

## Thermodynamics Equilibrium Analysis within the Entrained Flow Gasifier Environment

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### Abstract

A thermodynamic equilibrium approach is used to calculate the maximum cold gasification efficiency (CGE) of different feedstock within the entrained flow gasifier. The high temperature (1000 to 1500°K), the small feedstock size (10 $\mu$ m to 0.1mm), and the well mixing environment make them most amenable for equilibrium analysis. Four different feedstock, i.e. RTC coal, pine needles, ply-wood and lignite, are used for the gasification purpose. Using air as oxidizer a parametric study is conducted to show the behavior of CGE and product gasification composition by increasing oxidizer input. A gasification model is developed to calculate the seven unknowns in the gasification product. Using four elemental mass balance and three equilibrium constant relations a mathematical code is developed that also incorporate the solid un-burn carbon in product species. Energy equation is used to calculate the temperature of gasification using iterative approach. Result of model shows that the maximum CGE is achieved when all the solid carbon is converted into the carbon monoxide with nearly all hydrogen present in the feedstock converted into the hydrogen gas. Using this result as baseline, a global model to estimate the maximum CGE is developed in reference to Van Krevelen diagram. This model based on minimum requirement of air to convert all the carbon present in feedstock into carbon monoxide. Result shows a growing trend of CGE with the increase O/C and H/C ratio of feedstock.

**Keywords:** *Thermodynamics equilibrium, entrain flow gasifier, cold gasification efficiency*

### 1. Introduction

Fossil energy resources that can be exploited economically are believed to be finite. The developing economies are becoming major consumers of these resources that also add pressure on fossil fuel prices and supplies. The fear of depletion is a recurring theme in the discussion of the future of energy. Furthermore, the environmental concerns over the growing use of fossil fuels, especially with respect to carbon dioxide (CO<sub>2</sub>) emissions, have resulted in many calls for immediate action to curtail the possibility of dangerous emission level that may lead to global warming. Therefore, it should be a way to derive energy to meet the future energy demand without harming environment with the emissions associated with CO<sub>2</sub>, Nox Sox, and CH<sub>4</sub>.

Thermo-chemical conversion (combustion, gasification, and pyrolysis) is a core technology that can be utilized broadly to generate energy without polluting the environment. Because of its many applications, it is currently enjoying a considerable renaissance [1]. Gasification is one of a thermo-chemical conversion process through which clean fuels, chemicals and efficiency augmentation can be produced. Gasification is

compatible with new applications in the area of biomass conversion (when used with biomass, is carbon neutral); coal-to-liquid; superior environmental performance especially with regard to CO<sub>2</sub> capture and sulfur removal; and the prospect for substantial efficiency improvement when incorporated in Integrated Gasification Combined Cycle plants (IGCC) for electricity generation.

Gasification is a process in which a carbon containing feedstock is thermo-chemically converted into syngas comprising hydrogen (H<sub>2</sub>) and carbon monoxide (CO). Gasification adds value to low or negative value feedstocks by converting them into valuable fuel and/or chemical. Typical feedstock used in the gasification process are coal, biomass and industrial/municipal/agricultural as well as hazardous waste. The production of syngas using gasification is a complex process that depends on several factors including the composition of feedstock, the gasifier conditions, temperature and pressure, and the type and amount of oxidizer and moderator (CO<sub>2</sub> or Steam) [2]. The process of gasification utilizes the partial combustion of feedstock by carefully controlling the amount of oxidizer. The amount of oxidizer also controls the temperature of the gasification process, which is the most important parameter of gasifier, as reported by Walawender [3].

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Gasification process is a series of exothermic and endothermic process. Therefore a substantial amount of thermal energy is required to sustain the process which provided by either an external source of heat or by partial combustion of feedstock [4]. During the partial combustion a considerable amount (~25%) of feedstock is burned by the gasification process providing energy to moisture release, devolatilization, the endothermic Boudward and gas shift reactions as well as the unrecovered sensible heat of the product gas species and the ash. This amount is mainly depend upon the composition and the heating value of the feedstock. The gasification process mainly consists of initial preheating of the feedstock that leads to drying. Further increase in temperature causes pyrolysis during which light hydrocarbon (volatiles) start evolving from the feedstock. Finally, the char present in the feedstock either gasified or combusted leaving behind ash. Depending upon the process parameter gasification results mainly in formation of CO, H<sub>2</sub>, CH<sub>4</sub> and CO<sub>2</sub>.

The efficiency of gasification process is the major concern that decide the feasibility for the designed system. The efficiency is measured in term of product syngas heating value to the heating value of feedstock. This type of efficiency is termed as cold gasification efficiency (CGE) as it ignores the resulted gas and ash sensible heat and it is widely used to evaluate the effectiveness of gasification process [5-8]. The only major clean element present in the product gas is H<sub>2</sub>, because H<sub>2</sub> combust to produce water. On other hand both CO and CH<sub>4</sub> are inclined to produce CO<sub>2</sub> during the combustion and thus producing environmental problems[9]. The methane gas can be converted into H<sub>2</sub> and CO at high temperature but the problem still remain with CO as it combust to give CO<sub>2</sub>. Therefore, the shift reaction is widely used to convert CO into H<sub>2</sub> [10]. The remaining CO<sub>2</sub> is typically separated from the system prior to utilization of the Gasification product into power generation, i.e. Brayton Gas turbine cycle or fuel cell. In this way the clean fuel is produce in term of H<sub>2</sub> gas. So, the extent of H<sub>2</sub> from the gasification system is depending upon both the direct H<sub>2</sub> gas production from feedstock and indirect production via CO shift reaction. In this way CO also contribute in the formation of clean fuel and add the value in CGE.

Thermodynamic equilibrium modeling approach is widely used to evaluate the performance of gasification system in terms product gas composition and efficiency. Entrained flow gasifiers are the most amenable for equilibrium modeling than the fixed/moving and the bobbling bed gasifiers due to the higher conversion temperature (~1300°K), smaller particle size (10µm-0.1mm), higher mixing and heating rate environments (~3000-10,000K/s) and the fastest conversion rate. Abuadala [2] used equilibrium approach to improve the hydrogen production by optimizing operating parameters of gasifier. The study is mainly focused on the influence of gasification temperature, feedstock feeding and moderator (steam) injection on hydrogen yield and efficiency. Melgar [11] discuss the thermo chemical process of a downdraft biomass gasifier using thermodynamic equilibrium model. The work includes a parametric study of the influence of the gasifying relative fuel/air ratio and the moisture contents of the biomass on the characteristics of the process and the product gas composition. Using rubber wood as feedstock with 14.7% moisture a cold gasification efficiency of 80% was achieved. Sharma [12] proposed a full equilibrium model of global reduction reactions of a downdraft biomass gasifier in order to predict the accurate distribution of various gas species, unconverted char and reaction temperature. The maximum gasification efficiency of the system was calculated 81% and the results were compared with the experimental data. Zainal [13] develop a

thermodynamics equilibrium model to predict the gasification process in a downdraft gasifier. The parametric study in terms of initial moisture content in the feedstock and the temperature in the gasification zone has been investigated. Finally, the calorific value of product syngas was calculated to show its declining trend with the increase in the moisture content in the feedstock. Jarungthammachote [14] has developed a similar type of equilibrium as Zainal [13] to calculate the composition of product syngas for municipal solid waste using downdraft gasifier. To enhance the performance of the model a further modification was made by multiplying the equilibrium constants with coefficients. Then the results were compared with data reported by different experimental work. This model works on auto-thermal gasification cycle in which temperature of reaction zone was calculated using energy balance. This approach provided a better understanding for calculating the effect of moisture content and quantity of oxidizer on reaction temperature. Mountouris [15] studied the thermodynamic analysis of plasma gasification technology, which includes the prediction of the product syngas, energy and exergy calculations. This study also deals with the possibility of soot formation, as a solid carbon byproduct. It also accounts for the indirect energy provided to the gasifier from an additional out source. The literature [13-15] investigated the thermodynamics and kinetics involving the gasification process. It helps to identify the nature of syngas at different operating conditions. Also, different composition of feedstock can be handled.

In the view of above mention literature, a thermodynamic equilibrium model is established in this study. The focus of this study circles around the operating condition of an entrain flow gasifier for which a maximum cold gas efficiency can be achieved. This is accomplished by a parametric study of varying oxidizer concentration inside the gasifier. The results are present for the product gas composition, char consumption, gasification temperature and cold gasification efficiency. Based on the result derived from the equilibrium analysis approach, a case is developed of calculate the maximum cold gasification efficiency using Van Krevelen diagram. Following assumptions are made for this analysis:

- Samples are taken as dry and ash free.
- Steady state flow is considered inside the gasifier.
- Potential and kinetic energies are neglected.
- Only the major species are considered in the product gases, i.e CO, CO<sub>2</sub>, H<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub>.
- The contribution of ash in energy equation is neglected.
- Ideal gas behavior is considered for all gas phase.
- The gasifier is considered to operate isothermally.
- No heat losses are considered from the gasifier, i.e adiabatic condition.
- Infinite residence time is considered, so that the reaction have ample amount of time to take place.
- At each gasification step, all product gases are considered at same temperature.

## 2. Feedstock Characterization

The baseline calculations are performed using four different feedstocks. The feedstocks are selected to represent the different regions of Van Krevelen diagram. As shown in Figure 1, the Van Krevelen diagram characterizes different type of feedstocks according to their respective H/C and O/C ratio. The highest H/C and O/C ratio represent the biomass and the lowest represent the Anthracite, where coal, lignite and peat come in between them.

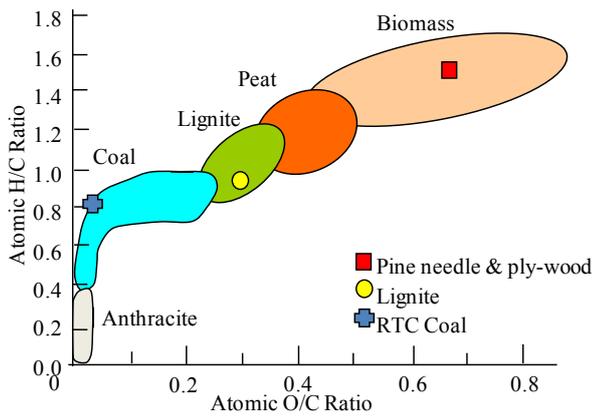


Figure 1: Van Krevelen Diagram [16]

Table 1 shows the ultimate analysis of dry ash free samples of four different feedstock performed at Masdar Institute (MI) in Waste to Energy laboratory using Flash (CHNS-O) analyzer. The percent weight of carbon present in coal is highest as compare to other three feedstocks. That shows the affinity of coal to form more CO when air-gasified. On the other hand, pine needles and ply-wood has high oxygen content that reduces the amount of oxygen required for gasification. The hydrogen contents of all feedstocks are within 1.65% to each other. Also, the close resemblance in the ultimate analysis of pine needles and ply-wood shows an expected same output during the gasification process.

Table 1: Ultimate analysis of feedstock based on dry ash free (DAF) basis

Feedstock	C %Wt	H %Wt	O %Wt	N %Wt	S %Wt
RTC coal	82.17	5.60	8.60	2.50	1.13
Pine needles	48.58	6.30	43.64	1.48	0.00
Ply-wood	49.59	6.28	43.74	0.39	0.00
Lignite[17]	66.03	4.65	25.64	2.07	1.62

The weight percent of each feedstock is used to calculate the empirical formula by considering only carbon, hydrogen, oxygen and nitrogen. Table 2 shows the empirical formula corresponding to each feedstock. These formulas are calculated on molar bases by normalizing through a single atom of carbon. The higher heating value (HHV), as shown in Table 2, are calculated using the following relation [18],

$$HHV \left( \frac{MJ}{Kg} \right) = 0.3491 C + 1.1783 H - 0.1043 O \quad (1)$$

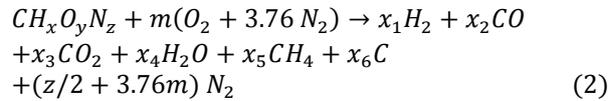
where C, H and O are the corresponding weight percentage of carbon, hydrogen and oxygen present in each feedstock. The results show that the coal has the highest HHV while pine needles and ply-wood have their HHV near to each other.

Table 2: Empirical formula and heating value (HHV) of feedstock

Feedstock	Empirical formula	HHV KJ/Kmole	HHV MJ/Kg
RTC coal	$CH_{0.7946}O_{0.0670}N_{0.0260}$	502928	34.38
Pine needles	$CH_{1.5550}O_{0.6736}N_{0.0261}$	489784	19.83
Ply-wood	$CH_{1.5196}O_{0.6615}N_{0.0067}$	487566	20.14
Lignite	$CH_{0.8450}O_{0.2912}N_{0.0268}$	469939	26.28

### 3. Gasification Model

The Global reaction of air gasification can be written as,



where x, y and z are number of atoms of hydrogen, oxygen and nitrogen based on a single atom of carbon. The right hand side of Equation (2) contains a single kmole of feedstock and known kmole of air (m). The left hand side of the Equation (2) composed of six unknowns, where,  $x_1, x_2, x_3, x_4, x_5$  and  $x_6$  are the kmole of each corresponding species. Nitrogen ( $N_2$ ) is not taken as an unknown because it is just a sum from the feedstock and oxidizer. Also,  $N_2$  is taken as un-reacted specie, so it goes in the reaction and comes out un-reacted. The one thing worth to mention at this point, that all the quantities x, y, z,  $x_1, x_2, x_3, x_4, x_5$  and  $x_6$  are based on single atom of carbon present in feedstock.

#### 3.1. Species mass balance

To calculate the value of six unknown, six equations are required. Three equations can be derived by the conservation of elemental mass present in the reactants and products. Followings are the mass balance of each element present in the Equation (2),

carbon balance

$$x_2 + x_3 + x_5 + x_6 - 1 = 0 \quad (3)$$

hydrogen balance

$$2x_1 + 2x_4 + 4x_5 - x = 0 \quad (4)$$

oxygen balance

$$x_2 + 2x_3 + x_4 - y - 2m = 0 \quad (5)$$

The nitrogen moles can directly be calculated by using of nitrogen present in feedstock and air, i.e.  $(\frac{z}{2} + 3.76m)$ . This value can be used to calculate the overall mole fraction, mass fraction of syngas and energy balance.

#### 3.2. Equilibrium constant formulation

Now three more equations are required that solved together with equation (3), (4) and (5) to calculate the equilibrium composition of product syngas. These equations are derived using the knowledge of equilibrium constants of elementary reactions. Higman [19] has described the elementary reactions as the intermediate reactions that leads to complete gasification. Solid carbon elementary reactions involving carbon (C), CO, CO<sub>2</sub>, H<sub>2</sub>, water (H<sub>2</sub>O) and CH<sub>4</sub> are necessary to describe the overall gasification process. The reactions are as follows,

boudouard reaction



CO shift reaction



methanation reaction



Therefore, the equilibrium constant is written for equation (6), (7) and (8) that enables to complete the six equation required to calculate the equilibrium composition of product syngas.

Equilibrium constant for boudouard reaction

$$K_1 = \frac{x_2^2}{x_3 x_{total}} \quad (9)$$

Equilibrium constant for CO shift reaction

$$K_2 = \frac{x_3 x_1}{x_2 x_4} \quad (10)$$

Equilibrium constant for methanation reaction

$$K_3 = \frac{x_5 x_{total}}{x_1^2} \quad (11)$$

where  $x_{total}$  is the total number of moles present in the product of Equation (2). That brings a new equation in the system and it is the total sum of moles of product species as follows,

$$x_{total} = x_1 + x_2 + x_3 + x_4 + x_5 + \left(\frac{Z}{2} + 3.76m\right) \quad (12)$$

The char ( $x_6$ ) represent the solid un- burnt carbon present in the product. Therefore charis excluded from the equation (12), that represent the sum of moles of gaseous phase.

The value of equilibrium constant is found out at constant temperature and pressure using the standard state Gibbs function of change( $\Delta G_T^o$ ) [21].

$$K_i = e^{-\frac{\Delta G_T^o}{RT}}, i = 1,2,3 \quad (13)$$

where  $R$  is the universal gas constant ( $R = 8.314 \frac{KJ}{Kmol K}$ ) and  $T$  is the absolute temperature in Kelvin. The value of  $\Delta G_T^o$  is calculated by taken the species present in the relevant elementary reactions. Therefore the value of  $\Delta G_T^o$  for boudouard, CO shift and methanation reaction is formulated,

$\Delta G_T^o$  for boudouard reaction

$$\Delta G_T^o = 2\Delta g_{f,CO}^o - \Delta g_{f,CO_2}^o \quad (14)$$

$\Delta G_T^o$  for CO shift reaction

$$\Delta G_T^o = \Delta g_{f,CO_2}^o + \Delta g_{f,H_2}^o - \Delta g_{f,CO}^o - \Delta g_{f,H_2O}^o \quad (15)$$

similarly,  $\Delta G_T^o$  for methanation reaction

$$\Delta G_T^o = \Delta g_{f,CH_4}^o - 2\Delta g_{f,H_2}^o \quad (16)$$

where  $\Delta g_{f,specie}^o$  represents Gibbs function of the pure species at standard state pressure (P=1 atm) at constant temperature. The value of  $\Delta g_{f,specie}^o$  at constant temperature can be expressed by the following empirical formula [20],

$$\Delta g_f^o = h_f^o - aT \ln(T) - bT^2 - \left(\frac{c}{2}\right)T^3 - \left(\frac{d}{3}\right)T^4 + \left(\frac{e}{2T}\right) + f + gT \quad (17)$$

The value of coefficients  $a, b, c, d, e, f, g$  and enthalpy of formation ( $h_f^o$ ) is presented in Table 3. The value of  $\Delta g_f^o$  for C and  $H_2$  is zero over the temperature range. Therefore, the contribution  $\Delta g_{f,C}^o$  and  $\Delta g_{f,H_2}^o$  in Equation (14), (15) and (16) is neglected.

Summarizing, the value of  $\Delta g_f^o$  from equation (17) is calculated for each species at corresponding temperature. Then this value is used in Equation (14), (15) and (16) to compute the value of  $\Delta G_T^o$  for boudouard, CO shift and methanation reaction. After that, the value of  $K_1, K_2$  and  $K_3$  are calculated using Equation (13). The value of equilibrium constants are used in Equation (9), (10) and (11) so that the only unknowns are the kmole of species. Finally, Equation (3), (4), (5), (9), (10) and (11) are solved simultaneously to find the equilibrium mole fraction of species.

### 3.3. Energy equation

In order to calculate the adiabatic temperature of gasification the energy balance between reactant and product is used,

$$\sum_{i=reactants} x_i h_{f,i}^o = \sum_{j=products} x_j (h_{f,j}^o + \Delta h_T) \quad (18)$$

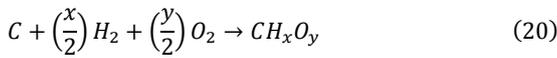
where  $x_i$  is the number of moles of reactants,  $h_{f,i}^o$  is the enthalpy of formation of reactants,  $x_j$  is the number of moles of product species,  $h_{f,j}^o$  is the enthalpy of formation of product species and  $\Delta h_T$  is the sensible enthalpy of product. The above equation can be expressed to the following expanded form when applied to equation (2)

**Table 3: The value of  $h_f^o$  and coefficients  $a, b, c, d, e, f, g$  in equation (17) for different species [20]**

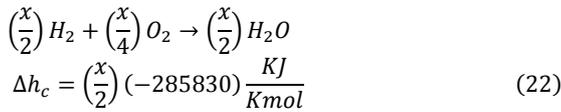
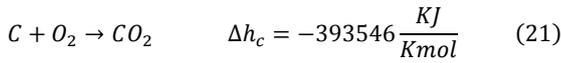
Species	$h_f$ (KJ/Kmole)	$a$	$b$	$c$	$d$	$e$	$f$	$g$
CO	-110.5	$5.619 \times 10^3$	$-1.190 \times 10^5$	$6.383 \times 10^9$	$-1.846 \times 10^{12}$	$-4.891 \times 10^2$	$8.684 \times 10^1$	$-6.131 \times 10^2$
CO <sub>2</sub>	-393.5	$-1.949 \times 10^2$	$3.122 \times 10^5$	$-2.448 \times 10^8$	$6.946 \times 10^{12}$	$-4.891 \times 10^2$	5.27	$-1.207 \times 10^1$
H <sub>2</sub> O	-241.8	$-8.950 \times 10^3$	$-3.672 \times 10^6$	$5.209 \times 10^9$	$-1.478 \times 10^{12}$	0	2.868	$-1.722 \times 10^2$
CH <sub>4</sub>	-74.8	$-4.620 \times 10^2$	$1.130 \times 10^5$	$1.319 \times 10^8$	$-6.647 \times 10^{12}$	$-4.981 \times 10^2$	$1.411 \times 10^1$	$-2.234 \times 10^1$

$$\begin{aligned} & \Delta h_{f,feedstock}^{\circ} + m h_{f,O_2}^{\circ} + 3.76 m h_{f,N_2}^{\circ} \\ & = x_1 (h_{f,H_2}^{\circ} + C_{p,H_2} \Delta T) + x_2 (h_{f,CO}^{\circ} + C_{p,CO} \Delta T) \\ & \quad + x_3 (h_{f,CO_2}^{\circ} + C_{p,CO_2} \Delta T) \\ & \quad + x_4 (h_{f,H_2O(vapor)}^{\circ} + C_{p,H_2O(vapor)} \Delta T) \\ & \quad + x_5 (h_{f,CH_4}^{\circ} + C_{p,CH_4} \Delta T) \\ & \quad + x_6 (h_{f,C}^{\circ} + C_{p,C} \Delta T) + \left(\frac{Z}{2} + 3.76m\right) \\ & \quad \left(h_{f,N_2}^{\circ} + C_{p,N_2} \Delta T\right) \end{aligned} \quad (19)$$

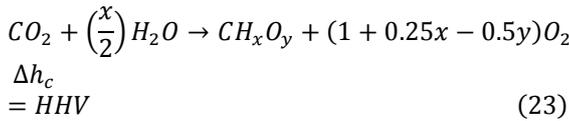
where  $C_p$  is the specific heat at constant pressure and  $\Delta T$  is the change in temperature with respect to reference temperature ( $T_1=298K$ ). The enthalpy of formation ( $h_f^{\circ}$ ) for  $O_2$  and  $N_2$  are zero at the reference state therefore the last two terms on left hand side of Equation (19) are eliminated. The enthalpy of formation of feedstock is calculated using the method defined by Zainal et al. [13]. In the calculation the presence of nitrogen in the feedstock is neglected as its contribution is small. The general formulation follows as,



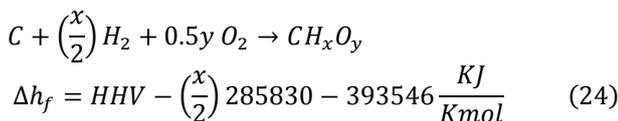
The above reaction is a hypothetical reaction showing the formation of feedstock. The near to realistic mechanism that contribute the formation feedstock follows as,



The value of heat of combustion in Equation (22) is based on the heating value of the feedstock. If the lower heating value (LHV) is used then it is necessary to use the heat of formation of water vapor. In the present calculations the HHV of the feedstock is used, therefore the heat of formation of liquid water is used. The resultant reaction attributed to HHV of feedstock and is written as,



Adding Equation (20), (21) and (22) yields,



The above formula is used to calculate the enthalpy of formation of feedstock. The enthalpy of formation of species in Equation (19) is used from Table 4.

The average specific heat over the temperature range used in Equation (19) is calculated by the following the formula of [22],

$$C_{p,i} = R \left( A + B T_{average} + \frac{C}{3} (4 T_{average}^2 - T T_1) + \frac{D}{T T_1} \right) \quad (25)$$

where  $T$  is the adiabatic gasification temperature acts like the only unknown in Equation (19),  $T_1$  is the reference temperature (298 K),  $R$  is the universal gas constant,  $T_{average}$  is the arithmetic mean of  $T$  and  $T_1$  i.e.  $\left(\frac{T+T_1}{2}\right)$  and  $A$ ,  $B$ ,  $C$  and  $D$  are the coefficients that are available in Table 5. The  $C_p$  for carbon is calculated from the following polynomial developed by using the NIST-JANAF table [23],

$$C_{p,C} = -6.7555 + 6.6253 \times 10^{-2} T - 5.8148 \times 10^{-5} T^2 + 2.4113 \times 10^{-8} T^3 - 3.812 \times 10^{-12} T^4 \quad (26)$$

**Table 4: Enthalpy of formation ( $\Delta h_{f,i}^{\circ}$ ) of species [22]**

Species	hf(KJ/Kmole)
Carbon dioxide (CO <sub>2</sub> )	394359
Carbon monoxide (CO)	137169
Methane (CH <sub>4</sub> )	50460
Water (liquid) (H <sub>2</sub> O)	237129
Water (vapor) (H <sub>2</sub> O)	228572
Hydrogen (H <sub>2</sub> )	0
Oxygen (O <sub>2</sub> )	0
Nitrogen (N <sub>2</sub> )	0
Carbon (C)	0

**Table 5: Constant used for specific heat capacity in Equation (25) [13]**

Species	T <sub>max</sub>	A	10 <sup>3</sup> B	10 <sup>6</sup> C	10 <sup>-5</sup> D
Methane	1500	1.702	9.081	2.164	0
Hydrogen	3000	3.249	0.422	0	0.083
Carbon monoxide	2500	3.376	0.557	0	0.031
Carbon dioxide	2000	5.457	1.047	0	1.157
Nitrogen	2000	3.28	0.593	0	0.04
Water	2000	1.771	0.771	0	0.121

Summarizing energy equation,

1. The value of  $m$ ,  $x_1$ ,  $x_2$ ,  $x_4$ ,  $x_5$  and  $x_6$  are known from previous step.
2. The enthalpy of formation of feedstock is calculated using Equation (24).
3. The enthalpy of formation of other species is taken from Table 4.
4. Specific heat at constant pressure is calculated using Equation (25) and (26).
5. Finally, the Equation (19) is solved for only unknown value of  $T$ , the adiabatic gasification temperature.

### 3.4. Calculation Procedure

At the start an initial value of  $T$  is assumed i.e.  $T=300$  K. At this value the equilibrium moles of product syngas is computed using Equation (3), (4), (5), (9), (10) and (11). After that, the values of moles are substituted in energy Equation (19) to

calculate the actual value of adiabatic gasification temperature ( $T$ ). Then the calculated value of  $T$  is again used to calculate equilibrium moles of species. This process is repeated until the value of  $T$  become stable and that gives the actual adiabatic gasification temperature and mole of product species.

#### 4. Result and Discussion

The model is run for all four feedstocks with varying air supply. The increasing amount of air causes to rise up the temperature to convert all the char, yet burning more of the feedstock. At every step the cold gas efficiency (CGE) is calculated using the following formula,

$$CGE = \frac{HHV_{product\ gases}}{HHV_{feedstock}} \quad (27)$$

The product gases that contribute in the higher heating value are carbon monoxide, hydrogen and methane. The inclusion of HHV of product gases gives the updated formula of CGE as,

$$CGE = \frac{x_1(283800) + x_2(283237.12) + x_5(889000)}{HHV_{feedstock}} \quad (28)$$

Now, using the gasification model the results are presented showing the product gas composition, temperature and CGE through parametric study of oxidizer input. Figure 2 shows the result of equilibrium analysis for RTC coal. It shows that the increase in the amount of air tends to raise the temperature of the product. The rise in temperature causes to produce more carbon monoxide in initial phase that directly increase the CGE. At 1024 K the CGE reaches to its maximum value of 68.5%. It is evident from the graph that CGE act like a normal distribution, i.e having a maximum value at certain point that tends to decrease at both ends. At maximum CGE, the kilo mole of CO, CO<sub>2</sub>, H<sub>2</sub> and H<sub>2</sub>O are 0.91, 0.09, 0.37 and 0.03, respectively. Further increase in air supply tends to convert CO into CO<sub>2</sub> and H<sub>2</sub> into H<sub>2</sub>O, that brings the CGE to lower value. The results are based on kilo mole of product per kilo mole of the feedstock, that shown a very small quantity of methane (nearly zero) in the results. Due to high HHV of methane, small quantity can lead to a significant change in the CGE, but the result of analysis shows that at point of maximum CGE the quantity of methane is of order minus four. It makes the contribution of methane almost negligible to account for maximum CGE.

Figure 2 show the results of equilibrium analysis for pine needles. The overall trend of the graph is similar to Figure 3. The maximum CGE of 76% is achieved at 978°K. This significantly increased value of maximum CGE as compare to RTC coal is achieved because of increased hydrogen and oxygen content in the pine needle. The rich hydrogen content in the pine needle enable to produce more hydrogen gas in product mixture and while the oxygen present in the mixture tends to react with solid carbon to make carbon monoxide. The high content of oxygen present in pine needles also enables to utilize lesser amount of air to achieve the desire temperature. Figure 4 shows the equilibrium analysis of ply-wood. The maximum CGE of 76.5% is achieved at 980° K. These values are in close proximity with the results achieved for pine needle. The difference in the temperature is by the virtue of small change in composition and HHV. Similarly, Figure 5 shows the maximum CGE of 74% for lignite at 1134°K temperature.

The results of all four feedstock shows that the maximum CGE is achieved when all the carbon present in feedstock is converted into CO or CO<sub>2</sub> while hydrogen content of feedstock

transformed in to H<sub>2</sub> gas or H<sub>2</sub>O. At maximum CGE, on average 15% of carbon is converted into CO<sub>2</sub> and rest form CO. Similarly, 10% of hydrogen present in the feedstock converted in H<sub>2</sub>O and rest goes to form H<sub>2</sub>. By using this conclusion, the maximum CGE of any feedstock present on Van Krevelen diagram can be calculated by using following reaction:

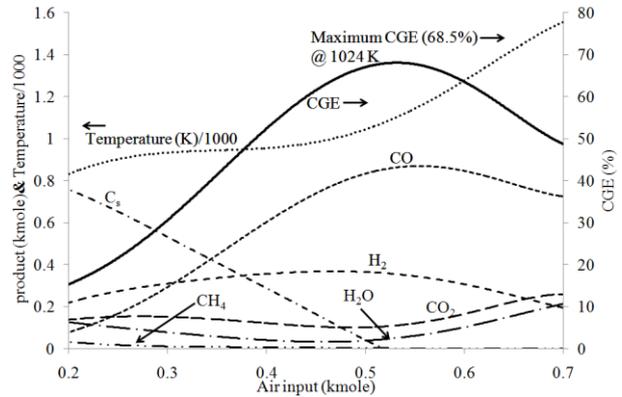
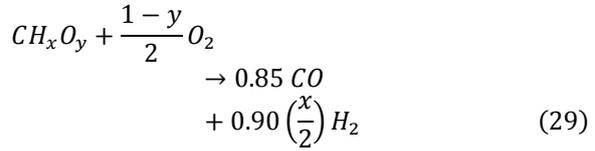


Figure 2: Equilibrium analysis for RTC coal showing CGE, Temperature and product gas composition

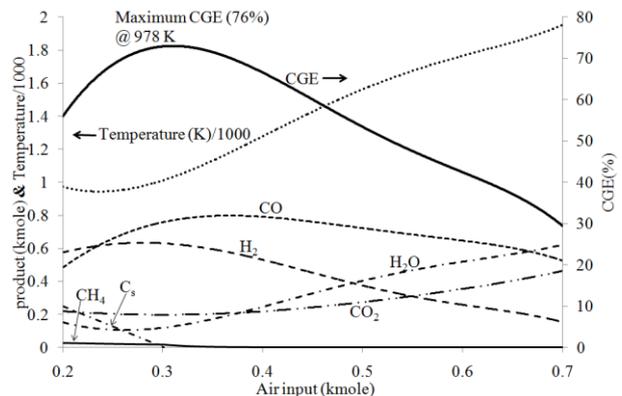
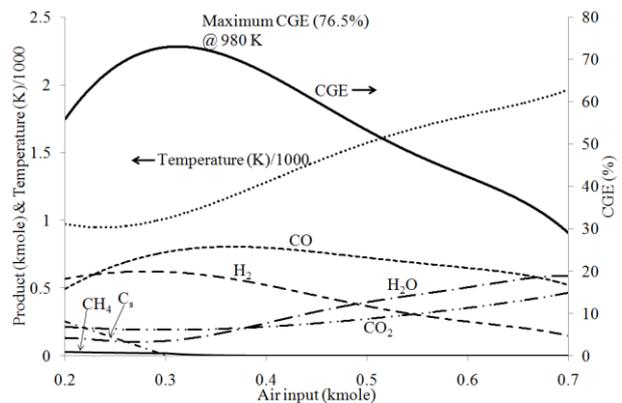
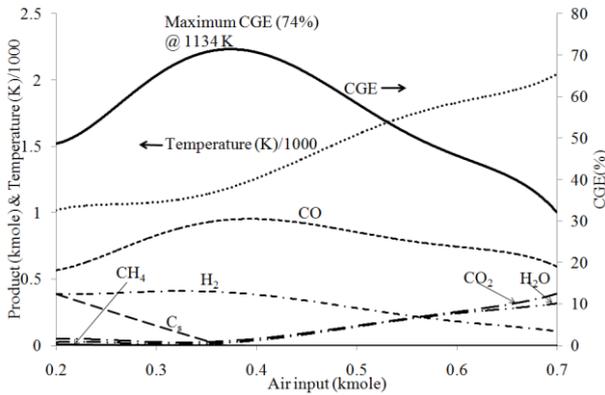


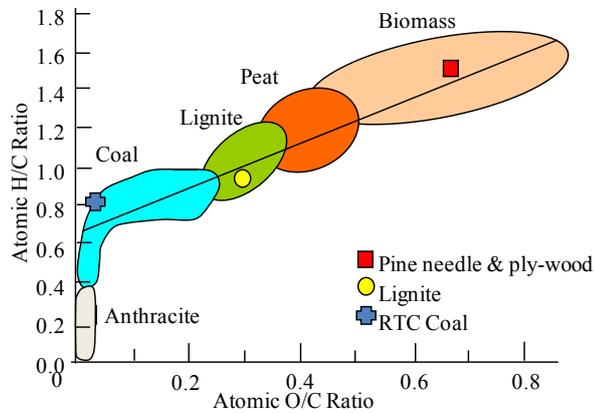
Figure 3: Equilibrium analysis for Pine wood showing CGE, Temperature and product gas composition



**Figure 4: Equilibrium analysis for Ply-wood showing CGE, Temperature and product gas composition**



**Figure 5: Equilibrium analysis for Lignite showing CGE, Temperature and product gas composition**



**Figure 6: Straight line approximation for Van Krevelen diagram**

As the O/C ratio on Van Krevelen diagram remains less than one, therefore the equation (29) remains valid for the entire region of the diagram. To demonstrate the process, a straight line is created on Van Krevelen diagram that passes through all major four zones, as shown in Figure 6. The equation (30) shows the equation of the line derived from Van Krevelen diagram. Only thing that account to develop the polynomial is to stay in the region inside the shaded area of diagram. The equation (30) provides the composition  $x$  of feedstock by specifying the amount of  $y$ . Although, a high order polynomial can be developed that account for all zones of the diagram, but for illustration, only a simplest line approach is used.

$$x = 1.1136 y + 0.6477 \quad (30)$$

The equation (1) is based on the weight percent of carbon, hydrogen and oxygen but it can be modified to produce the desired result of HHV by providing the value of  $x$  and  $y$ , as follows,

$$HHV \left( \frac{KJ}{Kmole} \right) = 418920 + 117830 x - 166880 y \quad (31)$$

The value of  $x$  and  $y$  in equation (30) and (31) are same as specified for the feedstock in equation (2). These values are actually H/C and O/C ratio used in Van Krevelen diagram. Now, to calculate the maximum CGE the value of  $x$  is calculated by increasing value of  $y$ . Once, the value of  $x$  and  $y$

are known then equation (31) is used to calculate the HHV of the corresponding feedstock. The maximum kmole of carbon monoxide and hydrogen is calculated using equation (29). After that, equation (28) is used to calculate the maximum CGE for the corresponding feedstock. The results are tabulated in Table 6 over the feedstock range on Van Krevelen diagram.

The result shows an increasing trend of CGE by increasing the amount of  $x$  and  $y$ . The mole of carbon monoxide is held 0.85 because it is assumed that 85% of carbon present in feedstock is converted into CO at CGE. Also, the excess amount of oxygen need to form a single mole of carbon monoxide is provided from the air input from outside the system. The formation of hydrogen is only dependent on the value of  $x$ , which is the only source of hydrogen in the system. So, as the value of  $x$  increase the number of moles of hydrogen increase. Table 6 shows a growing trend of CGE with increasing value of  $x$  and  $y$ . Practically, it is nearly impossible to achieve these high value of CGE. This high efficiency is because the usage of dry and ash free samples for the analysis. If the moisture and ash is considered for the analysis then they lower the temperature of the gasification process and eventually lower the system efficiency. But one thing is obvious from the Table 6 that increases in the value of  $x$  and  $y$  will also increase the CGE.

**Table 6: Maximum CGE by complete conversion of carbon into carbon monoxide**

#	y	x	HHV (kJ/kmole)	CO (kmole)	H2 (kmole)	CGE (%)
1	0.10	0.76	491672.04	0.85	0.34	68.74
2	0.20	0.87	488105.59	0.85	0.39	72.15
3	0.30	0.98	484539.14	0.85	0.44	75.61
4	0.40	1.09	480972.69	0.85	0.49	79.12
5	0.50	1.20	477406.24	0.85	0.54	82.69
6	0.60	1.32	473839.78	0.85	0.59	86.30
7	0.70	1.43	470273.33	0.85	0.64	89.98
8	0.80	1.54	466706.88	0.85	0.69	93.71

### 5. Conclusion

A thermodynamics equilibrium approach is used to calculate the maximum cold gasification efficiency of the gasification process. Air is used as oxidizer to gasify four different feedstock. Using the result of ultimate analysis of feedstock the empirical formula and heating values are calculated. The empirical formula is used to build the global gasification reaction that shows seven species (including solid carbon) as the product of gasification. To calculate the product composition seven equations are used that represented the four elemental balance equations and the three equilibrium constants. The gasification temperature is calculated using the energy equation following an iterative process. The result shows that, on dry and ash free basis, the maximum gasification efficiency of 68.5%, 76.0%, 76.5% and 74.0% can be achieved for RTC coal, pine needle, ply-wood and lignite, respectively. The trend of results shows that the maximum CGE is achieved when most of the solid carbon present in the feedstock is converted into carbon monoxide. Using the maximum potential of carbon monoxide, an idealized approach is used to calculate the CGE for Van Krevelen diagram. It shows increasing O/C and H/C ratio directly affects the CGE. The increase in the value of both ratios gives a raise to the CGE.

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