

SIMULATION OF ACACIA GASIFICATION PROCESS

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ABSTRACT

This electronic document presents the thermokinetic modelling of the gasification process done on acacia-tree with variable operating conditions and different humidity levels. Gasification does not produce flue gas, but due to imperfect burning, synthesis gas appears which is rich in flammable components (CO_2 and H_2). The chemical structure of this gas depends on the components of the fuel and the humidity level, but greatly affected by the technological parameters too, such as pressure and temperature, as well as the air-ratio. The study shows the change in the amount of the fuel and the reaction efficiency, caused by varying gasification temperature and pressure. Rising temperature results in improved efficiency, while higher pressure worsens reaction efficiency. However, at higher temperature intervals, the effect of the pressure is neglectable.

Keywords: acacia, gasification, pressure, temperature, air-ratio, reaction efficiency

1. INTRODUCTION

Nowadays one of the most important research fields is the energetics, which includes the production of energy, the consumption of energy and the improvement of the efficiency of the process. We can often hear about the gasification technology and wood-gas boilers taking part in heat-energy production. Gasification technology is not only able to produce heat, but electricity too, as the main product of the gasification process is the combustible synthesis gas, which can be utilized by gas engines and turbines with high efficiency. The poor calorific value and low-grade quality of gas can decrease efficiency and power of the gas powered machines, so the examination of wood gasification is inevitable due to the gas composition. Besides these facts, wood gasification gives a great opportunity to build wood and biomass fueled quick-start power plants, which would be able to provide a solution for the changing energy demand.

2. HISTORICAL REVIEW OF GASIFICATION

Gasification is one of the oldest processes used to convert solid fossils and renewable fuels into combustible synthesis gas and liquid fuel. This technology was first used by Thomas Shirley, who produced hydrogen in 1659. Robert Gardner filled the first patent in 1788 and the spread of gasification process began. Its industrial application is associated with William Murdoch and began in 1798 in England and France [1].

At the beginning, combustible gases (wood and carbon gas) were produced from wood and coal, and were mainly used for heating and public lighting purposes. By 1850, technology reached a level of development that allowed 75% of London's public lighting to be solved with the help of gases, produced this way. Some years later, the gasification technology appeared in the United States too, and by 1920, it was used in most of the cities for heating and public lighting [2].

Following the discovery of Texas oil fields, the first natural gas pipeline was built in Denver, which eliminated the predominance of synthesis gas. After discovering the oil field under the North Sea, gas plants went into oblivion in Europe over time too. Although the last one was unveiled in England in 1970, we can still find some functioning systems in the third world countries [1].

With the appearance of internal combustion engines, the gasification process was also used to generate alternative fuels. The first wood-gas powered car was designed and built by Thomas Hugh Parker in 1901,

but it was widespread only thirty years later. In the 1930s, the rapid development of military industry and the Second World War caused the use of alternative materials in the fuel industry.

During the Second World War, the Allies and the Soviet Union did not supply crude oil to European countries that were occupied by the Germans. The local small-scale exploitation was used by the German army (Wehrmacht). Since there was not enough fuel for the military industry, the Wehrmacht also experimented with wood-gas powered tanks, which were finally not applied because of their difficult and complicated operation. By the end of the Second World War, there were about a half million wood-gas powered vehicles only in Germany [1]. There were more than a million of such vehicles in Europe. In the occupied Denmark, 95% of civilian and agricultural vehicles were wood-gas powered [2].

The chemical composition and the energy content of the synthesis gas, produced during the gasification of wood, was appropriate to be the fuel of the rudimentary internal combustion engines [1]. Some decades later, the further developed gasification technology was used in waste management and power plant energetics. Special workshops had been set up to transform traditional cars into gas-powered ones, and fuel filling stations have been built, where people were able to buy firewood of the right size.

Gasification is a process based on the rapid heat dissipation of materials with partial oxidation, which has a smaller oxygen demand compared to the theoretical oxygen required for the perfect combustion. During the partial oxidation of the organic compounds found in the parent material synthesis gas is released, which can be utilized either as raw material, chemical synthesis or as fuel [1].

Due to the sensitivity of the process, it is important, that the characteristics (size, moisture content, consistency) of the fuel supplied remain within certain predetermined limits [3]. The effect of sensitivity typically occurs in energetic and environmental efficiency.

The main purpose of the process is to achieve the highest gas output and achieve optimum energetic efficiency. The synthesis gas, produced during the gasification process is a gas mixture, rich in hydrogen and carbon monoxide, which depends on the gasifying medium and contains energetically inert components. The most commonly occurring non-combustible components are the carbon dioxide and water steam, which take part in the operation, but leave the reactor as ballast. The gasifying medium significantly influences the chemical composition and energy content of the resulting synthesis gas. The gasifying medium helps to break down the solid carbon and the higher molecular weight carbon hydrogens resulting in the release of hydrogen and carbon monoxide [2]. Most commonly air, steam and pure oxygen are used, but a good ratio of carbon dioxide and oxygen can also yield good results. Incorrectly selected auxiliary gas can cause the fail of the technology.

It is recommended to cool the synthesis gas before the utilization and subjected to a complex purification process to remove harmful and corrosive substances. The purified synthesis gas is usually used to produce heat-energy and electricity by burning it in a gas-engine or in a gas-turbine. Gasification is a non-existent technology by its own, because in a reactor, formed for this purpose pyrolysis and combustion zones are both formed. However, the name is correct, because in case of thermodynamic equilibrium the reactions, which are taking place, with the exception of radiation losses, results a self-sustaining process [1]. In a thermodynamic equilibrium state, the system does not cool and does not heat up, therefore it does not require heat input (pyrolysis) or heat loss (combustion) and produces combustible synthesis gas. The gasification is carried out in four steps, which happens on different temperatures and stoichiometric proportions in the reactor. The relationship between the reactors are determined by the type of the reactor [2, 7].

Gasification is the only thermal treatment technology which can be an endothermic or an exothermic process too, depending on the excess air factor and on the temperature. When applying gasification, the main goal is to achieve a self-sustaining process. This only occurs, if the reactor, considering the radiation and heat losses, is in thermodynamic equilibrium state. After the start, the system reaches its steady state after a 5 - 20 minutes long transient. The thermodynamic equilibrium state is significantly affected by the moisture content of the dispersed war material. The excess air factor value can be determined basing on the moisture content and the thermal loss of the reactor [7].

3. BASIC EQUATIONS OF THERMOKINETICAL MODEL EXAMINATION

During thermokinetic model investigation, the chemical and energetic properties of gases, produced from different materials are determined. The thermokinetic model is used for the modelling of processes, which is based on the law of energy conservation [1]. By applying this model, approximate estimates of the chemical composition, viscosity and other properties of the produced gas can be given.

As the essence of the model is to make the calculations faster and easier, some ingredients, such as nitrogen oxide and ethylene, acetylene compounds were neglected during writing the simplified model equations. The model equation is written for the hydrogen and oxygen content of the fuel in one mole of carbon content [1, 5, 6].

Model examinations were carried out by using the equilibrium constants with predetermined gas composition at fixed temperature and operating pressure. The equilibrium constant method at the given temperature is the equation conversion. Its essence is to determine the composition of the produced product using the principle of Gibbs's free energy minimization. For the analyses, we used a software, called Gaseq, which is based on a NASA method. It was developed by Chris Morley and it is accessible for everyone, and can be used for educational and non-profit purposes. It is mainly used for solving equations describing interaction of gas reactants. In the case of the rate of the theoretical and practically used molar oxygen demand equals one ($\lambda=1$), or it is higher than one, then we get the combustion equations back.

The expanded model equation, based on the molar theoretical content may be written as the following:

$$\text{CH}_k\text{O}_l + n_m \cdot \text{H}_2\text{O} + m \cdot \text{O}_2 + (3.76 \cdot m + a_n) \cdot \text{N}_2 = x_1 \cdot \text{H}_2 + x_2 \cdot \text{CO} + x_3 \cdot \text{H}_2\text{O} + x_4 \cdot \text{CO}_2 + x_5 \cdot \text{CH}_4 + x_6 \cdot \text{O}_2 + x_7 \cdot \text{NO} + x_8 \cdot \text{NO}_2 + x_9 \cdot \text{N}_2 + x_{10} \cdot \text{N}_2\text{O} + x_{11} \cdot \text{C}_d\text{H}_f\text{O}_g \quad (1)$$

where:

n_m : is the moisture content of the fuel per mole of carbon content,

a : is the nitrogen content of the fuel,

x_1 : is the molar hydrogen content of the produced raw synthesis gas,

x_2 is the content of carbon-monoxide;

x_3 : is the content of water steam,

x_4 : is the content of carbon-dioxide,

x_5 : is the content of methane,

x_6 : is residual oxygen content,

x_7 : is the nitrogen-monoxide,

x_8 : is the content of nitrogen-dioxide,

x_9 : is content of nitrogen,

x_{10} : is the dinitrogen-oxide content,

x_{11} : is the residual solid carbon,

x_i : is the molar amount of other constituents that are formed (e.g.: ethylene, acetylene).

Model examinations were made to determine the chemical composition of the produced gas product to be able to determine the parameters and properties characterizing the technological and energetic efficiencies. Applying the parametric basic equations is necessary, because we have built up the model examinations by using them. To determine the right side of Equation (1), e.g. to determine the unknown quantities, we have chosen the equilibrium constant method, by knowing the input compositions and the resulting product [1, 6].

We applied the equilibrium constant method, for which we first wrote the molar material equation for each component, then we checked if the molar material retention met. In the end, the equilibrium conditions were determined [1, 6].

The value expressed in molar amounts of the resulting products is indicated by the equilibrium mole number (x). The equilibrium number shows how the resulting component is generated compared to other product components.

Gibbs's free energy can be written according to equation numbers pressure and temperature in accordance with Equation (2) [1, 8].

$$\frac{G}{R \cdot T} = \sum_{i=1}^n \left(\frac{x_i \cdot G_i^0}{R \cdot T} + x_i \cdot \ln \frac{x_i}{\sum x_i} + x_i \cdot \ln p \right) \quad (2)$$

where:

G: the Gibbs free energy,

G_i^0 : is the specific saturation energy of the i -th material with respect to 1 mole of material at atmospheric pressure,

R: is the universal gas constant,

T: is the temperature of the system,

p: is the pressure of the system,

x_i : is equilibrium mole number of component i , so the material quantity of the i -th parent material in the blend,

n: is the number of chemical elements,

$\sum x_i$: is the sum of the equilibrium numbers of the final product, the amount of the blend materials.

In case of thermodynamical state, the main purpose is to minimize the G/RT rate, which is determined by the elemental composition.

During the model examinations, we applied the equilibrium constant method at the pressure and the temperature fixed in the Gaseq software to solve the model equations. The software was created for analyzing chemical equilibrium processes, so applying it helps in the examination of thermic treatment technologies. During the simulations of gasification processes, we were able to see, how the variable input parameters determine the composition of the gas, produced during the gasification, which composition is really important to know to determine the efficiency of power and heat production, using the produced gas.

4. REACTION EFFICIENCY EXAMINATION

Energy efficiency is one of the central topics of our days. Energy efficiency policy is closely related to commercial, industrial and energy security activities, but environmental benefits have become increasingly important as one of the basic tools for reducing carbon emissions [3, 4]. Many conventional and non-conventional measurements are known and applied to determine the efficiency of energy conversion. The following non-conventional parameters are presented.

The reaction, or the chemical efficiency Equation (3) shows us what part of the energy content of the solid fuel is in the produced gas product [9, 10]. By knowing the reaction efficiency, the parameter that characterizing the perfection of combustion can be determined. Its calculation method is shown in Equation (4). According to these [4]:

$$\eta_r = \frac{M_{gt} \cdot F_{gt}}{M_{szt} \cdot F_{szt}} \quad (3)$$

$$\eta_c = 1 - \eta_r, \quad (4)$$

where:

η_r : is the reaction efficiency,

M_{gt} : is the mass flow of the gas product,
 F_{gt} : is the calorific value of the gas product,
 M_{szt} : is the mass flow of the solid fuel,
 F_{szt} : is fuel calorific value and η_c is the combustion efficiency.

5. EXAMINATION OF ACACIA GASIFICATION

This study was carried out applying the aforementioned 'Gaseq Chemical Equilibrium Program' using the equilibrium constant method. To perform an analysis, it is necessary to have the temperature, pressure and excess air factor values of the given process and the composition of the selected fuel. In this task, in all cases, there is acacia wood as a fuel. The composition of the dry solid fuel is shown in Table 1.

Table 1 The elemental composition of acacia tree of the dry base.

Component name	Amount
Carbon content	49.50%
Hydrogen content	5.90%
Oxygen content	43.30%
Nitrogen content	0.40%
Ash content	0.90%

In the process of modelling, the elemental molecules in the element must be given, not the elemental elements. The wood is made up of cellulose molecules, however cellulose was not included in the software, so I defined it from an chemical data book. Since the parameters of this data book are incomplete, therefore I did not can make totally successful analysis. So I looked for another molecule. This molecule was the phenol, with it I did make much more correct analysis. Furthermore the parameters of phenol are trusty, because they are included in the software, and the partial results were same as according to the cellulose. The corrected composition is given in Table 2.

Following the determination of the above data, the efficiency of the reaction (gasification) was examined on the basis of Equation (3), under different boundary conditions.

Table 2 The ecomposition of the dry acacia tree of the phenol content.

Component name	Amount
Carbon content	0.000%
Hydrogen content	1.746%
Oxygen content	32.311%
Nitrogen content	0.400%
Ash content	0.900%
Phenol content	64.644%

For the determination of efficiency of the calorific value of the released combustible gases and the actual heating value of the wood has been calculated. The amount of released gases was determined by the aforementioned Gaseq software. Carbon monoxide and hydrogen gases were present in the combustible constituents in a significant amount.

During these analyzes, we examined the gas composition and reaction efficiency change caused by the change of the excess air factor, the temperature of the reaction and the operating pressure.

During this simulation, we varied the temperature between 600 °C and 1,000 °C, and the pressure between 1-20 bar. The data are summarized in the following tables, than depicted in a diagram. During the test, the

moisture content of the acacia tree was kept constant at 15%, while the excess air factor was set to 0.5. In all cases 1kg of acacia was simulated to be gasified.

Table 3 shows that in case of low temperature, increasing the operating pressure decreases the hydrogen and carbon-monoxide production. As a result, the heating value of the produced wood-gas decreases and the reaction efficiency is drastically decreasing (Table 4).

Table 3 Hydrogen and carbon monoxide amounts at 600 °C.

Pressure [bar]	Hydrogen content [kg]	Carbon-monoxide content [kg]
1	0.03700	0.38466
5	0.02339	0.19235
10	0.01809	0.13551
15	0.01539	0.11033
20	0.01367	0.09534

Table 4 Heat value and reaction efficiency at 600 °C.

Pressure [bar]	Wood-gas heating value [MJ/kg]	Reaction efficiency [%]
1	8.3251	70.3682
5	4.7495	40.1458
10	3.5395	29.9174
15	2.9611	25.0292
20	2.6033	22.0049

Table 5 and Table 6 contain the results obtained for gasification at 800 °C. The deterioration of the energy efficiency caused by the increase of pressure is decreasing. While at 600 °C the reaction efficiency at 20 bar operating pressure decreased to less than its third compared to the examinations at 1 bar, at 800 °C this value did not reach 10%.

Table 5 Hydrogen and carbon monoxide amounts at 800 °C.

Pressure [bar]	Hydrogen content [kg]	Carbon-monoxide content [kg]
1	0.03438	0.52939
5	0.03412	0.52648
10	0.03339	0.51837
15	0.03240	0.50705
20	0.03129	0.49426

Table 6 Heat value and reaction efficiency at 800 °C.

Pressure [bar]	Wood-gas heating value [MJ/kg]	Reaction efficiency [%]
1	9.4724	80.0664
5	9.4118	79.5543
10	9.2423	78.1215
15	9.0092	76.1509
20	8.7468	73.9331

In case of gasification at 1,000 °C (Table 7 and Table 8) the effect of the pressure increase is negligible. On the basis of the results obtained, the increase of the operating pressure results in the reduction in the efficiency of gasification reaction, but the operating temperature influences in a positive direction. The

reaction efficiency decreasing effect of the pressure increase in the function of the temperature is exponential. The ideal gasification temperature for acacia is between 800 °C and 900 °C, because the gas has the best parameters in case of setting the temperature between these values. At 900 °C it can be noticed, that the rate of degradation of the reaction rate, caused by the pressure increase does not even reach 1%.

Table 7 Hydrogen and carbon monoxide amounts at 1,000 °C.

Pressure [bar]	Hydrogen content [kg]	Carbon-monoxide content [kg]
1	0.02967	0.59522
5	0.02966	0.59516
10	0.02964	0.59503
15	0.02962	0.59482
20	0.02960	0.59454

Table 8 Heat value and reaction efficiency at 1,000 °C.

Pressure [bar]	Wood-gas heating value [MJ/kg]	Reaction efficiency [%]
1	9.5721	80.9090
5	9.5703	80.8937
10	9.5666	80.8624
15	9.5621	80.8241
20	9.5569	80.7800

The above is illustrated in Fig 1. One can see how the reaction efficiency changes depending on the gasification temperature and on the operating temperature. It can be seen also, that at lower temperatures, the operating temperature has a greater effect on the efficiency of the gasification reaction than at higher temperatures.

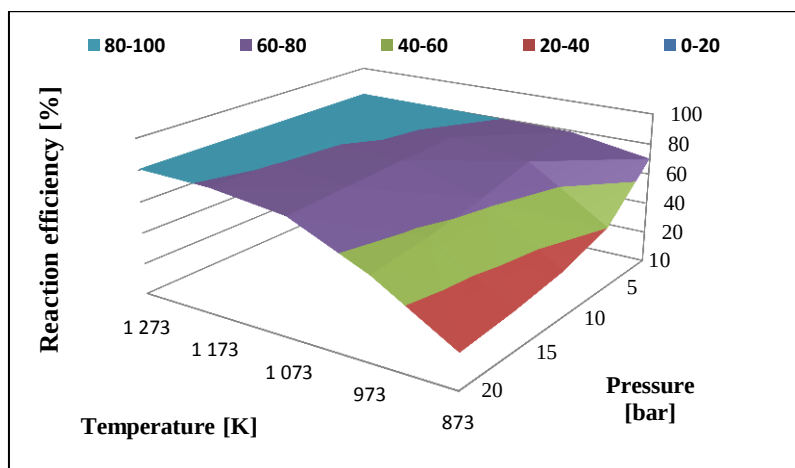


Figure 1. Reaction efficiency depending on the temperature and operating temperature, during acacia gasification.

We also investigated how the reaction efficiency changes with constant excess air factor and temperature and with constant moisture fuel.

Fig. 2. illustrates how the reaction efficiency varies depending on the pressure in case of 0.6 excess air factor. During gasification at 800 °C, 15% is the moisture content of the gaseous acacia wood. It can be noticed, that the increase in pressure exponentially reduces the efficiency of the reaction, so it is desirable to select an unreasonable high pressure during the gasification. Similar trend can be observed with varying the excess air factor, temperature and moisture content.

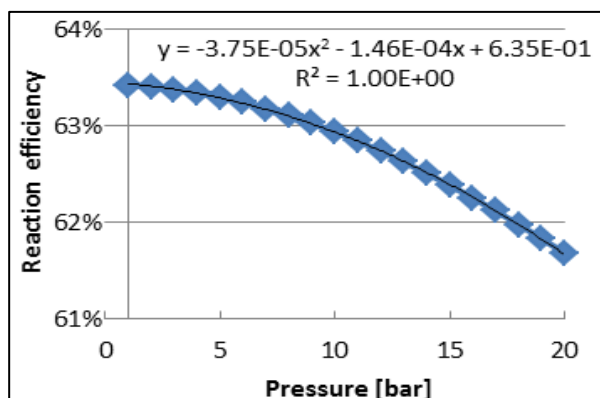


Figure 2. Reaction efficiency as a function of pressure, constant temperature, excess air factor and moisture content.

We also examined how the efficiency of the reaction changes, if the excess air factor and the moisture content of the solid fuel are varied, while the temperature is constant 800 °C and the pressure is 1 bar. It can also be observed that by increasing the excess air factor, the efficiency of the reaction decreases drastically. Increasing the moisture content of the fuel only slightly reduces the efficiency of the reaction. This is illustrated in Table 9.

At the end of the analyses, we investigated, how the electricity produced from the synthesis gas from the gasification of the wet wood relates to the electricity produced from the combustion of the wet wood. We call this amount electricity density change. The method of calculation is shown in Equation (5).

$$\Delta e_v = \frac{e_{k \text{ gasification}} \cdot \eta_{egv D}}{e_{k \text{ combustion}} \cdot \eta_{egv RC}} \quad (5)$$

where:

Δe_v : is the electricity density change,

$e_{k \text{ gasification}}$: is the specific energy output of the gasification,

$e_{k \text{ combustion}}$: is the specific energy output of combustion,

$\eta_{egv D}$: is the electrical efficiency of the Diesel cycle used during gasification,

$\eta_{egv RC}$: is electrical efficiency of the Rankine-Clausius cycle used during the combustion.

Table 9 Gasification reaction efficiencies at 800 °C temperature and 1 bar pressure.

Moisture content [%]	Excess air factor [-]		
	0.5	0.6	0.7
10	80.10%	63.65%	48.14%
20	79.49%	63.19%	47.77%
25	79.16%	62.93%	47.58%

The electrical efficiency of the Rankine-Clausius cycle was 27%, while the energy productions electrical efficiency with the help of a gas engine was 36%, which amounts are usual. The values obtained are shown in Fig. 3.

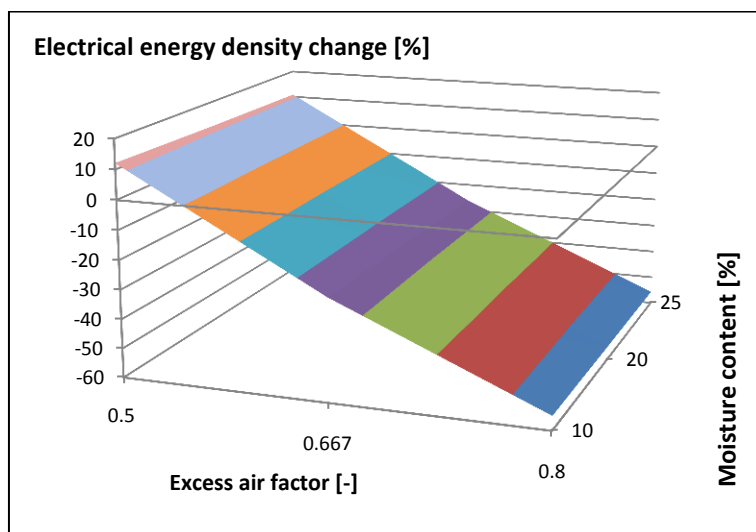


Figure 3. Change in density of electrical energy at 800 °C depending on the excess air factor and the moisture content.

From Fig. 3. it can be seen, that with both increasing excess air factor and moisture content, the energy density change varies in an unfavorable direction. Increasing the excess air factor results in a more intensive change in the density of electricity than the increase in moisture content, therefore in case of a higher moisture content fuel, gasification based electricity production may be favorable.

Over the excess air factor, the energy density change becomes negative, which means that it is not possible to produce more electricity from a unit of fuel using gasification technology, than using conventional combustion technology.

6. SUMMARY AND CONCLUSIONS

During the analyses, we have made sure that the simulation of the gasification of woody biomass is complex and complicated. Furthermore, it has become apparent that the moisture content of the raw material, as well as the parameters related to the technology can be influenced greatly by the excess air factor, temperature and pressure, which causes variation in the heating value of the synthesized gas produced. The analyses showed that the moisture content, the excess air factor and the pressure increase result in a reduction in the reaction efficiency while the temperature increase contributes to the increase of the reaction efficiency.

From the results above, we can conclude, that the efficiency of the gasification is the highest, in case of selecting the excess air factor as 0.5. Since the moisture content does not significantly influence the efficiency of gasification, it can be used well, in those cases, where the moisture content of the fuel is relatively high (20-25%).

By increasing the pressure, the efficiency decreases exponentially, so it does not worth choosing high pressure. Increasing the reaction temperature above 800 °C slightly increases the efficiency of the reaction, so its increase is not purpose-oriented based on economic considerations.

In our opinion, the efficient operation of a power plant, using gasification technology requires a very complex process, and requires careful engineering work, but it worth dealing with this technology. By applying gasification technology, we are able to build quick-start power plants to produce electricity with higher efficiency, than in case of conventional incineration.

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REFERENCES

- [1] Z.A. Zainal, R. Ali, C.H. Lean, K.N. Seetharamu, Prediction of performance of a downdraft gasifier using equilibrium modelling for different biomass material, *Energy Conversion and Management*, vol. 42. 2001. pp. 1499–1515.
- [2] T.B. Red, A. Das, *Handbook of biomass downdraft gasifier engine systems*, Solar Energy Research Ins., 1988. p. 148.
- [3] T. Hill, S. Downen, *Pyrolysis and gasification. Briefing (Draft 2)*, UK Without Incineration Network (UK WIN), 2010. p. 9.
- [4] M.G. Patterson, What is energy efficiency? Concepts, indicators and methodological issues, *Energy Policy*, vol. 24, No. 5. 1996. pp. 377–390.
- [5] Y. Wang, C.M. Kinoshita, Kinetic model of biomass gasification, *Solar Energy*, vol. 51. no. 1. 1993. pp. 19–25.
- [6] A. Mountouris, E. Voutsas, D. Tassios, Solid waste plasma gasification: equilibrium model development and exergy analysis, *Energy Conversion and Management*, vol. 47. 2006. pp. 1723–1737.
- [7] K.S. Hatzilyberis, Design of an indirect heat rotary kiln gasifier, *Fuel Processing Technology*, vol. 92. 2011. pp. 2429–2454.
- [8] C. Morly, Method for calculating equilibrium compositions at specified temperature, Gaseq, a chemical equilibrium program for windows. www.gaseq.co.uk, 2001. p. 6.
- [9] K.A. Rajvanshi, Biomass gasification, *Alternative Energy in Agriculture*, vol. 2. no. 4. 1986. pp. 83–102.
- [10] G. Schuster, G. Löffler, K. Weigel, H. Hofbrauer, Biomass steam gasification – an extensive parametric modeling study, *Bio resource Technology*, vol. 77. 2001. pp. 71–79.