

### IB01x - 3.6 - PDO continuous process design

Last unit we have established that our PDO producing organism has a lowest glucose/PDO ratio at  $\mu = 0.0245 \text{ h}^{-1}$ .

This is the logical condition at which to do the process design, because, knowing that substrate cost is the major cost factor for bulk chemicals, it leads to the lowest cost per mol PDO. We will design a continuous process.

Information needed for the design consists of information about the organism and about the process. Let us assume that a PDO producing organism is characterized by the PDO process reaction shown. This process reaction applies at  $\mu = 0.0245 \text{ h}^{-1}$ . The biomass coefficient of 1.090 equals  $\mu/q_p$ , leading to  $q_p = 0.02248$ .

The value for  $q_s$  follows from the glucose coefficient of 1.295 mol glucose / mol PDO and  $q_p$ , leading to  $q_s = 0.02911$ .

In a similar way all other  $q$ -values at  $\mu = 0.0245 \text{ h}^{-1}$  can be found from the process reaction. Furthermore it is known that the  $q_s$ -value requires a glucose concentration  $c_s = 85 \mu\text{mol glucose / kg broth}$ .

Note that we have replaced the N-source  $\text{NH}_4^+$ , present in the feed medium as e.g.  $(\text{NH}_4)_2\text{SO}_4$ , by  $\text{NH}_3$ , which is supplied as a sparged gas, together with the sparged air.

You should discuss why the choice of gaseous  $\text{NH}_3$  is advantageous compared to  $(\text{NH}_4)_2\text{SO}_4$ . The most important piece of information about the process is the production rate  $R_p$ , which is 165000 mol PDO/h, equivalent to 105 ton PDO/year when produced continuously, assuming 8000 hours per year.

We use the cheapest fermenter, which is a bubble column of 25 m high.

This allows  $\text{O}_2$  transport such that the mole fraction of  $\text{O}_2$  in the off-gas reaches 0.0725 mol  $\text{O}_2$ /mol gas, meaning that about 2/3 of the sparged oxygen is transferred. Furthermore it is assumed that the absolute pressure is 1 bar, that the temperature is 35 °C and that water of 35 °C evaporates at a partial pressure of 0.06 bar.

The fermentation feed consists of an aqueous glucose solution of 3 mol/kg and the N-source is  $\text{NH}_3$  sparged as gas.

The first action in design is to make a process scheme, to visualize all available information. The scheme shows gas in and outputs,  $F_{N,in}$  and  $F_{N,out}$  in mol/h, mass in and outputs for liquids,  $F_{m,in}$  and  $F_{m,out}$  in kg/h.

Also composition information for liquid (in mol/kg) and gas flows (in mol fraction) is shown. Furthermore, molecule traffic between gas and liquid is shown, e.g.  $\text{NH}_3$  and  $\text{O}_2$  from the gas to the liquid and water and  $\text{CO}_2$  from the liquid to the gas, and finally the heat removal is shown. The first step in design is to calculate all gas and liquid in and outputs, their

compositions and the heat output by combining the available information of the the process reaction stoichiometry with compound balances.

We start with the gas flows. We can set up the total gas phase balance, which states that the rate of gas molecules from sparged air plus transferred CO<sub>2</sub>, plus evaporated H<sub>2</sub>O must be equal to the rate of gas molecules present in the off-gas and the molecules of consumed O<sub>2</sub>. The second balance is the O<sub>2</sub>-balance in the gas phase, in mol O<sub>2</sub>/h, which speaks for itself. Note that consumed O<sub>2</sub> and produced CO<sub>2</sub> are calculated using the production rate of PDO, 165000 mol PDO/h, and the known process reaction stoichiometry coefficients for O<sub>2</sub> and CO<sub>2</sub>. Solving these balances gives the gas in and outflows  $F_{N,in}$  and  $F_{N,out}$  in mol gas / h.

Note that  $F_{N,out} > F_{N,in}$ , why is this? Knowing the outflow of gas, which carries out all produced CO<sub>2</sub> we can calculate the mol fraction of CO<sub>2</sub> in the off-gas using the gas phase CO<sub>2</sub>-balance which gives a CO<sub>2</sub> mol fraction in the off-gas of 0.1614.

We can now go to the liquid phase balances to obtain the liquid mass flows in kg/h. The glucose balance, in mol glucose per hour, neglecting the presence of glucose in the outflow, gives us the inflow of glucose feed solution of  $F_{m,in} = 71225$  kg/h. The total broth mass balance in kg/h, taking the mass inputs of glucose feed solution, O<sub>2</sub>, NH<sub>3</sub> and mass losses due to CO<sub>2</sub> and water, and broth outflow, leads to a mass outflow of  $F_{m,out} = 54920$  kg/h. Note that the mass outflow is much lower than the feed flow. We can now check the neglected glucose loss in the outflow. This is only 4.7 mol/h, which is negligibly small compared to a feed of 213675 mol glucose/h.

The biomass and PDO concentrations in the broth outflow follow from the biomass and PDO balances, which you should do yourself. The correct values are  $c_x = 3.275$  mol biomass / kg broth, and  $c_p = 3.00$  mol PDO/kg broth. We can calculate the required broth mass  $M$  in the fermenter because we know  $R_p$  and  $q_p$ , leading to the required biomass amount  $N_x$ .

Using  $c_x$ , one obtains the required broth mass. The correct values are  $M = 2250$  tonnes broth and  $N_x = 7.34$  million moles of biomass.

We can calculate the heat which must be removed by looking at the heat balance.

The temperature in the fermenter should be constant so the accumulation of heat should be zero.

We assume that the sparged air has a temperature equal to the fermentor temperature, because the hot compressed air has been cooled before sparging. The produced heat follows then from the heat produced per mol PDO (shown in the process reaction) and the PDO production of 165000 mol PDO/h.

The evaporated water removes heat because from thermodynamic tables we see that evaporation of 1 mol H<sub>2</sub>O requires 43 kJ of heat.

Note that water evaporation removes about 5% of the produced heat. The heat that needs to be removed by fermenter cooling follows from solving this balance.

Finally we calculate the  $\text{NH}_3$  balance in the broth which states that the consumed  $\text{NH}_3$ , calculated from the process reaction and  $R_p = 165000 \text{ mol PDO per hour}$ , equals the sparged  $\text{NH}_3$ .

This leads to  $35970 \text{ mol NH}_3/\text{h}$  to be sparged.

Note that we have assumed that there is no  $\text{NH}_3$  present in the broth outflow.

What would you do when it is found that the microorganism requires the presence of  $0.2 \text{ mol NH}_4^+/\text{kg broth}$ ?

We can now summarize the first stage of design calculations in the completed process scheme. This scheme shows all gas and liquid inputs and outputs and their composition.

To achieve these gas and liquid flows we need to design transport processes in the bubble column, which will be discussed in week 4 by Henk Noorman.

See you in the next unit!