Gasification - Gibbs reactor

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1 Thermodynamics

This is a short instruction of main task connected with simulating gasification process based on the Gibbs eactor approach. All necessary thermodynamic data can be found in file thermodynamics-data.xlsx

First step is to create thermodynamic basis of the process.

1. For the given set of coefficients create functions of heat capacity and calculate medium heat capacities for the necessary substances.

$$Cp(T) = a + b * 10^{-3}T + c * 10^{-6}T^2 + d * 10^{-9}T^3$$

2. Based on calculated heat capacities, calculate:

   (a) enthalpy

$$\Delta H(T) = H^0 + \frac{1}{Tx - T0}\int_{298}^{Tx} Cp(T)dT * (T - 298)$$

   (b) entropy

$$\Delta S(T) = \frac{1}{Tx - T0}\int_{298}^{Tx} \frac{Cp(T)}{T}dT$$

   (c) Gibbs free energy

$$\Delta G(T) = \Delta H(T) - T * \Delta S(T)$$

Now it's time to define streams of substrates and products.
We have two substrates:

1. coal - consist of 3 parts: "fixed carbon" + ash + moisture.

2. oxidant - given mixture of gases

Be careful to use as received as a reference state for your calcualtion. Coal is fed to the reactor in the standard temperature, while gas is fed in the temperature given in your task.

2 Gibbs function

The main part of calculation is to define an objective function, which will be minimised and create the system of constraining equation (mass balance). Gibbs function is defined as follows (include only gas products):

$$FG(R2,T) := \sum_{i=1}^{8} n_i * \Delta G_i(T) + \sum_{i=1}^{8} n_i ln(\frac{n_i}{\sum n_i}$$

Assuming that the conservation law can be applied to the mass balance in this case, number of moles of each element in inlet and outlet stream must be equal to each other. Composition of the outlet stream should be defined as a vector, starting with gaseous products and the rest of outlet stream components. Remeber to the define some initial values for these components before the *Given* - *Minimize* block.
the block for this solution shoul be as follows: Given
mass balance CARBON
mass balance HYDROGEN
mass balance OXYGEN
mass balance NITROGEN
mass balance SYLUPHUR

Solution(T):= Minimize(FG, outlet)

Because the final composition strictly depends on temperature, your solution must be a function of temperature (T). To minimize this function use Conjugate gradient method (right click on the Minimize -¿ nonlinear -¿ see which method is checked)

3 Energy balance

To calculate the temperature of the process you have to balance the energies in inlet and outlet streams, which consist of the following parts.
Inlet stream:

- enthalpy of formation of coal (calculated in dry and ash free state)
- standard enthalpies of ash and moisture
- standard and physical enthalpies of oxidant (depend on gas feed temperature)

OUTLET stream Calculating enthalpy of outlet stream is little bit complicated, because the stream of enthalpy of products depends on temperature and amount of products, so you have to create a fuction depending on the outlet stream composition vector. All components of utlet stream should be considered in the temperature if the inside of the reactor.

- enthalpy of ash
- enthalpy of gas products
- enthalpy of char (considered as four sepearate elements)

- enthalpy of tar

In the outlet stream tempreture you should also include heat loss coefficient (Φ). To calculate equilibrium temperature you should create a function:

$$Q(T) = \Delta H_{in} - \Delta H_{out}$$

and find for which temperature it is equal to zero. That is the equlibrium (or operating) temperature.

Example:
Let's define enthalpy of CO_2 in the outlet stream. First assume that the solution to the minimisation block is as follows and that CO_2 is a first element of vector R2 ($CO_2 = R2_1$:

$$Sol(T) = Minimize(FG, R2)$$

Now define variable representing changing temperature: $i := 1; ..8$, $temp_i := 800 + (i-1) * 50$ and then variable that will store the results (outlet composition vector) for each temperature $temp_i$:

$$res_i := F(temp_i)$$

$i - th$ vector res stores number of moles of each of the products in the $i - th$ temperature.
Using this notation strema of entahlpy of carbon dioxide will be formulated as follows;

$$Q(T, i) := (res_i)_1 * (\Delta H^0 + CpCO2(T) * (T - 298))$$

$$Q_i := Q(T_i, i)$$

Total enthalpy will be the sum of enthlapies for all products (solid, liquid, gaseous). At the end you just plot Q_i versus T_i and find 'zero' on the plot -¿ T_eq. The equlibrium composition (final result for the simulation is found as $Solution(T_{eq})$.
Please present your result as follows:

- gas compostion in mole fractions
- total yield of tar (kg/h)
- total yield of char (kg/h)