IB01x - 3.5 - Black box models: The PDO process reaction as function of µ

Previously we discussed the estimation of the PDO aerobic black box model and its parameters.

Such a parameterized black box model gives us the values of cs, qs and qp for different values of µ.

However, beside µ, qs and qp, there are many other q-rates which are all relevant in process design. For example, to quantify the heat removal in the fermenter we need q-heat, for oxygen supply we need qO2, for pH-control we need qH+, etcetera. The crucial understanding is that you only have to apply conservation principles of elements, charge and energy, to obtain all the other q-values from from qs, µ and qp, which are available from the aerobic PDO black box model.

Let us take the Herbert-Pirt relation of the PDO black box model, which tells us that the cell needs 0.25 mol glucose to make 1 mol biomass. This allows us to construct the biomass reaction where 1 mol X is produced from 0.25 glucose and where the other reactants are N-source NH4+, O2, CO2, H2O and H+, indicated by stoichiometric coefficients aN, aO, aC, aw and aH+ .

In a similar way we can formulate the product reaction where according to the Herbert-Pirt relation of the PDO black box model 0.80 mol glucose is needed to make 1 mol PDO.

The other reactants are O2, CO2 H2O and H+, with stoichiometric coefficients bO, bc, bw and bH+. The maintenance reaction is the aerobic combustion of 1 mol glucose.

Finally note that the biomass reaction has a rate µ, the product reaction has rate qp and the maintenance reaction has a rate -ms, which follows from the Herbert-Pirt relation to be 0.005 mol glucose per hour per mol biomass present in the vessel. The unknown stoichiometric coefficients ai and bi in the black box biomass and PDO reaction can be calculated from conservation principles.

The unknown stoichiometric coefficients ai in the black box biomass reaction can be found by setting up the conservation relations. In the biomass reaction there are 4 elements C, H, O, N and charge. This means that there are 5 conservation relations which are exactly needed to calculate the 5 unknown stoichiometric coefficients aN, aO, aC, aw and aH+ Let us do the carbon conservation. In the biomass reaction consumed glucose carbon equals -0.25 multiplied with 6 carbons per glucose. The consumed carbon is found back in biomass, plus 1 multiplied by +1, and in CO2 which is aC multiplied by +1.

In a similar way we can formulate the other element and charge conservation relations. Solving these 5 relations gives the 5 unknown stoichiometric coefficients of the black box biomass reaction.

We can do exactly the same for the coefficients bi of the black box product reaction. In this reaction we do not have the element nitrogen, because PDO doesn't contain N, so we have 4 conservation relations: for C,H, O and charge, leading to 4 equations and 4 unknowns, which can be solved.

These conservation calculations give the complete stoichiometry for:

- The black box biomass reaction, which runs at rate μ
- The black box PDO reaction which runs at rate qp
- The maintenance reaction which runs at rate 0.005

Knowing the stoichiometry we can use the first law of thermodynamics (energy conservation) to calculate the produced heat in each reaction.

From these black box model reactions we can formulate the total set of Herbert- Pirt relations by multiplication and addition. Let's consider O2.

For biomass formation at rate μ, the biomass specific O2-consumption rate equals $-0.45 * \mu$, because 0.45 mol O2 is consumed to produce 1 mol biomass.

In addition, there is O2 consumption for PDO production at a biomass specific rate of -0.80* qp and O2 is consumed for maintenance at a rate 6 times the glucose maintenance rate of 0.005. This leads to the Herbert-Pirt distribution relation for qO2 where total consumed O2 is used for growth, product and maintenance. Using the black box model reactions in a similar way, you should now calculate the Herbert pirt relation for qCO2, qNH4+, qH+ qw and qQ and give the units of the parameters in all the Herbert-Pirt relations.

From the completed BB model we can now calculate the process reaction, where the stoichiometric coefficients are the qi/qp ratios as shown.

As example we calculate the economically most important ratio, mol glucose consumed for 1 mol PDO, which is qs/qp. Using the qp/μ function and the Herbert Pirt relation for substrate it is easy to obtain the substrate coefficient in the process reaction, which is the ratio qs over qp. It is important to note that this ratio, which gives mol glucose consumed to produce 1 mol PDO, is only dependent on μ. This should not be surprising, because our black box model has only 1 free variable.

This ratio has a minimum, at μopt = 0.0245 h-1, of 1.295 mol glucose per mol PDO.

This value is higher than the value of 0.80 in the Herbert Pirt relation, because glucose is also used for growth and maintenance. It is also higher than the value of 0.666 in the theoretical PDO reaction, because we consume O2.

The other stoichiometric ratios of the process reaction also depend only on μ. These μ-functions are obtained by combining the relevant Herbert-Pirt relation with the qp(μ) function.

Please calculate yourself the μ-function for all remaining coefficients of the process reaction, make graphical plots of each coefficient against μ and calculate the μ-value where each coefficient is minimal.

Also compare each coefficient with the qp coefficient in the Herbert-Pirt relation and with the stoichiometric coefficient of the theoretical PDO reaction.

We can now summarize our complete black box PDO model. It consists of a hyperbolic substrate uptake relation, a qp(μ) relation and 7 Herbert Pirt relations. This model has only one free variable, μ.

When you choose a value for μ, all other q-values and cs are known.

The coefficients of the process reaction depend only on μ and are easily calculated from the 7 Herbert-Pirt relations and the qp(μ) function. The black box model shows that the consumed glucose per mol PDO is minimal at μopt = 0.0245 h-1.

It is economically logical to design the PDO process at this μ-value, which we will do later this week.

See you in the next unit!