Adiabatic temperature

The gas stream coming from the reformer unit is fed to a reactor where CO is converted to CO2 and H2 by means of the water gas shift (WGS) reaction:

CO + H2O ↔ CO2 + H2

The inlet gas stream is at 360 °C and 30 bar. The pressure drop across the reactor is negligible and the reactor is adiabatic.

By considering that a conversion of CO equal to 70% is achieved, evaluate the temperature and the composition of the stream leaving the reactor.



**DATA**:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Specie** | **mol/mol [%]** | **(298K)**  **[Cal/mol]** | **a** | **b \* 103** | **c \* 106** | **d \* 109** |
| **H2** | 34.8 | 0 | 6.483 | 2.215 | -3.298 | 1.826 |
| **CO** | 7.5 | -26420 | 7.373 | -3.070 | 6.662 | -3.037 |
| **CO2** | 5.0 | -94050 | 4.728 | 17.54 | -13.38 | 4.097 |
| **CH4** | 0.6 | -17890 | 4.598 | 12.450 | 2.860 | -2.709 |
| **H2O** | 37.9 | -57800 | 7.701 | 0.4595 | 2.521 | -0.859 |
| **N2** | 14.2 | 0 | 7.44 | -3.24 | 6.4 | -2.79 |

**Theory:**

The material balance for the reactor is:

Control volume = reactor

We define a new parameter . We can derive it:

Therefore, the mass balance will be written as follows:

Next step is to choose a basis of calculation. We assign as basis of calculations. In order to find we have to do …

For reaction components, we have this table:

|  |  |  |
| --- | --- | --- |
| In |  | Out |
|  |  |  |
|  |  |  |
|  |  |  |

For each single component, the molar fraction of “i” component will be calculated using this equation:

The energy balance for this system is:

Since we have no external heat exchange, the Q term will be equal to 0.

Assume that all gaseous components are Ideal Gas and for mixture we have Ideal Mixture.

The ideal gas is the simplest model that neglects all interactions between gas molecules.

For real gas, we have two options:

1. Ideal mixture
2. Real mixture

The enthalpy for stream “j” defined as:

The for elementary species in aggregation state is measured @ 298 K. (You can find it on Perry’s Handbook)

For Numerical Solution, please open .xlsx file.