

## **Modelling equations for the properties of producer gas generated from biomass gasifiers**

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### **Abstract**

Producer gas (PG) generated from biomass by thermo-chemical gasification process has been proved as a reliable, renewable and indigenous substitute for petroleum fuels to drive internal combustion engines. Since biomass gasification involves a set of various chemical reactions occurring simultaneously in the same reactor, it is being probed by many researchers to improve the yield of PG and its quality. The quality of PG is assessed on the basis of the values of certain desirable properties like heating value, Wobbe index, stoichiometric air-PG ratio, adiabatic flame temperature, burning velocity, etc. There are elaborate instrumental methods available for physically measuring these properties. However, they can also be calculated more conveniently by using modelling equations involving the properties of its constituent gases. In this article, modelling equations for the theoretical calculation of certain properties of PG are given. Using these equations, the properties of PG having a typical composition of CO-16 %, H<sub>2</sub>-17 %, CH<sub>4</sub>-1 %, CO<sub>2</sub>-13 %, N<sub>2</sub>-49 % and H<sub>2</sub>O-4 % have been determined and tabulated.

**Keywords:** Producer Gas, Biomass Gasifier, Modelling Equations

### **1. Introduction**

Thermo-chemical gasification of biomass involves a set of chemical reactions in which the solid biomass is reacted with sub-stoichiometric air at high temperature to generate Producer Gas (PG). The PG contains CO, H<sub>2</sub>, CH<sub>4</sub>, CO<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>O and small amounts of tar & particulates.

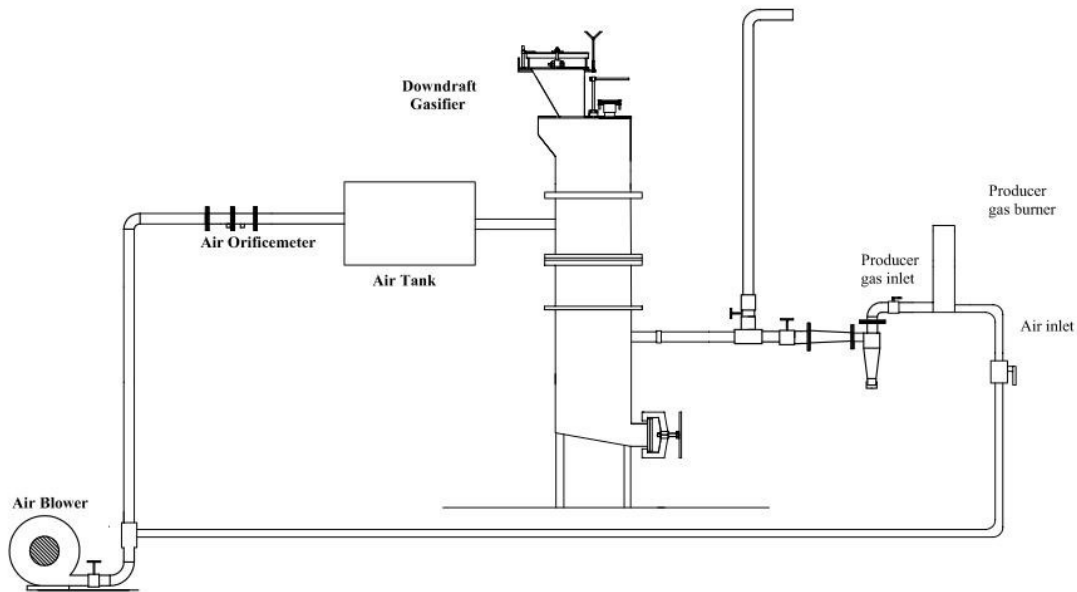
For the generation of PG, different types of biomass and different types of biomass gasifiers are available. Due to these, the generated PG will have properties varying within a range of values. The composition of PG generated from an air-blown,

downdraft biomass gasifier generally varies over a certain range: CO-15-20%, H<sub>2</sub>-15-20%, CH<sub>4</sub>-1-3%, CO<sub>2</sub>-12-14%, N<sub>2</sub>-45-50%, H<sub>2</sub>O-4-8%, on wet basis. In this mixture, the burnable constituents viz., CO, H<sub>2</sub>, and CH<sub>4</sub> sum up to about 35%.

To determine the various thermo-chemical, thermodynamic and transport properties of PG, costlier and sophisticated instruments are available. However, many of these properties can be theoretically calculated by using modelling equations for a preliminary information concerning PG. It is the objective of the present study.

## 2. PG and its generation

Before calculating the properties of PG, it may be useful to know about the method of generation of PG and its utility. Figure 1 is the schematic layout of downdraft type biomass gasification system. When PG is required for burning at a burner or for driving an engine, then it has to be simultaneously generated from a biomass gasifier. It is not economical to store PG in containers for using it later. It is due to its lower energy density than LPG. By feeding biomass into the gasifier and supplying sub-stoichiometric air into it, PG can be generated from the gasifier as a result of high temperature reactions under controlled conditions.



**Figure 1:** Layout of biomass gasification system

The generated PG has a good heating value and it can be burnt in a burner for heating application or it can be supplied to an engine for deriving mechanical work. Figure 2 illustrates the combustion of PG in a burner.



**Figure 2:** Flaring of PG in a burner

### 3. Calculation of thermo-chemical properties of PG using modelling equations

Each constituent gas of PG varies generally over a typical range as mentioned before. However, in this paper the composition of PG is taken as CO-16 %, H<sub>2</sub>-17 %, CH<sub>4</sub>-1 %, CO<sub>2</sub>-13 %, N<sub>2</sub>-49 % and H<sub>2</sub>O-4 % (Hall and Over end, 1987) for the purpose of calculation of various properties.

The pressure of PG generated by the biomass gasifier is slightly higher than atmospheric pressure. The partial pressures of component gases in PG mixture are lower than their respective critical point pressures. After cooling and cleaning, the temperature of PG is brought down to atmospheric temperature which is still higher than the critical point temperatures of component gases. Due to these factors, the PG has been treated as an ideal gas mixture while calculating the properties which are discussed below.

#### 3.1 Molar Mass

Assuming the gas mixture to behave ideally, the molar mass of PG mixture has been calculated using the equation (1).

$$M_m = \sum_i \frac{n_i}{n_m} M_i \quad (1)$$

In the calculation of molar mass, the subscript ‘i’ refers to CO, H<sub>2</sub>, CH<sub>4</sub>, CO<sub>2</sub>, N<sub>2</sub> and H<sub>2</sub>O. The calculated value of molar mass for PG is 25.14.

#### 3.2 Lower Heating Value

The lower heating value of the PG has been calculated using the equation (2).

$$\text{LHV}_m = \sum_i \frac{n_i}{n_m} \text{LHV}_i \quad (2)$$

The lower heating value of PG calculated using the above equation is 4042 kJ/m<sup>3</sup>. Many researchers (Madhukar and Goswami, 2007, Po-Chih Kuo et al, 2014) have experimentally determined the lower heating value of PG and found it to be in the range of 4000-5000 kJ/m<sup>3</sup>.

### 3.3 Wobbe index

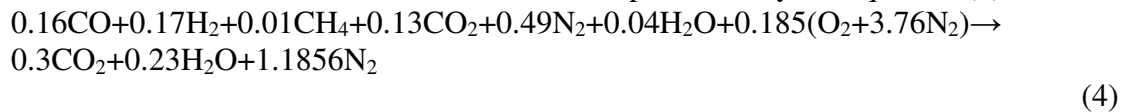
Wobbe index is a measure of energy per unit volume of gaseous fuels. It is given by the equation(3).

$$\text{Wobbe index} = \frac{\text{Heating value}}{\sqrt{\text{Specific Gravity}}} \quad (3)$$

A higher value of Wobbe index is considered desirable for gaseous fuels (Derek, 2008).

### 3.4 Stoichiometric air-PG ratio

The stoichiometric combustion of PG in air is represented by the equation (4).



The stoichiometric air-PG ratio for the above reaction has been calculated to be 1.01 on mass basis. The calculation of this quantity is considered vital before conducting experiments on gasifiers at various equivalence ratios.

### 3.5 Adiabatic flame temperature

The stoichiometric combustion of PG in air has earlier been represented by the equation (4). The adiabatic flame temperature of the above stoichiometric air-PG mixture has been calculated by using the equation (5).

$$\sum N_p (\bar{h}_f^\circ + \bar{h} - \bar{h}^\circ)_p = \sum N_r (\bar{h}_f^\circ + \bar{h} - \bar{h}^\circ)_r \quad (5)$$

This is the steady flow energy equation or the case of adiabatic combustion with no work transfer. By trial and error method, the adiabatic flame temperature has been found such that equation (5) is satisfied. NIST-JANAF thermo-chemical tables (Malcolm, 1998) have been referred for the specific enthalpy values. The adiabatic flame temperature has been found to be 1770 K for stoichiometric air-PG mixture.

### 3.6 Laminar burning velocity

The laminar burning velocity  $S_L$  is defined as the velocity with which the flame front advances through the un reacted gas in the direction normal to the flame surface. It cannot be treated as a constant for PG since it is a mixture of several constituent gases. It depends on several variables like composition of PG, equivalence ratio, pressure and temperature, etc. Therefore, its calculation is useful in the design and

construction of PG burners and engines. It is not obtained by solving a single equation, but by a set of equations such as those of reaction rate, burning velocities, specific enthalpies of constituent gases, etc. Ravindra Babu (2009) has given the procedure for the calculation of laminar burning velocity of producer gas-air mixture. The burning velocities for different species are calculated and the convergence of these burning velocities as well with time of integration was used to determine the steady state.

The laminar burning velocity  $S_{L,\infty}$  can be calculated based on mass fraction profiles using the following equations of individual species.

$$S_{L,k} = \frac{\int_{-\infty}^{+\infty} \dot{\omega}_k dx}{\rho(Y_{k,u} - Y_{k,b})}; k = 1, \dots, N_s \quad (6)$$

$S_L$  obtained from the above equations converge to the same value as the computations converged. It is about 0.4-0.5 m/s for PG-air mixture at atmospheric pressure and temperature.

Of the various components of PG, the inert gases  $N_2$  and  $CO_2$  reduce the flame speed. Also, the hydrocarbons like  $CH_4$  and higher molecular weight tar compounds reduce the flame speed. At the same time, the burnable gases like  $H_2$  increase the flame speed. Typically, the laminar burning velocity is high when the flame temperature is high (Gary and Kenneth, 1998).

#### 4. Calculation of thermodynamic properties of PG using modelling equations

##### 4.1 Molar specific heat capacities

If PG is considered as an ideal gas mixture containing a number of component gases, then the thermodynamic properties of the PG such as molar specific heat capacity at constant pressure  $\bar{c}_{p,m}$  and molar specific heat capacity at constant volume  $\bar{c}_{v,m}$  are given by equations (7) and (8).

$$\bar{c}_{p,m} = \sum_i \frac{n_i}{n_m} \bar{c}_{p,i} \quad (7)$$

$$\bar{c}_{v,m} = \sum_i \frac{n_i}{n_m} \bar{c}_{v,i} \quad (8)$$

In the calculation of molar specific heats using equations(7) and(8), the subscript 'i' refers to  $CO$ ,  $H_2$ ,  $CH_4$ ,  $N_2$ ,  $CO_2$  and  $H_2O$  which are the constituents of PG. The calculated values of molar specific heat capacities of PG at Normal Temperature of 298 K and Pressure of 1 atm (NTP) are listed in Table 2. The temperature dependence of molar specific heat capacity at constant pressure of a gas can be given by a cubic equation (9) (Yunus and Michael, 2006).

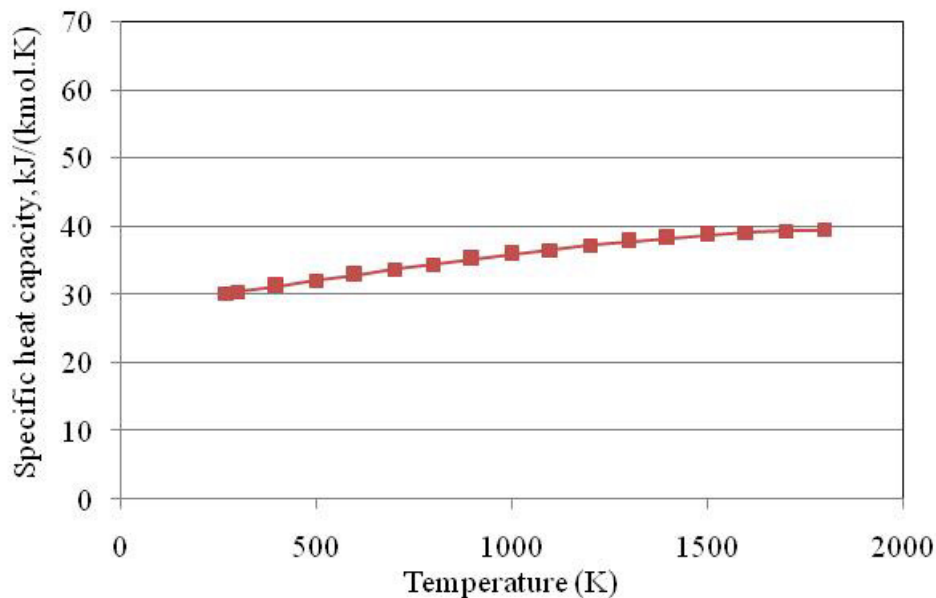
$$\bar{c}_p = a + bT + cT^2 + dT^3 \quad (9)$$

The coefficients of temperature employed in the equation (9) are given in Table 1.

**Table 1:** Coefficients of temperature employed in equation (9) for constituent gases

Constituent Gases of PG	a	b	c	d
CO	28.16	$0.1675 \times 10^{-2}$	$0.5372 \times 10^{-5}$	$-2.2220 \times 10^{-9}$
H <sub>2</sub>	29.11	$-0.1916 \times 10^{-2}$	$0.4003 \times 10^{-5}$	$-0.8704 \times 10^{-9}$
CH <sub>4</sub>	19.89	$5.0240 \times 10^{-2}$	$1.2690 \times 10^{-5}$	$-11.0100 \times 10^{-9}$
CO <sub>2</sub>	22.26	$5.9810 \times 10^{-2}$	$-3.5010 \times 10^{-5}$	$7.4690 \times 10^{-9}$
N <sub>2</sub>	28.90	$-0.1571 \times 10^{-2}$	$0.8081 \times 10^{-5}$	$-2.8730 \times 10^{-9}$
H <sub>2</sub> O	32.24	$0.1923 \times 10^{-2}$	$1.0550 \times 10^{-5}$	$-3.5950 \times 10^{-9}$

Using equation (9), the values of  $\bar{c}_{p,m}$  of PG at different temperatures are calculated and the results are shown in Figure 3.

**Figure 3:** Plot of molar specific heat capacity  $\bar{c}_{p,m}$  of PG at various temperatures

#### 4.2 Absolute entropy

Unlike enthalpy, the entropy of a gas depends not only on its temperature but also on its pressure. Gibbs theorem states that the total entropy of a mixture of gases is the sum of the partial entropies of the constituent gases. Thus, the entropy of PG is calculated as a weighted sum of the entropies of the constituent gases. The absolute entropy of PG at 298 K and total pressure 1 atm is given by equations(10) and (11).

$$s_{\text{mix}}(T, P) = \sum_i Y_i s_i(T, P) \quad (10)$$

$$s_i(T, P_i) = s_i(T, P_{ref}) - R \ln \frac{P_i}{P_{ref}} \quad (11)$$

In the calculation of absolute entropy of PG, 'i' refers to CO, H<sub>2</sub>, CH<sub>4</sub>, CO<sub>2</sub>, N<sub>2</sub> and H<sub>2</sub>O. The calculated value is given in Table 2.

### 4.3 Gibbs free energy

The Gibbs free energy is an important thermodynamic property when equilibrium approach is followed in the analysis of combustion of PG with air. Gibbs function for a mixture of ideal gases is given by equation (12).

$$G_m = \sum N_i \bar{g}_{i,T} = \sum N_i \left[ \bar{g}_{i,T}^\circ + R_u T \ln \left( \frac{P_i}{P^\circ} \right) \right] \quad (12)$$

For the calculation of Gibbs function of PG, 'i' refers to CO, H<sub>2</sub>, CH<sub>4</sub>, CO<sub>2</sub>, N<sub>2</sub> and H<sub>2</sub>O.

### 4.4 Reversible Work

It is the maximum work that can be done during a process. For the steady flow combustion process which involves heat transfer with only the surroundings at T<sub>o</sub>,

$$W_{rev} = \sum_i N_r \bar{g}_{i,r} - \sum_i N_p \bar{g}_{i,p} \quad (13)$$

The reversible work, that is the maximum possible work, obtainable from PG has been calculated using the equation (13) and it is given in Table 2.

## 5. Calculation of transport properties of PG using modelling equations

### 5.1 Mass density

It is the mass per unit volume of PG and it can be calculated using equation (14).

$$\rho_m = \frac{P_m}{T} \sum_i \frac{n_i}{n_m R_i} \quad (14)$$

### 5.2 Absolute viscosity

The absolute viscosity of PG has been calculated using the equation (15) which was proposed by Wilke (1950) for multi-component systems with ideal gas behaviour.

$$\text{Absolute viscosity } \mu_m = \sum_i \frac{\mu_i}{1 + \frac{1}{y_i} \sum_{j=1, j \neq i} (y_j \phi_{ij})} \quad (15)$$

where

$$\varphi_{ij} = \frac{\left[1 + \left(\frac{\mu_i}{\mu_j}\right)^{\frac{1}{2}} \left(\frac{M_j}{M_i}\right)^{\frac{1}{4}}\right]^2}{2\sqrt{2} \left[1 + \left(\frac{M_i}{M_j}\right)\right]^{\frac{1}{2}}} \quad (16)$$

In the relations (15) and (16), the subscript 'i' and 'j' refer to CO, H<sub>2</sub>, CH<sub>4</sub>, CO<sub>2</sub>, N<sub>2</sub> and H<sub>2</sub>O which are the constituents of PG.

### 5.3 Thermal conductivity

The thermal conductivity of PG has been calculated using the equation (17) which was used by Mishra (2010).

$$\text{Thermal conductivity } k_m = \sum_i \frac{k_i}{1 + \sum_{\substack{j=1 \\ j \neq i}} \varphi_{ij} \frac{y_j}{y_i}} \quad (17)$$

where

$$\varphi_{ij} = \frac{1.065 \left[1 + \left(\frac{k_i^\circ}{k_j^\circ}\right)^{\frac{1}{2}} \left(\frac{M_i}{M_j}\right)^{\frac{1}{4}}\right]^2}{2\sqrt{2} \left(1 + \frac{M_i}{M_j}\right)^{\frac{1}{2}}} \quad (18)$$

In the relations (17) and (18), the subscript 'i' and 'j' refer to CO, H<sub>2</sub>, CH<sub>4</sub>, CO<sub>2</sub>, N<sub>2</sub> and H<sub>2</sub>O which are the constituents of PG.

### 5.4 Diffusion coefficient

The diffusion coefficient when air diffuses into the constituent gases of PG have been calculated using the equation (19) which was proposed by Fairbanks and Wilke (1950) and the calculated value is listed in Table 2.

$$\text{Diffusion coefficient } D_{\text{air-PG}} = \frac{1 - y_{\text{air}}}{\sum_i \frac{y_i}{D_{\text{air-i}}}} \quad (19)$$

## 6. Results of calculation for the theoretical determination of various properties of PG

The values of various properties of PG have been calculated by using the modelling equations discussed above and these values are listed in Table 2.



**Table 2:** Properties of PG calculated by using the modelling equations

Parameters	Symbol	Units	Value
Chemical composition of PG:			
Carbon monoxide	CO	vol %	16
Hydrogen	H <sub>2</sub>	vol %	17
Methane	CH <sub>4</sub>	vol %	1
Carbon dioxide	CO <sub>2</sub>	vol %	13
Nitrogen	N <sub>2</sub>	vol %	49
Water vapour	H <sub>2</sub> O	vol %	4
Molar mass	M <sub>m</sub>	kg/kmol	25.14
Lower Heating Value	LHV <sub>m</sub>	kJ/m <sup>3</sup>	4042
Specific gravity at NTP	SG	-	0.87
Wobbe Index	WI	kJ/m <sup>3</sup>	4171
Stoichiometric air-PG ratio	(A/F) <sub>stoic</sub>	kg air/kg PG	1.01
Adiabatic Flame Temperature	T <sub>adfl</sub>	K	1770
Laminar burning velocity	S <sub>L</sub>	m/s	0.45
Molar specific heat capacity at constant pressure at NTP	$\bar{c}_{p,m}$	kJ/(kmol.K)	30.36
Molar specific heat capacity at constant volume at NTP	$\bar{c}_{v,m}$	kJ/(kmol.K)	22.05
Absolute entropy of PG	$\bar{s}_m^\circ$	kJ/(kmol.K)	196.44
Reversible Work	W <sub>rev</sub>	kJ/kmol	88021
Mass density at NTP	$\rho$	kg/m <sup>3</sup>	1.03
Absolute viscosity	$\mu_m$	kg/(m.s)	1.57263x10 <sup>-5</sup>
Thermal conductivity	k <sub>m</sub>	W/(m.K)	0.0344
Diffusion coefficient	D <sub>air-mixt</sub>	m <sup>2</sup> /s	0.209x10 <sup>-4</sup>

If more accurate property values are desired, then PG has to be treated as real gas mixture while doing property calculations, by incorporating pressure and volume corrections.

## 7. Conclusions

The properties of PG, which is a mixture of several constituent gases, have been calculated by using modelling equations and are given in a tabular form. In the development of these modelling equations, certain assumptions like ideal gas behaviour, frictionless processes, adiabatic conditions have been assumed. If more accurate results are required, then real gas behaviour of constituent gases, processes involving friction and non-adiabatic conditions have to be assumed.

## Nomenclature

n	-	Number of moles	
n <sub>m</sub>	-	Number of moles of the mixture	
M <sub>m</sub>	-	Molar mass of the mixture	kg/kmol
LHV <sub>m</sub>	-	Lower Heating Value	kJ/m <sup>3</sup>

$\bar{h}_f^\circ$	- Molar specific enthalpy of formation	kJ/kmol
$\bar{h}^\circ$	- Molar specific enthalpy at reference state	kJ/kmol
$\bar{h}$	- Molar specific enthalpy at any temperature	kJ/kmol
$\dot{\omega}_k$	- Volumetric production/consumption rate of chemical species	
$\rho$	- Density	kg/m <sup>3</sup>
Y	- Mass fraction	
R	- Characteristic gas constant	kJ/(kg.K)
R <sub>u</sub>	- Universal gas constant	kJ/(kmolK)
y	- Mole fraction	

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