University of Jyväskylä
Jukka Konttinen

SOLVING THE CALCULATION EXERCISE USING BALANCE SHEET SOFTWARE (EXCEL or corresponding)

- mark the inputs in their separate fields
- solve the material balance according to the way shown in the examples
- check the material balance (sum) total mass flow in (g/s) = total mass flow out (g/s)
- solve the elemental balance the way shown in the examples
- solving the energy balance: use this document as helping material

PLEASE NOTE THAT c_p IS NOT CONSTANT BUT IT IS DESCRIBED WITH A POLYNOMIAL FUNCTION, DEPENDENT ON TEMPERATURE (See **guide A** below)

- thus this cannot be calculated assuming as constant in integration ($T_{ref} \rightarrow T_{in}$ or $T_{ref} \rightarrow T_{out}$)

- determine the heat of reaction separately and add it into the energy balance (See **guide B** below)
- T_{out} is now a temperature, that has to be determined by iteration (See **guide C** below)

The idea of the exercise is to show the benefit of balance sheet programming, which is that when the balances have been correctly implemented, sensitivity analyses are possible – by changing the input values, the effect of those on the results can be seen.

b)- the idea of the item b) in the exercise is to show, how energy balance and chemical equilibrium can be solved simultaneously and how the affect each other.

Guide A: DETERMINATION OF ENERGY CONTENTS (ENTHALPIES) OF THE COMPONENTS IN ENERGY BALANCE

Otherwise the way to solve the calculation exercise is the same as those shown in the model examples, but the the cp-values are not constant. Instead they have been determined by using 4 constants.

When preparing the energy balance component by component, in and out, this can be done the following way:

$f(c_p, T) =$

$$\int_{T}^{T_2} c_p \, dT = \int_{T_1}^{T_2} \left(A + B \cdot 10^{-3} T + C \cdot 10^{5} \frac{1}{T^2} + D \cdot 10^{-6} T^2 \right) dT$$

$$= A(T_2 - T_1) + \frac{B \cdot 10^{-3}}{2}\left(T_2^2 - T_1^2\right) + C \cdot 10^{5}\left(\frac{1}{T_1} - \frac{1}{T_2}\right) + \frac{D \cdot 10^{-6}}{3}\left(T_2^3 - T_1^3\right)$$

, where $T_1 = T_{ref} = 298.15$ K. This expression (J/mol) will have to be multiplied with the molar flowrate of the component (mol/s), so that the entalpy or energy content (J/s) is obtained:

$H_i = n_i * f(c_{pi}, T)$

This term can be coded in Excel by using the following syntax:

```
=(A1*(F10-298.15)+B1*0.5*0.001*(F10^2-298.15^2)+C1*100000*(-1/F10+1/298.15)+D1*0.000001*(F10^3-298.15^3)/3)*D10
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Where the formula reads from the field A1 in the balance sheet the constant A of the component, constant B from field B1 etc. These constants have been given as inputs in the calculational exercise.
From field F10 the temperature in or out of the component is being read.
Field D10 contains the molar flowrate of component (mol/s).

When calculating the inputs, the temperatures of components are given and thus their enthalpies can be calculated with the above given formula. The same goes for calculation of outputs, provided that the output temperature has been given.

The enthalpies produced this way are summarised as one term. For the energy balance, the heat of reaction has to be determined separately.

In the exercises, the common output temperature of the components out will have to be determined. In case the temperature is in the field F10, a “starting value” is given to this temperature. Then the temperature, satisfying the energy balance, can be determined by using the Goal Seek-iteration subroutine (or corresponding) in balance sheet calculation.
Balancing the energy balance means:
Total energy in (J/s) – total energy out (J/s) = 0.

Guide B: HEAT OF REACTION

When the reaction is exothermic (producing energy), the heat of reaction is marked with minus (negative) in connection with the chemical reaction. The energy balance is then coded:

$\sum H_{i,in} + H_R = \sum H_{i,out}$

Where ΔH_R is the energy that is consumed in the reaction, heat of reaction (J/s). It is determined by:

$H_R = n_A * X_A * \Delta H_R * 1000$

where n_A is the molar flowrate of the limiting reactant (mol/s), X_A is the conversion (-) and ΔH_R is the heat of reaction (kJ/mol).

Thus in exothermic reaction the reaction heat brings energy to the process and thus is marked as positive in inputs (despite of the minus).

When the reaction is endothermic (consuming heat), its value is positive in connection with the chemical reaction. The consumption of energy in endothermic reaction is marked the following way:

$\sum H_{i,in} = \sum H_{i,out} + H_R$

In the chemical reactions, where the stoichiometric constants are not the same, for example in the following:

$SO_2(g)+0.5O_2(g) \rightarrow SO_3(g)$

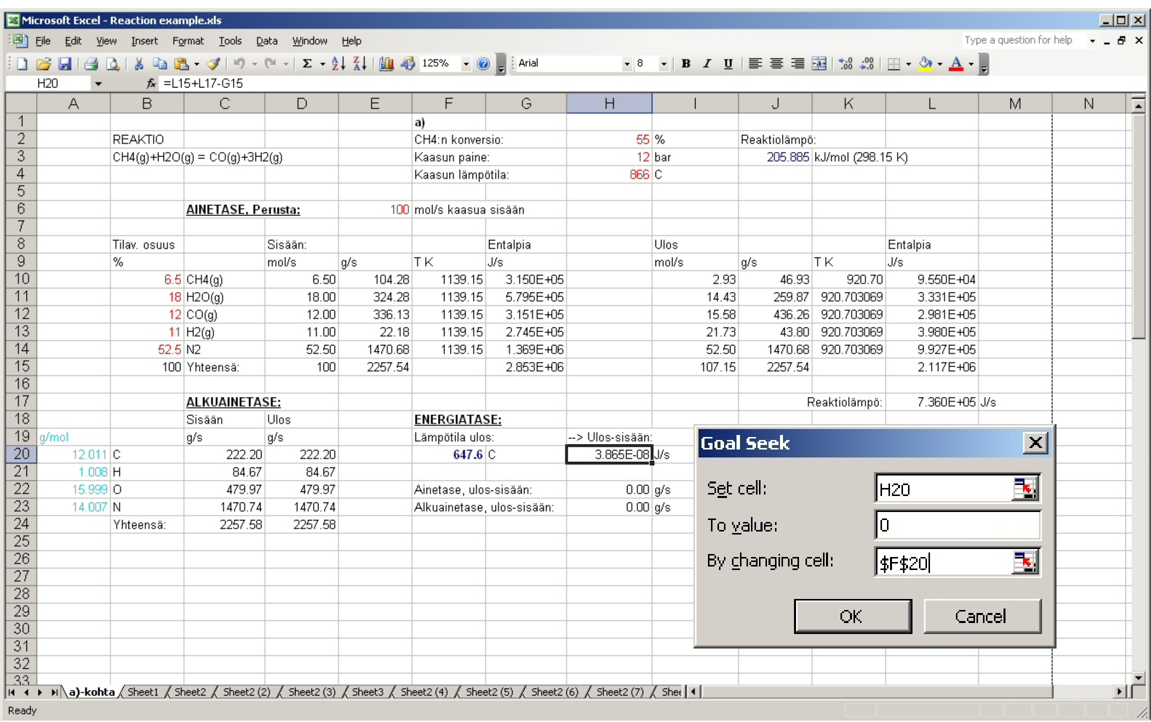
$3H_2(g)+N_2(g) \rightarrow 2NH_3(g)$

$NO(g)+0.5O_2(g) \rightarrow NO_2(g)$

$SO_2(g)+2H_2S(g) \rightarrow 3S + 2H_2O(g)$

For example in the lowest equation, the heat of reaction is given as -145.84 kJ/mol. This per 1 mol of SO_2, BUT in case H_2S would be the limiting reactant, the heat of reaction (per 1 mole of H_2S) is -145.84*0.5 = -145.84/2 = 72.92 kJ/mol (reaction equation can be formatted as 0.5 $SO_2(g)$ + $H_2S(g)$ --> 1.5 S + $H_2O(g)$) The heat of reaction is divided with the stoichiometric constant correspondingly in the other reactions above.

Guide C: HOW TO USE THE GOAL SEEK-SUBROUTINE



Problem b) **SOLVING THE CHEMICAL EQUILIBRIUM**

The equation to be solved in general format is:

$$(n_{C,o}^{\,c} * n_{D,o}^{\,d})/(n_{A,o}^{\,a} * n_{B,o}^{\,b})*(p_{tot}/n_{tot,o})^{(c+d-a-b)} - K_g = 0$$

where $K_g = K_0*\exp(-G/(8.315*T_g))$

Placing the molar flowrates of different species (from material balance "OUT"), the conversion X of the limiting reactant has to be determined so that the above equation (chemical equilibrium) is satisfied. Please note that there is a difference in here from the calculation in a), since in b) the conversion is not given as input, but instead it has to be calculated.

The parameters G ja K_0 are given as inputs and T_g is the mean temperature of the process (in Kelvins) which is the average of temperatures T_i and T_o.

T_i (K) is the same as in a). T_o which is the temperature of the system out (K) must now be solved so that the energy balance is satisfied, the same way as in a). Here it is a question of determining X and T_o simultaneously, so that the chemical equilibrium and energy balances are satisfied.

The determination of chemical equilibrium for different reactions are given in other documents.