

## CO conversion model

The conversion of CO in CO<sub>2</sub> is done according to the equilibrium reaction (1), equimolar and therefore not influenced by pressure.



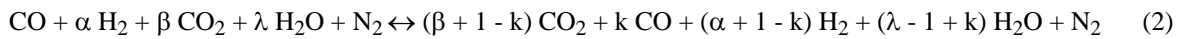
This reaction shows that, at stoichiometry, a mole of H<sub>2</sub>O is required per mole of CO.

Let us consider a gas of composition given figure 1 (in order for the CO conversion reaction to be as complete as possible, it is achieved with an excess of water close to 10%).

component name	molar fraction	mass fraction
H2O	0.4018773	0.3469813
CO	0.364922	0.4898814
H2	0.1344096	0.01298573
CO2	0.02284963	0.04819479
N2	0.07594142	0.1019568

Figure 1: composition of the inlet gas

On entering the CO unit conversion, the gas contains not only reactants but also products (CO<sub>2</sub> and H<sub>2</sub>) and N<sub>2</sub> which is inert. The actual reaction may be written as (2).



We have established a model for this reaction assuming it is in equilibrium, the equilibrium constant being given by the table on the left or by approximate equation (3).

Temperature °C	K
227	134
327	27.6
427	8.95
527	4.11
627	2.20
727	1.37

Between 500 K and 1000 K with an accuracy of about 0.5%, K<sub>p</sub> is given by equation (3), which has the advantage that it can be reversed without any particular problem: it is a second degree equation in 1/T.

$$\ln(K_p) = -3.69088 + \frac{3,710.59}{T} + \frac{292,593}{T^2} \quad (3)$$

Reaction (1) involving a constant number of moles, the equilibrium is independent of pressure and depends only on temperature. According to the law of mass action, we have here:

$$K_p = \frac{[\text{CO}_2][\text{H}_2]}{[\text{CO}][\text{H}_2\text{O}]} = \frac{(1 - k)^2}{(\lambda - 1 + k)k} = \frac{(\beta + 1 - k)(\alpha + 1 - k)}{(\lambda - 1 + k)k} \quad (4)$$

Knowing  $\alpha$ ,  $\beta$ ,  $\lambda$  and T, that is to say K<sub>p</sub>, k is also given by a quadratic equation.

In practice, however, T, K<sub>p</sub> and k are the solution of a system of three equations with three unknowns, unfortunately not linear. The first two are (3) and (4), while the third (5) is the reactor enthalpy balance: heat released by the reaction is used to heat the reactants and products, up to temperature T.

To express this, we must calculate the composition of the reaction products and the adiabatic temperature at the end of reaction.

T<sub>ad</sub> is obtained by writing the reaction energy balance for 1 kmol of fuel.

The enthalpy of products is equal to that of reactants plus heat released during the reaction. Total mass flow is conserved. Heat released is used to heat the product at temperature T<sub>ad</sub>.

$$m h_2(T_{ad}) = m h_1 + Q \eta_{\text{react}}$$

We can possibly introduce an additional term to account for reactor losses: thermal efficiency  $\eta_{th}$ . In these conditions, we no longer speak of end of reaction adiabatic temperature, but rather of end of reaction temperature  $T_{react}$ .

The enthalpy equation is then:  $\dot{m} h_2(T_{react}) = \dot{m} h_1 + Q \eta_{react} \eta_{th}$  (5)

$T_{react}$  can be obtained by inversion of the enthalpy function.

$Q \eta_{react}$  is easily calculated from reaction (1) or (2):

$$Q \eta_{react} = -\Delta H_r = (1 - k) h_{fCO} + (1 - k) h_{fH_2O} - (1 - k) h_{fCO_2}$$

$$Q \eta_{react} = 41,170 (1 - k) \text{ kJ/kmol de CO}$$

component name	molar fraction	mass fraction
H2O	0.08026623	0.06930195
CO	0.04331098	0.05814185
H2	0.4560207	0.04405759
CO2	0.3444607	0.7265418
N2	0.07594142	0.1019568

*Figure 2: Composition of the converted gas*

The search algorithm is a dichotomy for  $k$  ranging from 0.01 to 0.999. Two values of  $T$  are estimated, one based on equations (3) and (4), the other from (5). The algorithm iterates until they are equal.

With a two reactor conversion unit, the final composition of the converted gas is given in Figure 2.