# HYDROGEN PRODUCTION FROM COAL GASIFICATION USING SOLAR ENERGY: THERMODYNAMIC EQUILIBRIUM MODELLING AND EXERGY ANALYSIS

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## ABSTRACT

In this study the merits of hydrogen production using solar energy are discussed. The primary focus of the paper is to perform thermodynamics analysis of coal gasification via solar energy. Initially the chemical properties of coal are determined using proximate analysis, ultimate analysis and calorimeter. Using the coal properties a thermodynamics model bases on equilibrium constant approach is developed. The model is tested against the experimental data and further exergetic and cold gas efficiency is calculated. The effect of temperature and moisture contents is studied which shows that efficiency as high as 70% can be achieved with hydrogen yield of around 57% by volume. The model is further used to explore the potential of solar energy along with the partial combustion of coal. The result shows a sharp decline in the  $CO_2$  emission, while 43% increase in the yield of Hydrogen is calculated.

# INTRODUCTION

Hydrogen is an emerging sustainable fuel that has a potential to offset a larger amount of the existing fossil fuel that provides a solution to the world energy demand with benign emission. Still however its production is neither unsustainable nor environmental friendly while its storage is quite challenging. Also, the transition from conventional fossil fuel to more sustainable is a long goal, but a bridging technology is required for the countries which are highly dependent on fossil fuel to fulfil their energy demand. Coal is one of the major fossil resources that is currently utilized for energy and electricity generation and the conventional method of its usage makes it one of the most environmentally unfriendly fuels, in term of CO<sub>2</sub> generation. The integration of CO<sub>2</sub> sequestration with existing/new coal power plants is costly or penalizing in terms of power plant efficiency. On other hand, coal can be converted into benign emission fuel when converted into hydrogen using the solar energy. In this process coal is mixed with water/steam at a high temperature to produce high quality syngas of equi-molar amount of H<sub>2</sub> and CO. The CO again is reformed into H<sub>2</sub> through the shift reaction to ensure the high

yield of  $H_2$ . The  $CO_2$  produced during the process without the combustion emission can be relatively easily separated and sequestrated. This whole process of Coal conversion is highly endothermic and thus the solar energy is the primary source of providing the process heat. The hydrogen production through solar gasification provides three-fold advantages: 1) Coal is converted in the highly upgraded fuel in term of calorific value, 2) Combustion by-product are avoided, and 3) under the common oxy-gasification, it facilitates easy  $CO_2$  separation and potential sequestration.

The viability for the production of hydrogen via gasification can be calculated through process thermodynamic modelling. Previously, several studies were performed at Masdar Institute that target the thermodynamics modelling of gasification process at different points of view [1-4]. There is considerable literature also available which deal with the modelling of gasification processes. These models can be mainly classified into three broad categories: 1) Kinetic rate models [5-7]; 2) Thermodynamic equilibrium model [8, 9] of which ASPEN Plus model can belong to this category [10, 11]; and 3) neural network based gasification model [12, 13]. Except thermodynamics equilibrium model, other two models are computationally expensive or contain parameters that limit their applicability for a special scenario of power plant. Thermodynamic equilibrium model provides the flexibility to assess the gasifier performance independently with other plant or process related parameters.

In this analysis a thermodynamic bases solar gasification modelling of coal is performed using the equilibrium constant stoichiometric based approach. The viability of using solar energy for gasification process is performed by calculation the second law efficiency (exergetic efficiency) of the system. The effects of temperature and moisture contents are studies and discussed. Finally, the viability of using solar energy with the conventional gasification power plant is studies by replacing the process heat produce by the air combustion with solar heat.

## MATERIAL AND METHODS

**Coal Properties:** The coal composition are measured using proximate, ultimate and calorimeter analysis. The analysis are performed earlier and can be found in the literature [2] and are given in Table 1.

$1 u 0 0 1 \cdot 1 \cdot 1 0 \Lambda m u 0 u 0 u 0 u 0 0 0 0 0 0 0 0 0 0 0 0$	Table	1: Proximate	and ultimate	analysis of	Coal	(Ash free)	[2]
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Element	Weight (%) as received
С	81.90
Н	5.61
0	8.86
Ν	2.49
S	1.13
HHV (kJ/kg)	30420
Volatile matter	40.76
Fixed carbon	58.92
Moisture	0.32
Empirical formula	$C_{0.0683}H_{0.0561}O_{0.0055}N_{0.0018}S_{0.0040}$
Normalized formula	$CH_{0.8173}O_{0.0785}N_{0.0260}S_{0.0052}$
M.weight (kg/kmol)	14.43

**Gasification Model:** The gasification model used in this study is defined by the following reaction,

$CH_x O_y N_z + \alpha H_2 O + heat + \beta (O_2 + CH_z O_2 + C$	
$3.76 \text{ N}_2 ) \rightarrow aH_2 + bCO + cCO_2 + dCH_4 +$	(1)
$eH_2O + \left(\frac{z}{2} + 3.76\beta\right) N_2$	
The mass balance of carbon is,	
b + c + d - 1 = 0	(2)

The mass balance for hydrogen is,

 $\begin{array}{l} 2a + 4d - x - 2\alpha = 0 \quad (3) \\ \text{The mass balance for oxygen is,} \\ b + 2c - y - \alpha - 2\beta = 0 \quad (4) \\ \text{To solve for a, b, c, d and e we need another equation using the equilibrium constant for the following reaction,} \\ C + 2H_2 \rightarrow CH_4 \quad (5) \\ \text{And,} \\ CO + H_2O \rightarrow CO_2 + H_2 \quad (6) \\ \text{The equilibrium constant for the equation (5) is given below,} \end{array}$ 

$$K_1 = \frac{a^2 \cdot N}{d}$$
(7)  
And for equation (6),

 $K_2 = \frac{a.c}{b.e} \tag{8}$ 

Where, N is the total number of moles of product, as given,

$$N = a + b + c + d + e + \left(\frac{2}{2} + 3.76\beta\right)$$
(9)

The value of equilibrium constant can be calculated from the following equation using the properties of methane and hydrogen,

$$K = \exp{-\frac{\Delta G}{RT}} \tag{10}$$

The model details of the equilibrium can be found in previous study of the authors [1].

**Exergy Evaluation:** The chemical exergy of coal can be calculated using the following reaction from the literature [14]  $(c C + h H + o O + n N + s S) + v_{02} O_2 \rightarrow$ 

$$\nu_{CO_2} CO_2 + \nu_{H_{2O}} H_2 O(l) + \nu_{SO_2} SO_2$$
(11)  
+  $\nu_{N_2} N_2$ 

For the coal used in this study,  $v_{CO_2} = c = 0.0683$ ,  $v_{H_{2O}} = \frac{1}{2}h = 0.02805$ ,  $v_{SO_2} = s = 0.0040$  and  $v_{N_2} = \frac{1}{2}n = 0.0009$ and  $v_{O2} = c + \frac{1}{4}h + s - \frac{1}{2}o = 0.0836$ .

Using the values mentioned above the following formula can be used to calculate the chemical exergy  $(e_{DAF}^{Ch})$  of coal on dry ash free bases.

$$e_{DAF}^{CR} = (HHV)_{DAF} - T_o [s_{DAF} + v_{O_2} \bar{s}_{O_2} - v_{CO_2} \bar{s}_{CO_2} - v_{H_2O} \bar{s}_{H_2O} - v_{SO_2} \bar{s}_{SO_2} - v_{N_2} \bar{s}_{N_2}] + [v_{CO_2} \bar{e}_{CO_2}^{CH} - v_{H_2O} \bar{e}_{H_2O}^{CH} - v_{SO_2} \bar{e}_{SO_2}^{CH} - v_{N_2} \bar{e}_{N_2}^{CH} + (12) + v_{O_2} \bar{e}_{O_2}^{CH}]$$

The higher heating value (HHV) is in kJ/kg. The value of coal entropy ( $s_{DAF}$ ) can be calculated using the following formula [15],

$$S_{DAF} = c \left[ 37.1653 - 31.4767e^{-0.564682\frac{h}{c+n}} + 20.1145\frac{o}{c+n} + 54.3111\frac{n}{c+n} + 44.6712\frac{s}{c+n} \right]$$
(13)

The value of standard state entropy of substance used in equation (12) is given in Table 2.

Table 2: Value of standard entropy [16]

Substance	Entropy (kJ/kmol-K)
Oxygen $(0_2)$	205.146
Carbon dioxide ( $CO_2$ )	213.794
Water (liquid) $(H_2 0)$	69.948
Sulphur di oxide $(SO_2)$	284.094
Nitrogen $(N_2)$	191.610

The standard state chemical exergy of substance used in equation (1) is given in Table 3,

Table 3: Standard state chemical exergy (E<sub>xo</sub>) [16]

Substance	Exergy (kJ/kmol)
Oxygen $(0_2)$	3951
Carbon di oxide $(CO_2)$	14176
Water (liquid) $(H_2 0)$	45
Water (gas) $(H_2 0)$	9500
Sulphur di oxide $(SO_2)$	301939
Nitrogen $(N_2)$	639
Hydrogen $(H_2)$	236100
Carbon mono oxide (CO)	275100

Using equation (13) and values given in Table 1, Table 2 and Table 3 the coal entropy  $(s_{DAF})$  is found to be  $1.5473 \frac{kJ}{kg-K}$ . Further using equation (12) for  $T_o = 298.15 K$  the value of chemical exergy of coal  $(e_{DAF}^{Ch})$  is calculated as 30204.18  $\frac{kJ}{kg}$ ,

care must be taken while using the right units and conversion. The proximate analysis on coal is performed on as received bases which show only 0.32% of moisture present in the sample. Therefore we can assume the coal on dry bases. The empirical formula, as given in Table 1, is derived by normalizing the quantity of ash, therefore the empirical formula can be treated as ash free. The exergy calculated can be taken for the moister sample as the moisture is present in small quantity.

The exergetic efficiency is calculated using the following equation,

$$\eta = \frac{Ex_{gas}}{Ex_{coal} + Ex_{steam} + Ex_{solar}}$$
(14)  
And,  
$$\eta_{H, SCO} = \frac{Ex_{CO} + Ex_{H_2}}{(15)}$$

 $Ex_{coal} + Ex_{steam} + Ex_{solar}$ 

where Ex is the exergy of the respective substances. It is assumed that coal is crushed and prepared as water slurry and enters the reactor at ambient condition, Guaranteeing a zero state for coal chemical exergy and steam. As the solar heat calculated by the model is actually the quantity of useful solar radiation in the form of heat, the exergy of solar radiation is taken equivalent to the heat calculated from the model.

The exergy of the product gases are calculated by accounting both chemical and physical exergy, as shown by the following equation,

$$Ex = Ex_{chemical} + Ex_{physical} \tag{16}$$

The chemical exergy is calculated by considering the mole fraction of each individual species as given by the following equation,

$$Ex_{chemical} = N\left(\sum_{i} X_{i}E_{xo} + RT_{o}\sum_{i} X_{i}lnX_{i}\right)(17)$$

Where N is the total number of moles in product,  $X_i$  is the respective mole fraction of each product species that can be calculated from a, b, c, d and e using equation (1), R is the universal gas constant and  $T_o$  is the reference temperature, i.e. 298.15 K. The standard state reference exergy  $(E_{xo})$  is given in Table 3.

The physical exergy  $(Ex_{physical})$  is calculated using the following equation,

$$Ex_{physical} = N\left(\sum_{i} X_{i}(\Delta h_{i} - T_{o}\Delta S_{i})\right)$$
(18)

Where  $\Delta h$  is the enthalpy and  $\Delta S$  is the entropy change for the respective species. The change in enthalpy is calculated using a fourth order polynomial using six coefficient [17], as follows,

$$h = RT \left( a_1 + a_2 \frac{T}{2} + a_3 \frac{T^2}{3} + a_4 \frac{T^3}{4} + a_5 \frac{T^4}{5} + \frac{a_6}{T} \right)$$
(19)

A similar equation is used to calculate the entropy of substance, as follows,

$$S = a_1 \ln(T) + a_2 T + a_3 \frac{T^2}{2} + a^4 \frac{T^3}{3} + a_5 \frac{T^4}{4} + (20)$$
  
$$a_7$$

The coefficients used in equation (19) and (20) are presented in Table 4 and Table 5 for different temperature ranges.

Specie a7  $a_1$  $a_2$ a3  $a_4$ as  $a_6$ CO 2.72 -9.99E-7 2.30E-10 -2.04E-14 -1.42E4 2.06E-3 7.82 2.27  $CO_2$ 3.86 4.41E-3 -2.21E-6 5.23E-10 -4.72E-14 -4.88E4 H<sub>2</sub>O 3.03 2.18E-3 -1.64E-7 -9.70E-11 1.68E-14 -3.00E4 4.97  $H_2$ 3.34 -4.94E-5 4.99E-7 -1.80E-10 2.00E-14 -950 3.21 CH₄ 7.49E-2 1.34E-2 -5.73E-6 1.22E-09 -1.02E-13 -9.47E3

18.4

Table 4: Coefficients used in equation (19) and (20) for

temperature range 1000-3500 K

Table 5: Coefficients used in equation (19) and (20) fo
temperature range 200-1000 K

Specie	$a_1$	$a_2$	a <sub>3</sub>	$a_4$	a <sub>5</sub>	$a_6$	a <sub>7</sub>
СО	3.58	-6.10E-4	1.02E-6	9.07E-10	-9.04E-13	-1.43E4	3.51
$CO_2$	2.36	8.98E-3	-7.12E-6	2.46E-9	-1.44E-13	-4.84E4	9.90
$H_2O$	4.20	-2.04E-3	6.52E-6	-5.49E-9	1.77E-12	-3.03E4	-0.849
$H_2$	2.34	7.98E-3	-1.95E-5	2.02E-8	-7.38E-12	-918	6.83E-1
$CH_4$	5.15	-1.37E-2	4.92E-5	-4.85E-8	1.67E-11	-1.02E4	-4.64

MODEL VALIDATION USING EXPERIMENTAL DATA

The model validation is performed by comparing the results with the literature [18]. The chemical composition of the coal sample is given below,

Table 6: The chemical properties of coal[18]

Element	С	Н	0	Ν	S
Weight%	80	4.5	3.5	1	1
Normalized	d formu	la	$CH_{0.6750}O_{0.0328}N_{0.0107}S_{0.0046}$	M. Wt. (kg/kmol)	13.5

The model runs using the coal, as given in Table 6, at the temperature of 700°C (973°K). As the percentage of the moisture in the literature was not given, different moisture content is assumed in order to get the desire value of hydrogen molar rates. The moisture contents are calculated using the equation (22), but for the corresponding molecular weight of 13.5 kg/mol. The comparison between the model results and experimental data is given in Table 7 for the moisture content of 57%. Although the moisture content is very high but not all the moisture is consumed, some portion of it remains in the product. For this case around 22% of water is calculated in the product, therefore the effective moisture content is 35%.

Table	7:	Comparison	between	model	and	experimental	results

	$n_{H_2}\left(\frac{mol}{kg}\right)$	$n_{CO}\left(\frac{mol}{kg}\right)$	$n_{CH_4}\left(\frac{mol}{kg}\right)$	$n_{CO_2}\left(\frac{mol}{kg}\right)$
Experiment	15.30	4.85	1.66	1.33
Model	15.30	11.53	1.0667	0.89

It is evident from the Table 7 that there is an obvious difference between the results of experimental data and the model calculations. The model considered the process as a steady state, whereas the experimental study is inherently unsteady. The model neglects the effect of potential and kinetic energy present in experiment. The model considers that gases obeying the ideal gas law with isothermal and equilibrium condition. All these assumption pollute model results. But this difference in the results can be compensated by incorporating the effectiveness factor, which is the ratio of experiment to model results. The effectiveness factor calculated for this study is given in Table 8.

Table 8: Effectiveness factor

Specie	$H_2$	СО	CH <sub>4</sub>	<i>CO</i> <sub>2</sub>
Factor	1	0.42	1.55	1.49

The factors listed in Table 8, however, are not used in this study. It is worth mentioning that the residence time of coal water slurry is greatly influenced by the coal particle size and consequently, change in gas composition and coal conversion raise. Nevertheless, the generalized agreement to the experimental results can be inferred, such as the increase in the steam results in a higher yield of hydrogen and the increase in the temperature leads in a better conversion, etc.

## **RESULT AND DISCUSSION**

Using the model, as explained through equations (1)-(20), various studies can be performed. Beacause the coal sample used in this study has a small moisture contents, the moisture counts only the water used in the coal slurry. The moisture content (MC) is calculated using the following formula:

$$Moisture \ contents = \frac{mass \ of \ water}{mass \ of \ wet \ coal}$$
(21)

The mass of water is  $18\alpha$  and the mass of dry coal is taken as molecular weight of coal, the equation (21) becomes:

$$MC = \frac{18 \,\alpha}{18 \,\alpha + 14.6} \tag{22}$$

The stoichiometric reaction for the solar gasification of coal is given by the following equation,

 $CH_x O_y + (1-y)H_2 O$ 

$$\rightarrow \left(1 + \frac{x}{2} - y\right)H_2 + CO \tag{23}$$

Using equation (23) the amount of water required ( $\alpha$ ) required is calculated to be 1 - y = 1 - 0.0785 = 0.9215. This amount is corresponds to a moisture content of 53.18%.

Effect of Temperature: Initially the model is run to calculate the effect of temperature on the composition of product gas. The moisture content of 0.9215 moles is used per kilogram of coal (which is equivalent to 1.15 kg of water). The temperature range from 700-1800°K is used. The results are given in Figure 1 thru 3. Figure 1 shows the composition of product gas in kilogram per kilogram of coal. It is evident that as the temperature increases the mass of CO and H<sub>2</sub> increase. As CO have higher molecular weight, it gains higher mass percentage in the result. On the other hand, the mass of CO2 and CH4 decrease as the temperature increase. Around 1.8 kg and 0.194 kg of  $H_2$  and CO is produced per kg of coal at 1500 °K, respectively. Figure 2 shows the volume of H<sub>2</sub> is far greater then CO in the product gas. After 1,100°K the composition of the product gas remains constant. Around 57% and 43% of H<sub>2</sub> and CO is produced per kg of coal, respectively.



Figure 1 Product gas composition in kilogram



Figure 2 Product gas composition by volume percent

Figure 3 shows the efficiency and the solar heat required for the gasification. The exergetic efficiency of the process continues to rise as the physical exergy of the product gases are increasing due to temperature increase. The cold gas efficiency of the process initially is increased, but after  $960^{\circ}$ K a decreasing trend is calculated. The reason for the decline is due to near stagnation of H2 and CO production beyond  $960^{\circ}$ K and with an increase in solar heating. The maximum cold gas efficiency reaches near 71.5% achieved at  $1000^{\circ}$ K, whereas a 67% maximum exergy efficiency is attained at  $1,500^{\circ}$ K



Figure 3 Efficiencies and solar heat for the gasification

Effect of Moisture: The effects of moisture contents are also studied covering a wide range {5 to 60%} and two constant values of temperatures are considered  $800^{\circ}$ K and  $1500^{\circ}$ K. Figure 4 shows results of the  $800^{\circ}$ K temperature. It shows an initial and slow increase in CO mass with respect to the increase in the moisture content that accelerated beyond 25% until 45% then a quick drop beyond 45% of moisture contents. The reason for the sharp decrease after 45% moisture contents is due to the formation of CO<sub>2</sub>. Figure 5 shows that at 50% of moisture contents equal volume of CO and H<sub>2</sub> is achieved. The rise in CO2 concentration beyond 45% moisture contents results in a sharp decrease in the CO concentration.



Figure 4 Product gas composition in kilogram at 800 °K



Figure 5 Product gas composition by volume percent at 800 °K

Figure 6 shows that the maximum cold gas efficiency and exergetic efficiency is achieved at 45% of moisture contents. The decrease in the efficiency is due to the formation of CO<sub>2</sub>.

The maximum cold gas efficiency of 77% and 70% of exergetic efficiency is achieved.



Figure 6 Efficiencies and solar heat gasification at 800 K

The result of 1500°K temperature is given in Figure 7, Figure 8 and Figure 9. The results in Figure 7 show that 1.9 kg of CO and 0.2 kg of H<sub>2</sub> is form per kg of coal at 55% moisture level. These values are quite high as compare to the results at 800°K temperature. It shows that even at higher moisture level the high yield of H<sub>2</sub> and CO can be achieved at 1,500°K.



Figure 7 Product gas composition in kilogram at 1500 °K

The results in Figure 8 show that maximum concentration of 55% of  $H_2$  and 62% of CO can be achieved by volume. Although as the moisture contents increase the concentration of CO continuously decrease while the concentration of  $H_2$  continue to increase at 25% moisture level. The methane initially shows an increasing behaviour in concentration and after 25% of moisture contents it shows a sudden decreasing trend. The concentration of other gases, CO<sub>2</sub> and N<sub>2</sub>, remains relatively lower in the whole study of 1500°K temperature.

The results in Figure 9 show that the both cold gas efficiency and exergetic efficiency initially increase, but after 25% of moisture contents it starts decreasing. Although both decrease by 10% for the whole range of moisture content (i.e. 5-60%). The reason for initial increase is mainly due to the formation of methane, which has high contribution to the cold gas efficiency and in the chemical exergy. As soon as methane concentration start to decrease, efficiencies are started to descend. A maximum of 70% in both cold gas and exergetic efficiencies are calculated. At the maximum efficiency, a 57% of CO and 47% of CH<sub>4</sub> are calculated by volume, the concentration of other gases remains negligible. The solar heat required to obtain this maximum efficiency is calculated to be 11.40 MJ/kg of coal.



Figure 8 Product gas composition by volume percent at 800 °K



Figure 9 Efficiencies and solar heat for gasification at 1500 °K

The results of both  $800^{\circ}$ K and  $1500^{\circ}$ K temperature are compared in Figure 10. It shows that the exergetic and cold gas efficiency are higher for 800 compare to  $1500^{\circ}$ K temperature study. The reason for higher efficiency is due to the fact that at  $800^{\circ}$ K more methane is present in the system.



Figure 10 Comparison of 800K and 1500 °K results

**Co-combustion:** Another study is performed in which potential of solar gasification is explored to retrofit the existing gasification power plants. The idea is to replace some part of partial combustion with the solar heat. For this purpose 1500 °K temperature is maintained in the gasifier and gradually decreasing the amount of air in the system by offsetting the equivalent heat with the solar heat. The results are shown in

Figure 11. It shows that as the quantity of air is start decreasing the amount of  $CO_2$  and  $H_2O$  starts falling and more CO and  $H_2$  forming.



Figure 11 result of co combustion and solar gasification

#### CONCLUSION

The study shows the thermodynamics viability of using solar energy to perform coal gasification. At constant, moisture contents increase in temperature produce high yield of product syngas, while beyond  $1100^{\circ}$ K any further increase in temperature does not increase the yield of syngas. Around 57% and 43% of H<sub>2</sub> and CO is produced per kg of coal, respectively. The study on the effect of moisture content shows that increase in moisture contents can enhance the yield of methane. For  $1500^{\circ}$ K study, at maximum efficiency, 57% of CO and 47% of CH<sub>4</sub> is calculated. The results of co-combustion and solar gasification show that when the amount of air in the system deceases and is replaced by equivalent amount of heat by solar energy then CO<sub>2</sub> emission can be reduced and the system efficiency is increased.

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