Elemental Balance -- Yeast fermentation with ethanol production -- Given Y_x and RQ, find Y_p

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$$a\ C_6H_{12}O_6 + b\ O_2 + c\ NH_3 \longrightarrow C_6H_{10}O_3N + d\ H_2O + e\ CO_2 + f\ C_2H_6O$$

(glucose) (yeast) (ethanol)

Molecular Weight

$MW_{glucose} := 180$ $MW_{yeast} := 144$ $MW_{ethanol} := 46$

Elemental Balance Given

C: $6\cdot a = 6 + e + 2\cdot f$

O: $6\cdot a + 2\cdot b = 3 + d + 2\cdot e + f$

N: $c = 1$

H: $12\cdot a + 3\cdot c = 10 + 2\cdot d + 6\cdot f$

Note: "e" means exponential in Mathcad. "ε" works in Mathcad v5, but is strictly treated as an antisymmetric tensor function and does not work in Mathcad v7. Here we add a period (which is invisible) to fool Mathcad.

Measurements: $RQ = \frac{e}{b}$ $\frac{MW_{yeast}}{a\cdot MW_{glucose}} = Y_x$

As far as setting up the equations are concerned, the problem is considered solved at this point. Now, let the computer find the analytical solution symbolically (|Math|SmartMath|) or you can do it manually.

$$Find(a,b,c,d,e,f) \rightarrow \begin{bmatrix} \frac{4}{(5\cdot Y_x)} \\ \frac{-1}{10}\cdot\frac{(55\cdot Y_x - 48)}{[Y_x\cdot(-2+3\cdot RQ)]} \\ 1 \\ \frac{1}{20}\cdot\frac{(-220\cdot Y_x + 165\cdot RQ\cdot Y_x + 96)}{[Y_x\cdot(-2+3\cdot RQ)]} \\ \frac{-1}{10}\cdot RQ\cdot\frac{(55\cdot Y_x - 48)}{[Y_x\cdot(-2+3\cdot RQ)]} \\ \frac{-1}{20}\cdot\frac{(-120\cdot Y_x + 125\cdot RQ\cdot Y_x + 96 - 96\cdot RQ)}{[Y_x\cdot(-2+3\cdot RQ)]} \end{bmatrix}$$

Alternative Approach with Linear Algebraic Equations. Express the six algebraic equations in the standard linear form: A·x=B, where x is a vector of stoichiometric coefficients. The solution is $x=A^{-1}\cdot B$.

$$A = \begin{bmatrix} 6 & 0 & 0 & 0 & -1 & -2 \\ 6 & 2 & 0 & -1 & -2 & -1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 12 & 0 & 3 & -2 & 0 & -6 \\ 0 & RQ & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad x = \begin{bmatrix} a \\ b \\ c \\ d \\ e \\ f \end{bmatrix} \quad B = \begin{bmatrix} 6 \\ 3 \\ 1 \\ 10 \\ 0 \\ \dfrac{MW_{yeast}}{Y_x \cdot MW_{glucose}} \end{bmatrix}$$

$$\begin{bmatrix} 6 & 0 & 0 & 0 & -1 & -2 \\ 6 & 2 & 0 & -1 & -2 & -1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 12 & 0 & 3 & -2 & 0 & -6 \\ 0 & RQ & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}^{-1} \cdot \begin{bmatrix} 6 \\ 3 \\ 1 \\ 10 \\ 0 \\ \dfrac{MW_{yeast}}{Y_x \cdot MW_{glucose}} \end{bmatrix} \rightarrow \frac{1}{(8-12\cdot RQ)} \cdot \begin{bmatrix} \dfrac{-16}{5} \cdot \dfrac{(-2+3\cdot RQ)}{Y_x} \\ \dfrac{2}{5} \cdot \dfrac{(55\cdot Y_x - 48)}{Y_x} \\ 8 - 12\cdot RQ \\ \dfrac{-1}{5} \cdot \dfrac{(-220\cdot Y_x + 165\cdot RQ\cdot Y_x + 96)}{Y_x} \\ \dfrac{2}{5}\cdot RQ \cdot \dfrac{(55\cdot Y_x - 48)}{Y_x} \\ \dfrac{1}{5} \cdot \dfrac{(-120\cdot Y_x + 125\cdot RQ\cdot Y_x + 96 - 96\cdot RQ)}{Y_x} \end{bmatrix}$$

Of course, both approaches give the same solution. Each coefficient is now described in terms of RQ and Y_x. For example the ethanol coefficient is the last item in the above solution vector:

$$f(RQ, Y_x) := \frac{1}{20} \cdot \frac{96 - 120\cdot Y_x + 125\cdot RQ\cdot Y_x - 96\cdot RQ}{(2 - 3\cdot RQ)\cdot Y_x}$$

Example:

$Y_x := 0.5$

$f(1, Y_x) = -0.25$ ... A negative coefficient means consumption of ethanol.

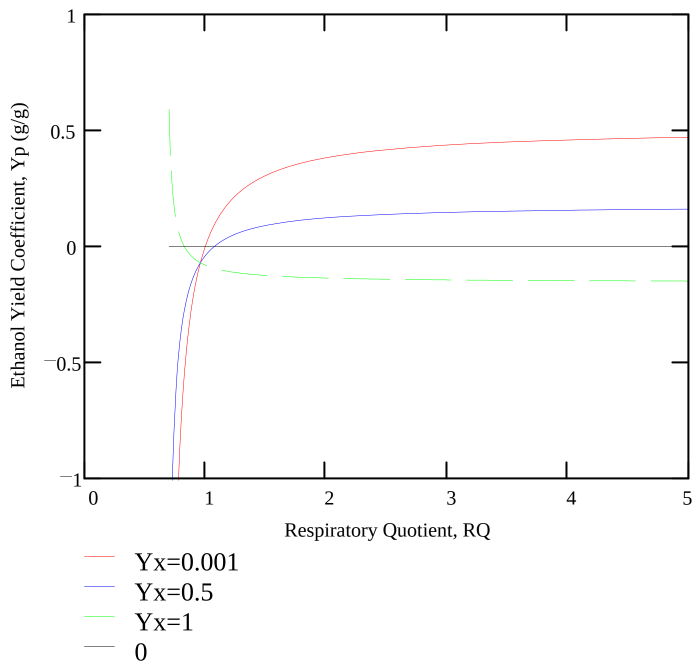
$f(1.07, Y_x) = -0.013$ ... ethanol is consumed for RQ<1.08.

$f(1.08, Y_x) = 0.015$ ... ethanol is produced for RQ>1.08.

Ethanol Yield (g ethanol produced per g glucose consumed): $Y_p=(f\cdot MW_{ethanol})/(a\cdot MW_{glucose})$

$$Y_p(RQ, Y_x) := \frac{f(RQ, Y_x)\cdot MW_{ethanol}}{\dfrac{4}{5\cdot Y_x}\cdot MW_{glucose}}$$

$RQ := 0.7, 0.71 .. 5$



As RQ increases (i.e., more CO_2 evolution per O_2 consumption), more ethanol is produced; thus, CO_2 production drags ethanol production along with it. As Y_x increases (i.e., more glucose is directed more toward biomass), less ethanol is produced. Furthermore, even for high values of RQ and very little biomass formation, one achieves only 0.5g of ethanol per g of glucose. (If someone approaches you and claims that he can achieve 0.6g of ethanol per g glucose, you should suspect his claim.)