

# Thermodynamics of the Reaction $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$

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## Abstract

The paper presents the values of thermodynamic functions  $\Delta H$ ,  $\Delta G$ ,  $\Delta S$  reactions  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  in the temperature range 298 - 1500 K. In the considered temperature interval, the reaction is exothermic ( $\Delta H < 0$ ) with a negative entropy change ( $\Delta S < 0$ ). Free reaction enthalpy ( $\Delta G$ ) is determined by the ratio of the enthalpy and entropy terms. This means that the reaction is  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  thermodynamically favorable at lower temperatures. Above 1092 K the free reaction enthalpy is positive ( $\Delta G > 0$ ) so the reaction enters thermodynamically unfavorable conditions. At lower reaction temperatures the equilibrium reaction constant  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  is much larger than one ( $K_p \gg 1$ ) which means that the products of the reaction are in excess of the reactants, *i.e.* the reaction is shifted in the direction of building up the products of the reaction. In an equilibrium mixture with a stoichiometric ratio of reactants  $\text{CO} : \text{H}_2\text{O} = 1 : 1$  and at an ambient temperature of 298 K, the degree of conversion of reactants into products is 99.69% and at 1500 K it is 38.08%.

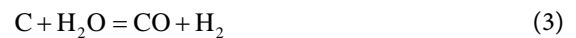
## Keywords

Temperature, Thermodynamic Functions, Equilibrium Constant

## 1. Introduction

Solid fuels are still the main sources of primary energy in the world today and provide about 30% of global production [1]. The increasing need for energy requires the increasing use of various technologies for upgrading solid fuels such as gasification and pyrolysis. The problem of landfilling municipal solid waste is a major environmental problem, especially in developing countries. Therefore, cer-

tain thermal processes such as gasification or pyrolysis of solid fuels or municipal solid waste enable the production of high-quality gaseous fuel. Gaseous fuel is known as synthetic gas and contains valuable compounds such as: CO<sub>2</sub>, CO, H<sub>2</sub>, H<sub>2</sub>O, CH<sub>4</sub> and N<sub>2</sub>. In gasification, the starting fuel is partially oxidized either by air, oxygen, or water vapor. Many authors [2]-[5] theoretically and experimentally investigate the influence of gasification process parameters on the yield of synthetic gas. In this regard, various types of gasifiers have been developed [6] [7]. However, the choice of gasifier depends on the properties of the feedstock and the desired quality of the syngas. In industrial practice, two types of gasifiers are most commonly used: fixed-bed gasifiers and fluidized-bed gasifiers. Recently, mathematical models of solid fuel gasification have been widely used in engineering practice. Various studies have been conducted to model the gasification process in order to predict the performance of solid fuel gasifiers and the composition of the produced syngas [8]-[13]. The composition of the synthetic gas depends on the type of fuel, its composition, the gasification medium such as air, oxygen or water vapor, as well as the process parameters of the gasification process such as temperature and pressure. A number of authors [14] [15] assumed that during the gasification of solid fuel the following reactions take place:



Equilibrium constants ( $K_{p_1}, K_{p_2}, K_{p_3}$ ) chemical reactions (1), (2) and (3) depending on temperature can be determined using the expression [16]:

$$\log K_{p_1} = -18.06361 + \frac{4662.80}{T} - 2.09594 \times 10^{-3} T + 0.38620 \times 10^{-6} T^2 + 3.034338 \log T \quad (4)$$

$$\log K_{p_2} = 8.26730 - \frac{8820.690}{T} - 1.208714 \times 10^{-3} T + 0.153734 \times 10^{-6} T^2 + 2.295483 \log T \quad (5)$$

$$\log K_{p_3} = -28.45778 - \frac{4825.986}{T} - 5.671122 \times 10^{-3} T + 0.8255488 \times 10^{-6} T^2 + 14.515760 \log T \quad (6)$$

of which:

$$K_{p_1} = \frac{P_{\text{CH}_4}}{P_{\text{H}_2}^2}, \text{Pa}^{-1} \text{—equilibrium constant of a chemical reaction (1).}$$

$$K_{p_2} = \frac{P_{\text{CO}^2}}{P_{\text{CO}_2}}, \text{Pa} \text{—equilibrium constant of a chemical reaction (2).}$$

$$K_{p_3} = \frac{P_{\text{CO}} \cdot P_{\text{H}_2}}{P_{\text{H}_2\text{O}}}, \text{Pa} \text{—equilibrium constant of a chemical reaction (3).}$$

$T$ —absolute temperature during the considered chemical reactions, K.

$P_{\text{CH}_4}, P_{\text{H}_2}, P_{\text{CO}}, P_{\text{CO}_2}, P_{\text{H}_2\text{O}}$ —partial pressure of methane, hydrogen, carbon

monoxide, carbon dioxide and water vapor in an equilibrium mixture, Pa.

When calculating the composition of synthetic gas in gasification processes, some authors [17] start from the molecular formula of the solid fuel  $CH_xO_yN_z$  of which  $C, H, O, N$  are mass fractions (kg/kg) of carbon, hydrogen, oxygen and nitrogen in the fuel a  $x, y$  and  $z$  are determined using the expression:

$$x = \frac{H}{C} \cdot \frac{M_C}{M_H} \quad (7)$$

$$y = \frac{O}{C} \cdot \frac{M_C}{M_O} \quad (8)$$

$$z = \frac{N}{C} \cdot \frac{M_C}{M_N} \quad (9)$$

of which:

$M_C, M_H, M_O$  and  $M_N$  are molar masses of carbon, hydrogen, oxygen and nitrogen, kg/kmol.

Authors [18] investigate the water-gas shift reaction and the steam reforming of methane:

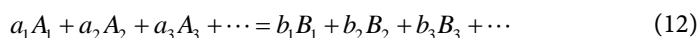


The thermodynamics of reaction (10) as well as its composition of the equilibrium mixture is dominant during the gasification of solid fuel, which is the aim of the research in this paper.

## 2. Mathematical Formulation

### 2.1. Thermodynamic Functions

For a chemical reaction:



of which:

$A_i, B_j$ —labels for chemical substances;

$a_i$ —stoichiometric coefficients for reactants;

$b_j$ —stoichiometric coefficients for products.

Thermodynamic functions  $\Delta H, \Delta S, \Delta G$  at 298 K and  $1.013 \cdot 10^5$  Pa are defined by the expression [18]:

$$\Delta H = \sum_j b_j \cdot \Delta h_j - \sum_i a_i \cdot \Delta h_i \quad (13)$$

$$\Delta S = \sum_j b_j \cdot s_j - \sum_i a_i \cdot s_i \quad (14)$$

$$\Delta G = \sum_j b_j \cdot \Delta g_j - \sum_i a_i \cdot \Delta g_i \quad (15)$$

of which:

$a_i$ —the number of kilomoles of the  $i$ -th reactant components;

$b_j$ —the number of kilomoles of the  $j$ -th component for products;

$\Delta h_i$ —bond enthalpy of the  $i$ -th component;

$\Delta h_j$ —bond enthalpy of the  $j$ -th component;

$s_i$ —specific entropies and connections of the  $i$ -th component;

$s_j$ —specific entropies and connections of the  $j$ -th component;

$\Delta g_i$ —specific free enthalpies of the  $i$ -th component;

$\Delta g_j$ —specific free enthalpies of the  $j$ -th component.

The dependence of enthalpy, entropy and free enthalpy of reaction (12) on temperature are defined by the expressions:

$$\Delta H_T = \Delta H_{298} + \int_{298}^T \Delta c_{mp}(T) dT \quad (16)$$

$$\Delta S_T = \Delta S_{298} + \int_{298}^T \frac{\Delta c_{mp}(T)}{T} dT \quad (17)$$

$$\Delta G = \Delta H - T \cdot \Delta S \quad (18)$$

of which:

$$\Delta c_{mp} = \sum_j b_j \cdot c_{mpj} - \sum_i b_i \cdot c_{mpi} \quad (19)$$

the sum of the specific molar heat capacities of the components.

$$c_{mp}(T) = a + b \cdot T + c \cdot T^2 + d \cdot T^3 + e \cdot T^4, \text{ kJ}/(\text{kmol} \cdot \text{K}) \quad (20)$$

dependence of molar heat capacity on temperature.

$a, b, c, d, e, f$ —polynomial coefficients  $c_{mp}(T)$ .

If  $\Delta G > 0$ , the reaction proceeds from right to left, *i.e.* in the direction of the formation of reactants of the reaction. If  $\Delta G < 0$  the reaction proceeds from left to right, *i.e.* in the direction of the formation of reaction product.

Values of enthalpy, entropy and free enthalpy of reaction components

$\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  at 298 K and  $1.013 \times 10^5$  Pa are shown in **Table 1**, in **Table 2** the values of the polynomial coefficients (20) are shown.

**Table 1.** Thermodynamic data of the reaction components  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  at 298 K and  $1.013 \times 10^5$  Pa [19].

	$\Delta h$ (kJ/kmol)	$\Delta g$ (kJ/kmol)	$s$ kJ/(kmol·K)
CO	-110,520	-137,150	197.56
H <sub>2</sub> O(g)	-241,820	-228,590	188.72
CO <sub>2</sub>	-393,510	-394,360	213.64
H <sub>2</sub>	0	0	130.57

**Table 2.** Numerous coefficient values  $a, b, c, d, e$  polynomial (20) [20].

	$a$	$b$	$c$	$d$	$e$	Temperature range, K
CO	29.5560	$-6.5807 \cdot 10^{-3}$	$2.0130 \cdot 10^{-5}$	$-1.2270 \cdot 10^{-8}$	$2.2617 \cdot 10^{-12}$	60 - 1500
H <sub>2</sub> O(g)	33.9330	$-8.4186 \cdot 10^{-3}$	$2.9906 \cdot 10^{-5}$	$-1.7825 \cdot 10^{-8}$	$3.6934 \cdot 10^{-12}$	100 - 1500
CO <sub>2</sub>	27.4370	$4.2315 \cdot 10^{-2}$	$-1.9555 \cdot 10^{-5}$	$3.9968 \cdot 10^{-9}$	$-2.9872 \cdot 10^{-13}$	50 - 5000
H <sub>2</sub>	25.3990	$2.0178 \cdot 10^{-2}$	$-3.8549 \cdot 10^{-5}$	$3.1880 \cdot 10^{-8}$	$-8.7585 \cdot 10^{-12}$	250 - 500

For a chemical reaction:

$$\sum_i a_i \cdot A_i = \sum_j b_j \cdot B_j \quad (21)$$

The chemical equilibrium constant expressed in terms of partial pressures is:

$$K_p = \frac{\prod_j (p_{B_j})^{b_j}}{\prod_i (p_{A_i})^{a_i}} \quad (22)$$

Value of chemical equilibrium constant  $K'_p$  reduced to pressure  $p_0 = 1.013 \times 10^5$  Pa is determined by the expression:

$$K'_p = e^{-\frac{\Delta G}{R_u \cdot T}} = K_p \cdot p_0^{-\left(\sum_j b_j - \sum_i a_i\right)} \quad (23)$$

of which:

$R_u = 8.314$  kJ/(kmol · K) — universal gas constant.

Using numerical thermodynamic data for the pure components involved in the reaction  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  at 298 K and  $1.013 \times 10^5$  Pa (**Table 1** and **Table 2**) and using expressions from (13) to (23) the values of the thermodynamic functions  $\Delta H, \Delta S, \Delta G, K'_p$  reaction can be calculated considered depending on the reaction temperature (**Table 3**).

Reaction equilibrium constant  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  (reaction (10)) can also be determined by combining Equations (2) and (3), *i.e.*

$$K_p = \frac{K_{p3}}{K_{p2}} \quad (24)$$

Substituting Equations (6) and (5) into Equation (24) gives:

$$\log K_p = -36.72508 + 3994.704/T - 4.462408 \times 10^{-3} \cdot T + 0.6718146 \times 10^{-6} \cdot T^2 + 12.220277 \cdot \log T \quad (25)$$

concluding that the equilibrium reaction constant is  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$ :

$$K_p = 10^{-36.72508 + 3994.704/T - 4.462408 \times 10^{-3} \cdot T + 0.6718146 \times 10^{-6} \cdot T^2 + 12.220277 \cdot \log T} \quad (26)$$

Values of reaction equilibrium constant  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  obtained using expression (23) is in agreement with the values of the equilibrium constant presented in the literature (Equation (26)) (**Table 3**).

In the temperature interval 298 K to 1500 K, thermodynamic functions  $\Delta H$  and  $\Delta S$  are negative, so the sign is  $\Delta G$  determined by the relative ratio of the enthalpy and entropy terms (Equation (18)) (**Figure 1**). This means that the reaction temperature is the decisive factor for the thermodynamic equilibrium of the reaction under consideration. In the temperature range 298 K to  $\approx 1090$  K, the free reaction enthalpy is less than zero ( $\Delta G < 0$ ) and the equilibrium reaction constant under consideration is very large  $K_p \gg 1$  (**Figure 2**), which means that the reaction is shifted towards the formation of reaction products. Above 1090 K, the reaction enters an unfavorable area and the reaction equilibrium shifts towards the formation of reaction reactants.

The values of the thermodynamic functions of the considered reaction shown in **Table 3** are in agreement with data from the literature [21] [22].

## 2.2. Determining the Composition of the Equilibrium Reaction Mixture $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$

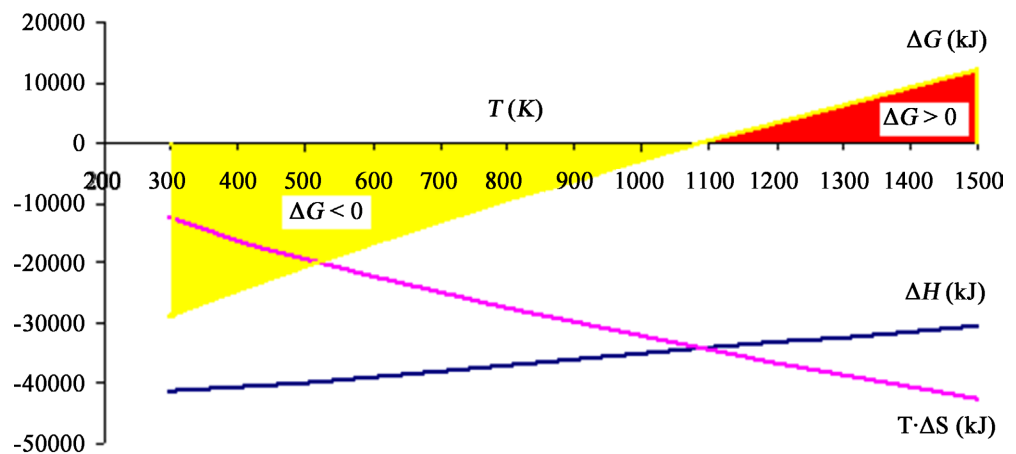
Balance of reaction components:



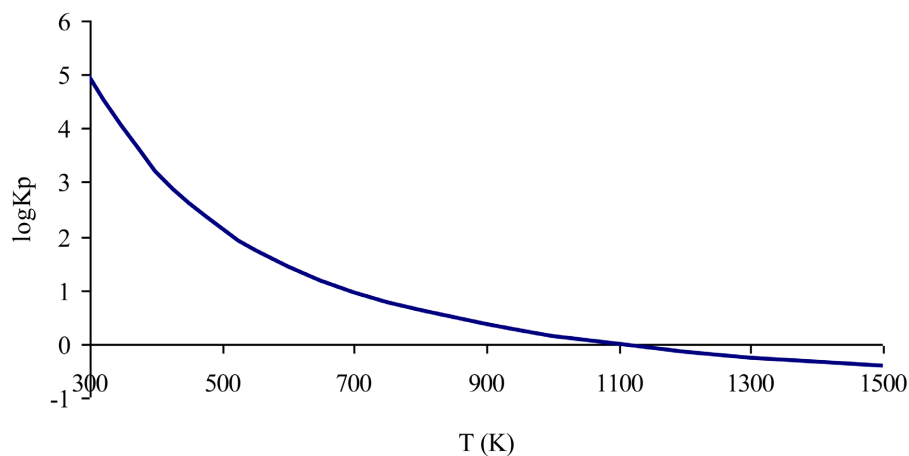
can be formulated as follows.

**Table 3.** Thermodynamic reaction functions  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  depending on temperature.

$T$ (K)	$\Delta H$ (kJ)	$\Delta S$ (kJ/K)	$T \cdot \Delta S$ (kJ)	$\Delta G$ (kJ)	$K_p$ (-) Equation (23)	$K_p$ (-) Equation (26)
298	-41,170	-42.07	-12,537	-28,633	$1.05 \cdot 10^5$	$4.42 \cdot 10^5$
400	-40,583	-40.39	-16,156	-24,426	$1.55 \cdot 10^3$	$2.41 \cdot 10^3$
500	-39,814	-38.68	-19,342	-20,472	$1.38 \cdot 10^2$	$1.52 \cdot 10^2$
600	-38,930	-37.08	-22,245	-16,686	$2.84 \cdot 10^1$	$2.80 \cdot 10^1$
700	-37,985	-35.62	-24,933	-13,052	9.42	9.02
800	-37,014	-34.32	-27,458	-9556	4.21	4.03
900	-36,038	-33.17	-29,856	-6183	2.28	2.20
1000	-35,068	-32.15	-32,151	-2918	1.42	1.38
1100	-34,107	-31.23	-34,358	251	0.97	0.95
1200	-33,154	-30.40	-36,487	3332	0.72	0.70
1300	-32,210	-29.65	-38,544	6334	0.56	0.54
1400	-31,278	-28.96	-40,542	9264	0.45	0.44
1500	-30,368	-28.33	-42,496	12,128	0.38	0.37



**Figure 1.** Determining the reaction area for an exothermic reaction  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$ .



**Figure 2.** Dependence of the reaction equilibrium constant  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  of temperature.

- CO  $n_{\text{CO}} = a - y, \text{ kmol}$  (28)

- H<sub>2</sub>O  $n_{\text{H}_2\text{O}} = b - y, \text{ kmol}$  (29)

- CO<sub>2</sub>  $n_{\text{CO}_2} = y, \text{ kmol}$  (30)

- H<sub>2</sub>  $n_{\text{H}_2} = y, \text{ kmol}$  (31)

of which:

$a$  —the number of kilomoles of carbon monoxide that enters the reaction (27);

$b$  —the number of kilomoles of water (water vapor) that enters the reaction (27);

$y$  —the number of kilomoles of carbon dioxide or hydrogen in the mixture after establishing chemical equilibrium balance.

The total number of kilomoles in the mixture at any conversion time is equal to:

$$n_{\Sigma} = n_{\text{CO}} + n_{\text{H}_2\text{O}} + n_{\text{CO}_2} + n_{\text{H}_2}$$

$$n_{\Sigma} = (a - y) + (b - y) + y + y = a + b, \text{ kmol} \quad (32)$$

The molar fraction of the components in the mixture after establishing chemical equilibrium is:

$$y_{\text{CO}} = \frac{n_{\text{CO}}}{n_{\Sigma}} = \frac{a - y}{a + b}, \text{ kmol/kmol} \quad (33)$$

$$y_{\text{H}_2\text{O}} = \frac{n_{\text{H}_2\text{O}}}{n_{\Sigma}} = \frac{b - y}{a + b}, \text{ kmol/kmol} \quad (34)$$

$$y_{\text{CO}_2} = \frac{n_{\text{CO}_2}}{n_{\Sigma}} = \frac{y}{a + b}, \text{ kmol/kmol} \quad (35)$$

$$y_{\text{H}_2} = \frac{n_{\text{H}_2}}{n_{\Sigma}} = \frac{y}{a + b}, \text{ kmol/kmol} \quad (36)$$

The partial pressures of the components in an equilibrium mixture are:

$$p_{\text{CO}} = y_{\text{CO}} \cdot p = \frac{a-y}{a+b} \cdot p, \text{ Pa} \quad (37)$$

$$p_{\text{H}_2\text{O}} = y_{\text{H}_2\text{O}} \cdot p = \frac{b-y}{a+b} \cdot p, \text{ Pa} \quad (38)$$

$$p_{\text{CO}_2} = y_{\text{CO}_2} \cdot p = \frac{y}{a+b} \cdot p, \text{ Pa} \quad (39)$$

$$p_{\text{H}_2} = y_{\text{H}_2} \cdot p = \frac{y}{a+b} \cdot p, \text{ Pa} \quad (40)$$

of which:

$p$  —total pressure in the reactor space after equilibrium is established, Pa.

By changing partial pressures  $p_{\text{CO}_2}$ ,  $p_{\text{H}_2}$ ,  $p_{\text{CO}}$  and  $p_{\text{H}_2\text{O}}$  into equation (22) the equilibrium reaction constant  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  is given by the expression:

$$K_p = \frac{p_{\text{CO}_2} \cdot p_{\text{H}_2}}{p_{\text{CO}} \cdot p_{\text{H}_2\text{O}}} = \frac{\frac{y}{a+b} \cdot p \cdot \frac{y}{a+b} \cdot p}{\frac{a-y}{a+b} \cdot p \cdot \frac{b-y}{a+b} \cdot p}$$

and after rearranging the previous expression, we obtain a quadratic equation of the form:

$$(K_p - 1) \cdot y^2 - K_p \cdot (a+b) \cdot y + ab \cdot K_p = 0 \quad (41)$$

By solving equation (40) for the unknown quantity  $y$  two solutions are obtained:

$$y_{1/2} = \frac{(a+b) \cdot K_p \pm \sqrt{(a+b)^2 \cdot K_p^2 - 4 \cdot ab \cdot K_p \cdot (K_p - 1)}}{2 \cdot (K_p - 1)}, \quad (K_p \neq 1) \quad (42)$$

That solution is taken  $y$  for which mole fractions  $y_{\text{CO}}$ ,  $y_{\text{CO}_2}$ ,  $y_{\text{H}_2\text{O}}$  and  $y_{\text{H}_2}$  they make physical sense. At an equimolar ratio  $a = b = 1 \text{ kmol}$  from equation (42) we get:

$$y_{1/2} = \frac{K_p \pm \sqrt{K_p}}{K_p - 1}, \quad (K_p \neq 1) \quad (43)$$

Under the given conditions  $0 < y < 1$  equation (42) takes the form:

$$y = \frac{K_p - \sqrt{K_p}}{K_p - 1}, \quad (K_p \neq 1) \quad (44)$$

Degree of conversion of reactants CO and H<sub>2</sub>O is determined using the expression:

$$\eta_{\text{CO}} = \frac{a - (a - y)}{a} = \frac{y}{a}, \text{ kmol/kmol} \quad (45)$$

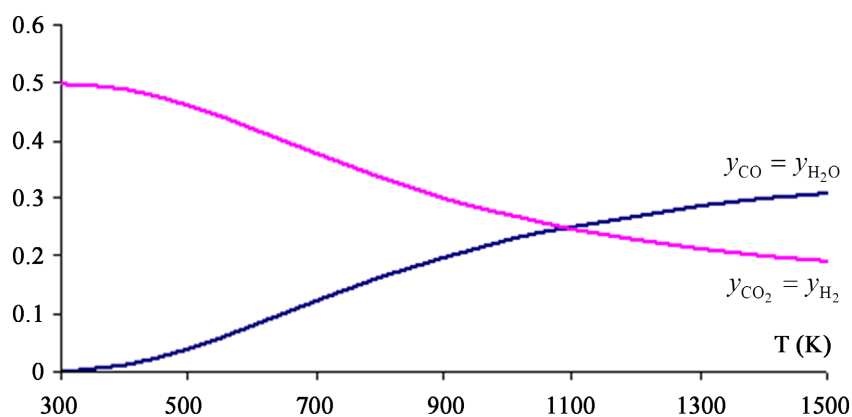
$$\eta_{\text{H}_2\text{O}} = \frac{b - (b - y)}{b} = \frac{y}{b}, \text{ kmol/kmol} \quad (46)$$

Results of the calculation of the composition of the equilibrium reaction mix-

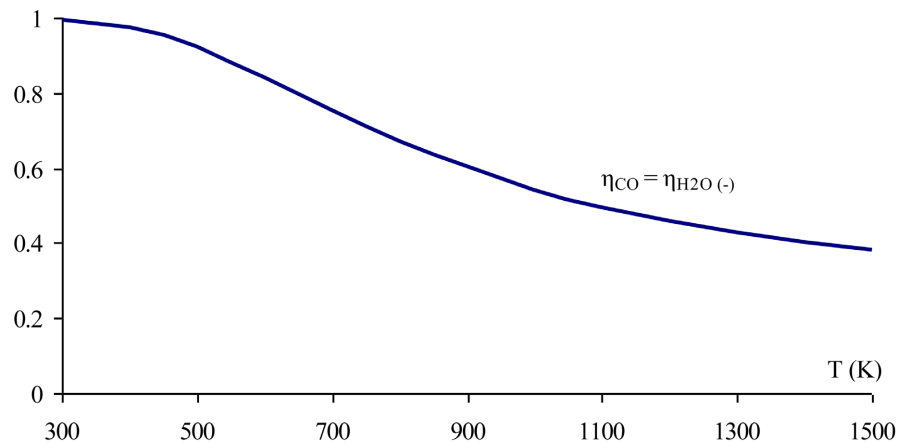
ture  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  at an equimolar ratio of reactants in the temperature range 298 K to 1500 K and pressure  $p = 1.013 \times 10^5$  Pa are shown in **Table 4** and graphical dependence on **Figure 3**. It can be seen that at an ambient temperature of 298K, the degree of conversion of reactants into products is 99.69% (**Figure 4**). Since the reaction  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  occurs without changing the number of moles  $\Delta n = 0$  (Equation (23)), changing the pressure in the system has no effect on changing the equilibrium composition. The equilibrium constant depends only on temperature (Equation (26)).

**Table 4.** Change the composition of the equilibrium reaction mixture  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  at an equimolar ratio of reactants  $\text{CO}:\text{H}_2\text{O} = 1:1$  at constant pressure of  $1.013 \times 10^5$  Pa of temperature.

$T$ (K)	$y_{\text{CO}}$ (kmol/kmol)	$y_{\text{H}_2\text{O}}$ (kmol/kmol)	$y_{\text{CO}_2}$ (kmol/kmol)	$y_{\text{H}_2}$ (kmol/kmol)	$\eta_{\text{CO}} = \eta_{\text{H}_2\text{O}}$ (kmol/kmol)
289	0.0015	0.0015	0.4985	0.4985	0.9969
400	0.0124	0.0124	0.4876	0.4876	0.9752
500	0.0392	0.0392	0.4608	0.4608	0.9216
600	0.0790	0.0790	0.4210	0.4210	0.8420
700	0.1229	0.1229	0.3771	0.3771	0.7542
800	0.1638	0.1638	0.3362	0.3362	0.6723
900	0.1992	0.1992	0.3008	0.3008	0.6016
1000	0.2281	0.2281	0.2719	0.2719	0.5437
1100	0.2519	0.2519	0.2481	0.2481	0.4962
1200	0.2705	0.2705	0.2295	0.2295	0.4590
1300	0.2864	0.2864	0.2136	0.2136	0.4273
1400	0.2991	0.2991	0.2009	0.2009	0.4018
1500	0.3096	0.3096	0.1904	0.1904	0.3808



**Figure 3.** Changing the structure of the reaction equilibrium mixture  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  at an equimolar ratio of reactants  $\text{CO}:\text{H}_2\text{O} = 1:1$  at constant pressure of  $1.013 \times 10^5$  Pa of temperature.



**Figure 4.** Change in the degree of conversion of the reactants of a reaction  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  at constant pressure of  $1.013 \times 10^5$  Pa of temperature

### 3. Conclusions

The thermodynamic equilibrium model of the reaction  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  presented in this manuscript predicts the maximum product yield in the reaction system. Although thermodynamic equilibrium will not be achieved inside the gasifier, the results presented in this manuscript provide a reasonable prediction of the yield of the desired product and the following conclusions are reached:

- The reaction is exothermic with a negative entropy change in the temperature interval 298 - 1500 K.
- The sign of the free enthalpy of reaction  $\Delta G$  is determined by the ratio of the enthalpy and entropy terms (equation (18)), which means that the reaction temperature is the decisive factor for the thermodynamic equilibrium of the reaction.
- The reaction is favorable in the temperature interval 298 K to  $\approx 1090$  K ( $\Delta G < 0$ ).
- Above 1090 K the response enters the unfavorable region ( $\Delta G > 0$ ).
- The equilibrium reaction constant under consideration is very large ( $K'_p \gg 1$ ) at lower temperatures, which means that the products of the reaction are in excess of the reactants, *i.e.* that the reaction has shifted in the direction of building reaction products.
- At higher temperatures above 1090 K the equilibrium constant decreases slightly so the reaction equilibrium shifts slightly towards the reactants of the reaction.
- At an ambient temperature of 298 K, the degree of conversion of the reactants CO and H<sub>2</sub>O is 99.69%. By increasing the reaction temperature, the conversion of the reactants decreases slightly, reaching only 38.08% at 1500 K.

Research on the kinetics of  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  was not the goal of this manuscript further studies of reaction thermodynamics  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$  should focus on reaction kinetics under different conditions and the possibility of using catalysts to accelerate the reaction in order to obtain a higher yield CO and H<sub>2</sub> which is of practical importance in the gasification of solid fuel.

## Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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