liquid phase and then towards the cells. At the interface, the concentration of oxygen in the liquid is in equilibrium with the concentration of oxygen in the gas phase. We call this the equilibrium concentration, or solubility,C_o^*.

A good question now is: how to maximize solubility? For this, we look at Henry's gas law, which correlates the solubility of oxygen to its partial pressure. The partial pressure can be raised by changing the gas composition and increasing the total pressure. The second option is to increase the value of the Henry constant, by reducing temperature, minimizing the amount of salt, or using a solvent that is added to the broth. An opposite effect is that the oxygen content in the outlet gas can be much lower than the 21% of the inlet air. Such oxygen depletion will lower the C_o^*.

You will recognize this picture from what Sef discussed in week 2. The transfer rate $T_{N,o}$can be calculated using the oxygen gas phase balance. It is determined by 4 different terms:

- The C_o^*, the solubility
- C_o, which is the actual concentration of oxygen in the liquid
- K_L, which is the resistance coefficient
- and A is the total surface area of the bubbles present in the fermentation broth

The difference between $C_o^*$and C_o is called the driving force for oxygen transfer. Further, usually we deal with the specific bubble area, small a, which is capital A, divided by the total liquid volume. The product of K_L and small a determines the well-known volumetric mass transfer coefficient K_La.

When increasing the oxygen transfer, you cannot influence K K_L very much because it is only weakly dependent on the bubble size and medium composition. Because the minimum oxygen concentration which organisms can handle in a fermentation is usually quite fixed, it is also hard to vary C_o. This leaves two parameters that can be changed. First is the solubility C_o^*as explained before. The other option is to increase the bubble surface area; you can do this by increasing the amount of energy that you put in your bioreactor either via the gas or via the impeller plus the gas. This affects the number of bubbles, the size of bubbles, and the velocity at which bubbles rise. The maximum oxygen transfer rate is achieved at the maximum driving force, when the actual oxygen concentration in the liquid is zero.

For dissolved CO_2a similar reasoning can be applied, with two important differences. The first is that CO2 moves in the opposite direction of oxygen. It is carried away from the cells that produce it in the metabolic network, quantified by the process reaction. CO_2 is transferred all the way to the bubbles, after which it leaves the reactor. The second is that the solubility of $CO_2$is very high, at least 30 or 40 times higher than for oxygen. It can easily be demonstrated that the actual concentration of CO_2 in the liquid, C_c, is usually almost the same as the solubility of CO_2. This is challenging, because it means that you have to deal with phenomena like the inhibition of CO_2, reducing the performance of the cells and the rate of the reaction.

If we apply these concepts to bioreactors, stirred tanks or bubble columns for example, then you have to deal with these four quantities: the resistance coefficient, the total bubble area capital A, or small a if expressed per m^3 broth, the solubility, and the actual oxygen concentration. In this diagram you can see that these four terms are determined by multiple bioreactor characteristics, which are mutually dependent.

One important consideration is that there can be roughly two types of bubbles. Bigger bubbles that are quite mobile and smaller bubbles that are rigid. When rigid bubbles meet each other in the fermentation, they usually bounce like billiard balls and continue their way. Larger bubbles, on the other hand, often merge when they collide, we call this coalescence, and later on break up again elsewhere in the reactor. This results in two different bubble dynamics: coalescing and non-coalescing, and these have a prominent impact on the mass transfer rate. When coalescing, larger bubbles are formed with less surface area per amount of volume, in this example from 100% down to 79%.

Now let's see how mass transfer coefficients can be calculated and what values do they take.

An important concept in gas transfer is the superficial gas velocity v_{gs}, which is defined as the actual gas flow rate in m^3/s divided by the cross-sectional area of the reactor. It is an artificial term that, however, correlates well with experimentally determined mass transfer coefficients. In a bubble column, for example, you can see how this works out, for two reported correlations.

For a stirred tank, apart from the superficial gas velocity, also the impeller power input per volume is required. The parameters in the correlation are different for coalescing and non-coalescing liquids, and in general it can be said that non-coalescent liquids give at least a twofold higher K_{La}.

A final remark is devoted to scale-up and operation in tall bioreactors. There will be a vertical gradient in the solubility: the pressure decreases with about 0.1 bar per meter height, and the gas phase is depleted with about 0.55% oxygen per meter. For a 25 meter tall bioreactor, the solubility can decrease from 0.919 mol/m^3 at the bottom, to a poor 0.091 mol/m^3 at the top. Apart from this, there is an opposite gradient in the superficial gas velocity and K_{La}, due to expansion of the bubbles. This can be easily quantified.

We will now apply this information to the PDO case at the optimal μ of 0.0245 h-1, in which we use the bubble column in a continuous mode of operation. According to the literature, the most efficient mass transfer rate (kWh/mol O_2 transferred) in the bubble column, is achieved with a height H of 25 m. In this case, the average broth pressure is 2.25 bar. Assuming a cylindrical shape, the vessel diameter is then 10.7 meter, and the aspect ratio, H/D, is 2.34. The required oxygen transfer rate is 193 mol/tonne h.

With an average gas flow rate of 11.1 m^3/s, to be calculated from the molar gas flow rate via the gas law, we can now quantify the superficial gas velocity, the oxygen solubility, the K_{La}, and the maximum oxygen transfer rate, all averaged over the height. The CO_2concentration can be calculated in a similar way, which I leave to you. The result of such calculation will be around 7mol/m^3. It is noted that in this example the required oxygen transfer rate cannot be met by the gas flow and pressure settings, so the bioreactor is under-designed. I invite you to think about suggestions how to overcome this issue.

To finalize this unit: the mass transfer rate is dependent on different, interrelated aspects. You have several choices for the design of your large scale fermentation.

The most important ones are:

- Gas phase composition and pressure
- Power input: air, impeller + air
- Interface mobility: coalescence behavior and bubble size
- Reactor type: bubble column, stirred tank reactor, etc.
- Reactor geometry and scale.

Here it is noted that in large bioreactors there will be vertical gradients of the transfer rates and the oxygen and CO_2 concentrations, causing scale-up issues such as oxygen starvation and CO_2inhibition.

Finally, gas/liquid flow patterns, mixing and gas holdup also play an important role but we will explain that in more detail in the next units.