

IVANA ČEKOVIĆ¹
 NEBOJŠA MANIĆ²
 DRAGOSLAVA
 STOJILJKOVIĆ²
 MARTA TRNINIĆ²
 DUŠAN TODOROVIĆ²
 ALEKSANDAR JOVOVIĆ²

¹Innovation Center, Faculty of
 Mechanical Engineering, Belgrade,
 Serbia

²Faculty of Mechanical
 Engineering, University of
 Belgrade, Serbia

SCIENTIFIC PAPER

UDC 621.8.036:674:519

MODELING OF WOOD CHIPS GASIFICATION PROCESS IN ASPEN PLUS WITH MULTIPLE VALIDATION APPROACH

Article Highlights

- Modeling of wood chips gasification in downdraft gasifier was carried out in ASPEN Plus
- Due to the mathematical model development issues, three cases are considered and described
- Experimental work was carried out within commercial small-scale CHP system
- Multiple validation approach was applied for model verification

Abstract

A thermochemical equilibrium model is formulated for wood chips downdraft gasification. Steady state ASPEN Plus simulator was utilized to evaluate producer gas composition and low heating value. Three cases are considered, due to mathematical model developed issues, and described in details. Experimental work was carried out within commercial small-scale CHP system where twelve beech wood samples were taken. Equivalence ratio is between 0.32 and 0.38 and air-fuel ratio ranges from 1.49 to 1.81, when gasifier capacity is optimal, at 250 kW. Mole fractions of CO₂, H₂, CO, CH₄ and N₂, in dry producer gas, are respectively, 16.06-17.64, 17.98-20.33, 13.71-17.26, 1.65-2.89 and 43.21-48.36. Multiple validation approach was applied for model verification. The results are in reasonable agreement with different literature sources (experimental work and modeling) and in a great agreement with the modified equilibrium model developed in Engineering Equation Solver found in the literature. Result deviations are explained by two major facts: wood downdraft gasification experiments are to a certain extent different and the model parameters could not be adjusted enough to fully minimize differences between model results. Predicted low heating value of dry producer gas is between 4.67-5.61 MJ/Nm³.

Keywords: ASPEN, downdraft gasification, experiment, modeling, multi validation approach, wood chips.

The efficient utilization of biomass is of great importance when it comes to replacing fossil fuels that are still used in large amounts [1,2]. Thermochemical conversions of biomass fuels are challenging not only in terms of physical and chemical transformations, but also in terms of a large number of product species [3]. Biomass gasification is a thermochemical process and a highly efficient way of con-

verting biomass, in the presence of air, oxygen or steam, into a mixture of combustible (CO, H₂ and CH₄) and non-combustible (CO₂ and N₂) gases in a gasifier [4]. Beside the mentioned gas mixtures, the products of gasification are water vapor, other gaseous hydrocarbons, small quantities of char, ash, condensable compounds (tars and oils), etc. [5]. It is a complex process of partial oxidation of biomass followed by sequential and parallel physical processes and chemical reactions [6]. Generated gas could be classified as producer gas or syngas. In general, producer gas is formed at a low gasification temperature, <1000 °C, and syngas is formed at high gasification temperature, >1200 °C [7]. Both producer gas and

Correspondence: I. Čeković, Innovation Center, Faculty of Mechanical Engineering, Kraljice Marije 16, 11120 Belgrade, Serbia.

E-mail: ivanacekovic@yahoo.com

Paper received: 9 July, 2018

Paper revised: 21 November, 2018

Paper accepted: 10 December, 2018

<https://doi.org/10.2298/CICEQ180709034C>

syngas can be standardized in their quality and can be used to power gas engines and gas turbines (*e.g.*, combined heat and power (CHP) systems) or as a chemical feedstock (*e.g.*, liquid fuel production), which means that gasification adds value to low- or negative-value feedstock by converting it into marketable fuels and products [5]. Since biomass gasification within CHP system is in the focus of this paper, it is important to emphasize the importance of such systems in terms of climate change mitigation, energy security and increasing energy efficiency [2]. Good quality gas has high heating value and low tar content. The gas quality is affected by parameters such as biomass characteristics (size, density, ultimate and proximate analysis), process parameters (biomass consumption rate, equivalence ratio (ER) and gasification temperature and pressure) and gasifier design [4,5,8]. Depending on the direction of biomass and producer gas/syngas flow in the gasifier, fixed-bed gasifiers can be generally categorized as updraft, downdraft and cross-draft [6,7,9]. Since the downdraft gasifier is in the focus of investigation, other types of fixed-bed gasifiers will not be discussed. Typically, downdraft gasifiers have a capacity of 10 kW-1 MW [4]. Biomass feedstock is fed from the top. Gasifying agent, typically air, oxygen or steam, is fed from the top (open-core) or from the side (throated), Figure 1 [10]. The main advantages of downdraft gasifiers are easy fabrication and operation, suitability for biomass with low moisture content and low tar and ash content in a produced gas. On the other side, disadvantages are related to biomass type and feed size limitations, moisture content sensitivity, low heating value of produced gas, scale limitations, appearance of grate blocking, channeling and bridging [4,5,11,12].

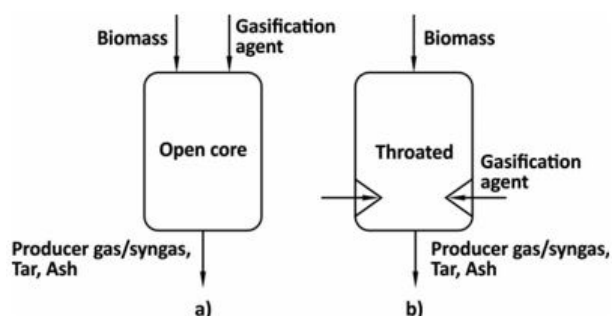


Figure 1. Downdraft gasifiers: a) open-core; b) throated.

Due to the complexity of biomass gasification, simulation and prediction of the process performance are continuously developing research areas and subjects of lots of studies. Mathematical modeling of gasification could be categorized into thermodynamic equilibrium model, kinetic model, artificial neural net-

work (ANN) model and computational fluid dynamic model (CFD) approaches. Diverse to the thermodynamic equilibrium models that are predicting maximum possible product quantity, kinetic models are predicting product quality features (composition and fractions of products in different reactor zones). There are parameters within kinetic models that are limiting their application. On the other side, thermodynamic equilibrium models are suitable for investigating different parameter impact on producer gas/syngas composition and are not limited with gasifier design. Still, difficulties caused by low process temperatures (low outlet gas temperatures) may occur while reaching thermodynamic equilibrium [5,13]. In this study, equilibrium modeling was carried out within Aspen Plus with a purpose to investigate wood chips gasification in downdraft gasifier in order to determine gas composition and heating value of producer gas. ASPEN Plus was very convenient for such an investigation because it is reliable, problem-oriented and a user-friendly process simulator and a great tool for utilization when there is a need to avoid complex processes such as gasification and to develop very simple models. There are also process model simulators that are combining thermodynamic equilibrium model and kinetic model approaches. Within Aspen Plus, there is such a possibility, but it was not considered in this study.

Theoretical background

Broadly speaking, the principle stages of gasification are drying, devolatilization (pyrolysis), oxidation (combustion) and reduction, Figure 2 [5]. Normally, suitable moisture content of biomass for downdraft gasifiers ranges from 5 to 35% [4,5,9]. Drying stage occurs at about 100-200 °C, when the moisture starts converting into water vapor, and it takes place due to the heat transfer from the hotter oxidation zone [4].

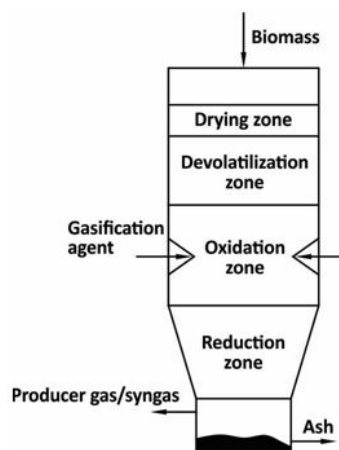


Figure 2. Stages of gasification inside the downdraft gasifier.

Higher moisture content requires more heat for drying. The rate of drying depends on the surface area of the biomass feed, the temperature difference between the feed and its external environment and the internal diffusivity of moisture within the feed. It is important to point out that drying is not a discreet process and it also occurs alongside pyrolysis as temperature increases [10]. Devolatilization (pyrolysis) occurs at about 200–700 °C in the absence of a gasification (oxidation) agent. Biomass starts decomposing irreversibly, due to the partial oxidation heat released (thermal degradation), into a mixture of non-condensable gases (CO, H₂, CO₂ and CH₄), tar and char. Decomposition of tar into gas, char and liquid occurs in the secondary tar-cracking reactions [4]. The release of volatiles begins at about 250 °C, until under the conditions in a downdraft gasifier, 80–95% of the original mass is converted, leaving 5–20% highly reactive charcoal [10]. During this stage, both homogeneous and heterogeneous reactions take place. Oxidation (combustion) provides heat not only for drying and pyrolysis, but also for endothermic gas-

ification reactions during the reduction stage. It occurs between solid carbonized biomass and air, oxygen or steam, at about 800–1400 °C, resulting in formation of CO₂, CO and H₂O [4,5,9]. The volatile products of pyrolysis are partially oxidized in highly exothermic reactions resulting in rapid temperature increase. The oxidation reactions of volatiles are very rapid and oxygen is consumed before it can diffuse to the surface of the char. Therefore, no oxidation of the char can take place [10]. Combustible gases in producer gas/syngas are formed during the reduction stage when main gasification reactions occur. Reduction occurs at about 800–1000 °C followed by endothermic reactions in majority [4,5,9]. Solid char is converted into gas by reactions with the hot gases from zones above. Gases are reduced to form a greater proportion of H₂ and CO. The gasification reactions of the liquid products of pyrolysis are complex and are not widely discussed in literature [10]. Characteristic reactions of the gasification process and the principle stages are presented in Table 1.

Table 1. Characteristic gasification reactions [4,5,8,9]

Drying and Devolatilization (pyrolysis)	
Biomass	$\xrightarrow{\text{Heat}} \text{H}_2\text{O} + \sum_{\text{gas}} \text{C}_b\text{H}_b\text{O}_c + \sum_{\text{liquid}} \text{C}_x\text{H}_y\text{O}_z + \text{Char}$
Oxidation (combustion)	
R1:	$\text{C} + \text{O}_2 \rightarrow \text{CO}_2 - 394 \frac{\text{kJ}}{\text{mol}}$
	$\text{C} + \frac{1}{2}\text{O}_2 \rightarrow \text{CO} - 111 \frac{\text{kJ}}{\text{mol}}$
	$\text{H}_2 + \frac{1}{2}\text{O}_2 \rightarrow \text{H}_2\text{O} - 242 \frac{\text{kJ}}{\text{mol}}$
Reduction	
Main reactions	
	$\text{C} + \text{CO}_2 \leftrightarrow 2\text{CO} + 172 \frac{\text{kJ}}{\text{mol}}$ - Boudouard reaction
	$\text{C} + \text{H}_2\text{O} \leftrightarrow \text{CO} + \text{H}_2 + 131 \frac{\text{kJ}}{\text{mol}}$ Water-gas reaction
	$\text{CO} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2 - 41.2 \frac{\text{kJ}}{\text{mol}}$ - Water-gas Shift reaction
	$\text{C} + 2\text{H}_2 \leftrightarrow \text{CH}_4 - 74.8 \frac{\text{kJ}}{\text{mol}}$ Methane reaction
Additional reactions of importance	
Oxidation reaction	
	$\text{CH}_4 + 2\text{O}_2 \leftrightarrow \text{CO}_2 + 2\text{H}_2\text{O} - 803 \frac{\text{kJ}}{\text{mol}}$
Methanization reactions	
R2:	$2\text{CO} + 2\text{H}_2 \rightarrow \text{CH}_4 + \text{CO}_2 - 247 \frac{\text{kJ}}{\text{mol}}$

Table 2. Continued

Methanization reactions	
$\text{CO} + 3\text{H}_2 \leftrightarrow \text{CH}_4 + \text{H}_2\text{O}$	$-206 \frac{\text{kJ}}{\text{mol}}$
$\text{CO}_2 + 4\text{H}_2 \rightarrow \text{CH}_4 + 2\text{H}_2\text{O}$	$-165 \frac{\text{kJ}}{\text{mol}}$
Steam reactions	
$\text{CH}_4 + \text{H}_2\text{O} \leftrightarrow \text{CO} + 3\text{H}_2$	$+206 \frac{\text{kJ}}{\text{mol}}$
$\text{CH}_4 + \frac{1}{2}\text{O}_2 \rightarrow \text{CO} + 2\text{H}_2$	$-36 \frac{\text{kJ}}{\text{mol}}$

MATERIALS AND METHODS

Experimental setup within the CHP facility

The experiment was performed within a commercial small-scale CHP plant, Figure 3. Wood chips are stored in the outdoor covered bunker, located close to the plant. When the level of chips gets below the recommended value in the bunker next to the gasifiers, it is necessary to fill it with a new batch. Warm air-drying comes after the batch is being transported from one bunker to another by an excavator, to reduce moisture content in the wood. Afterwards, dried wood chips are transported by conveyer directly to atmospheric throated downdraft gasifiers. It takes approximately 24 h from the moment when a new batch is transported to the “drying” bunker until wood chips are gasified in the presence of air. Producer gas proceeds through filtration and cooling before being combusted in the gas engine.

Room temperatures, where gasifiers are located, and outlet temperatures of producer gas (t_1 and t_2) were recorded on SCADA, Supervisory Control and Data Acquisition system within CHP, Table 2. Since CHP consists of same two gasifiers and since

SCADA gives information about both producer gas outlet temperatures, the average of those temperatures, t_1 and t_2 , is considered as the relevant one for further gasification modeling of the downdraft gasifier.

Biomass material

The feedstock used in the investigation was beech wood chips that are approximately rectangular in a shape with average dimensions of 40 mm×65 mm. Based on a feed level difference in the bunker next to the gasifiers, within 24 h, it was estimated that feedstock mass flow per gasifier is approximately 200 kg/h (wet basis). Twelve samples were taken after drying, directly from the conveyor, just before entering gasifiers. Sampling, sample preparation and fuel characterization was fulfilled following the relevant ISO/TC 238 standard [14] procedures for solid biomass. The wood chips properties are summarized in Table 3.

Aspen Plus model

Advanced System for Process Engineering (ASPEN) is a software package that gives a complete integrated solution to chemical processes and reactors. Steady state ASPEN Plus simulator was

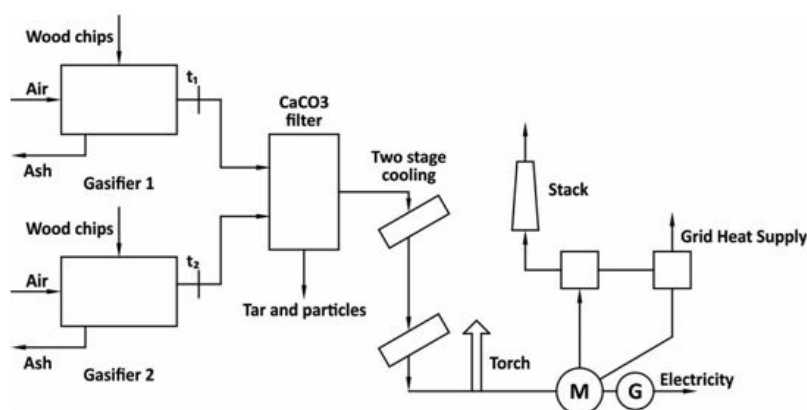


Figure 3. Schematic of CHP system-plant.

Table 3. Room temperatures during wood chips sampling and proper producer gas temperatures

Sample	Room temperature (°C)	Outlet temperature of producer gas, gasifier 1 (t_1 , °C)	Outlet temperature of producer gas, gasifier 2 (t_2 , °C)	Average outlet temperature of t_1 and t_2 (°C)
S1	20.5	403	405	404
S2	20.4	407	394	400.5
S3	21.7	405	391	398
S4	21	415	398	406.5
S5	20	412	415	413.5
S6	19.2	402	399	400.5
S7	15.4	405	402	403.5
S8	14.7	405	393	399
S9	14.7	398	398	398
S10	13.0	393	390	391.5
S11	12.9	404	395	399.5
S12	13.5	395	384	389.5

Table 4. Characterization of wood chips, samples S1-S12

Property	Min	Average	Max
Proximate analysis			
C (% , dry basis)	43.63	43.77	43.91
H (% , dry basis)	6.06	6.08	6.09
O (% , dry basis)	48.73	49.49	49.82
N (% , dry basis)	0.13	0.13	0.13
S (% , dry basis)	0.00	0.00	0.00
Ultimate analysis			
Moisture (%)	4.94	5.26	5.61
Volatiles (% , dry basis)	84.41	85.71	86.98
Fixed carbon (% , dry basis)	12.69	13.76	14.98
Ash (% , dry basis)	0.28	0.53	1.30
HHV (kJ/kg, dry basis)	18588	19106	19735

developed to evaluate producer/syngas constituents [15]. After placing the blocks, models of specific process operations, on the flowsheet, the user is specifying material, inlet and outlet streams of the blocks. As the ASPEN Plus process simulator does not have a built-in gasifier model, a number of reactor types defined in ASPEN are used to model each zone of gasification [16].

In order to simulate wood chips gasification in a downdraft gasifier based on the experiment that was carried out, four different blocks were considered, Figure 4. The first one: wood decomposition (DECOMP block), within RYield reactor, where wood is converted into its components including carbon, hydrogen, oxygen, nitrogen, moisture and ash, according to its ultimate analysis. This type of reactor is used when reaction stoichiometry or reaction kinetics are unknown or unimportant, while the yield distribution is known [17]. The second one: volatile reactions with air (combustion and reduction stages) (GASIFIER

block), within RGibbs reactor, where the raw producer gas (RAWSG stream) is generated. This type of reactor is used when reaction stoichiometry is unknown, while temperature and pressure in the reactor are known [17]. The third one: Solid Separator-Cyclone (FILTER block), in which the separation of ash from the raw producer gas occurs, resulting with SYNGAS and ASH streams. The fourth one: Heat Exchanger (HEATEXC block), heat generated from the decomposition (HEATDEC stream) and from combustion and reduction processes in gasifier (QCOMB stream) is used for water heating water from 20 to 100 °C, Table 4. More detailed specifications of each of the reactors, RYield and RGibbs, are presented in Table 5.

The following assumptions [18] were considered while modeling the gasification process:

- The whole process is steady state and isothermal in the same section;

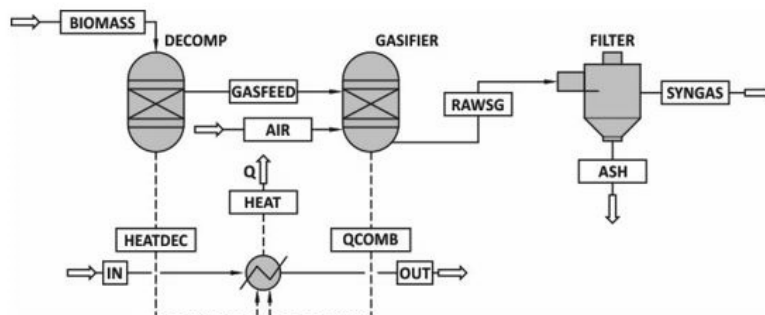


Figure 4. Flowsheet of ASPEN Plus simulation of wood chips gasification in downdraft gasifier.

Table 5. List of blocks in Aspen Plus utilized in the simulation

Name of the block	Reactors/Solid Separators/ Exchangers	Description
DECOMP	RYield reactor	Elemental decomposition of wood chips and product distribution
GASIFIER	RGibbs reactor	Modeling chemical equilibrium by minimizing Gibbs free energy
FILTER	Cyclone	Gas-solid separation
HEATEXC	Heater	Heat exchange

Table 6. Specifications of RYield and RGibbs reactors

Reactor	Input	Output
RYield	Specifications: Operating conditions Reactor outlet temperature Reactor outlet pressure/pressure drop Valid phases Vapor-Liquid Yield: Defining components generated after decomposition on mole basis with no defined yield H ₂ , O ₂ , N ₂ , H ₂ O, C and ash Component attributes: Biomass/ash Ultimate/proximate analysis of samples/ash	Product distribution
RGibbs	Specifications: Calculation option Defining gasifier regime Operating conditions Pressure Temperature Air feed Products: Identification of possible products CO ₂ , CO, CH ₄ , N ₂ , H ₂ , H ₂ O, NO, NO ₂	Product distribution, ER, low heating value of the product gas, gasifier capacity

- Reactions reach chemical equilibrium with volatile products mainly made of CO₂, H₂, CO, CH₄, N₂ and H₂O;
- Char only contains carbon and ash. Ash is inert and it does not participate in any of the chemical reactions;

- Tars are assumed to be negligible in the producer gas and are not taken into account.

Considered cases

In the first stage, cases 1, 2 and 3 of model development tests were carried out only for wood chips sample S1. When the model was improved and

validated, a simulation run was carried out for all twelve samples S1-S12. A sensitivity analysis was fulfilled by varying types of regime in the gasifier and the operating parameters, gasifier capacity, temperature and air feed. In the first stage model predicted producer gas composition and low heating value (LHV) were only validated with [11] by comparing model results with typical producer gas composition and LHV ranges for downdraft gasification of wood. ER was validated with [19] by comparing it with the range for ideal and theoretical gasification (0.19, 0.43). Due to the technical difficulties in CHP, it was not possible to measure air feed rates and to take producer gas samples. Wood chips flow, 200 kg/h (wet basis) and pressure value, inside and outside of gasifier, 1 bar, are considered as equal and constant. Inlet temperature of each sample and inlet air temperature are taken into account as equal to proper room temperature recorded on SCADA. The average of twelve average outlet temperatures of t_1 and t_2 (Table 2) is considered as producer gas outlet temperature in the first stage. Brief methodology for all considered cases is presented in Table 6. All presented cases were considered due to mathematical model developed issues. Multiple validation approach was applied for model verification.

RESULTS AND DISCUSSION

The results of proximate and ultimate analysis of the wood chips sample S1 used for different case analyses are presented in the Table 7.

Table 8. Characterization of wood chips sample S1

Proximate analysis	
C (% dry basis)	43.66
H (% dry basis)	6.09
O (% dry basis)	49.71
N (% dry basis)	0.13
S (% dry basis)	0.00
Ultimate analysis	
Moisture (%)	5.04
Volatiles (% dry basis)	86.34
Fixed carbon (% dry basis)	13.25
Ash (% dry basis)	0.41

Case 1 Results

Simulation results for Case 1 are presented in Table 8. Graphical presentation of these results is available as supplementary material. For the average measured value of producer gas temperature, 400 °C, ER and LHV are in the ranges, Table 9, only for the 350 kW gasifier. As the capacity increases, CO₂ has a trend of decreasing. However, when capacity is 400 kW, the fraction of CO₂ in producer gas is still high above the range. High values are probably caused by very a dominant carbon oxidation reaction, reaction R1 in Table 1. Predicted H₂ and CO fractions in the producer gas are very low. Contribution of CH₄ is almost as high as CO₂ for the 150 kW gasifier. By increasing capacity, CH₄ has a trend of more rapid decrease, compared to CO₂, but still it does not reach the range. The cause of consumption of H₂ and CO and generation of CO₂ and CH₄ is the methanization reaction, reaction R2 in Table 1.

Table 7. Considered cases and implemented methodology

Case	Methodology
1	Establishing the optimal value of gasifier capacity (unknown value) was achieved through varying air feed within the RGibbs reactor, until fitting into recommended ranges, Table 8. Calculations were carried out using the "Calculate phase equilibrium and chemical equilibrium" gasifier regime. By choosing this calculation option, operating conditions pressure in the gasifier and outlet temperature of producer gas have to be defined, so the composition, LHV and ER could be calculated for the equilibrium state. Outlet temperature in the RYield reactor is the same as the temperatures of sample S1 and air (room temperature), 20.5 °C, Table 2. The gasifier capacity varied from 150 kW to 400 kW. Producer gas outlet temperature was varied, 400 (average measured), 600 and 800 °C, to examine the effect of it on gas composition and heating value.
2	The next set of calculations was carried out using the "Restrict chemical equilibrium - specify temperature approach or reactions" gasifier regime. By choosing this calculation option, beside operating conditions, pressure in the gasifier and outlet temperature of producer gas, the temperature approach for entire system has to be defined as well. It means that the number of degrees above the gasifier temperature at which chemical equilibrium is computed has to be specified. Again, the gasifier capacity was varying from 150 to 400 kW. Also, outlet temperature in the RYield reactor (DECOMP outlet temperature) was varying, 20.5, 400, 600 and 800 °C. Producer gas outlet temperature is fixed, 400 °C. Chemical equilibrium occurs at 800 °C.
3	After defining gasifier capacity, further analysis is conducted to study the effect of chemical equilibrium temperature on producer gas and CH ₄ . Gasifier regime and producer gas outlet temperature are kept the same as in Case 2. Chemical equilibrium temperature is varied from 550 to 800 °C, with 50 °C temperature difference.

Table 8. Simulation results for Case 1, sample S1

Gasifier capacity (kW)	Producer gas outlet temperature (°C)	ER	Producer gas composition (mol %, dry basis)					LHV _{dry basis} (kJ/Nm ³)
			CO ₂	H ₂	CO	CH ₄	N ₂	
150	400	0	39.36	1.08	8.1	38.41	13.05	15433
	600	0.26	16.16	21.01	19.48	4.64	38.71	6626
	800	0.38	12.35	19.60	20.79	0.00	47.26	4922
200	400	0.11	37.22	2.46	3.06	29.29	27.97	11544
	600	0.34	16.70	19.62	16.18	2.65	44.85	5299
	800	0.44	13.73	16.69	17.60	0.00	51.98	4176
250	400	0.18	33.66	3.50	1.81	21.71	39.32	8685
	600	0.41	17.30	17.99	13.52	1.47	49.72	4331
	800	0.51	14.97	14.03	14.70	0.00	56.30	3498
300	400	0.26	30.86	4.04	1.33	16.34	47.43	6691
	600	0.48	17.92	16.20	11.25	0.78	53.85	3578
	800	0.57	16.06	11.66	12.15	0.00	60.13	2897
350	400	0.34	28.73	4.31	1.07	12.41	53.48	5229
	600	0.54	18.53	14.32	9.26	0.39	57.50	2963
	800	0.63	17.05	9.50	9.84	0.00	63.61	2354
400	400	0.42	27.08	4.43	0.89	9.42	58.18	4107
	600	0.61	19.12	12.32	7.45	0.18	60.93	2422
	800	0.69	17.95	7.50	7.72	0.00	66.83	1852

Table 9. Literature recommended composition of producer gas for downdraft gasification of wood [11] and literature recommended ER [19]

Biomass	Gasifier	Mole %, dry basis					MJ/m ³
		CO ₂	LHV	CO	CH ₄	N ₂	LHV
Wood	Downdraft	10-15	16-20	17-22	2-3	50-55	5-5.86
Ideal and theoretical gasification							
ER		0.19-0.43					

Case 2 Results

Case 2 results are presented in Table 10. Graphical presentation of these results is available as supplementary material. ER, composition and LHV of producer gas do not depend on DECOMP outlet temperature. ER and LHV are in/close to the recommended ranges, Table 9, for 150, 200 and 250 kW gasifiers. In general, the model showed reasonable agreement with [11] with the exception of CH₄. This time, the methanization reaction, reaction R2 in Table 1, did not take the place, resulting in CH₄ concentration being close to zero. Based on the results, the manufacturer's recommendations and additional consultations with CHP designers, the conclusion is that the optimal gasifier capacity in this regime is 250 kW.

Case 3 Results

The final results, for S1 wood chips sample, are presented in Table 11. Graphical presentation of these results is available as supplementary material. ER, producer gas composition and LHV of producer

gas are in a very good agreement with the ranges from Table 9 for 600 °C chemical equilibrium temperature. It means that equilibrium is reached when the temperature in the gasifier is 200 °C above the outlet temperature of the producer gas (400 °C measured). Chemical equilibrium temperature decrease has affected CH₄ by providing its increase.

Model validation for all wood chips samples

Model predictions, for all the samples, S1-S12, are in reasonable agreement with different literature sources [5,11] and [20-26], Tables 12 and 13. The first group of authors, Table 12, present a too general review of data related to wood gasification, lacking relevant information. The second group of authors, Table 13, present their experimental work or model development. The presence of result deviations are explained by two main facts, wood downdraft gasification experiments are to a certain extent different and the model parameters could not be adjusted enough to fully minimize differences between model results.

Table 9. Simulation results for Case 2, sample S1

Gasifier capacity (kW)	DECOMP block outlet temperature (°C)	ER	Producer gas composition (mol %, dry basis)					LHV _{dry basis} (kJ/Nm ³)
			CO ₂	H ₂	CO	CH ₄	N ₂	
150	20.5	0.28	9.84	24.84	26.61	0.02	38.69	6278
	400	0.28	9.84	24.84	26.61	0.02	38.69	6278
	600	0.28	9.84	24.84	26.61	0.02	38.69	6278
	800	0.28	9.84	24.84	26.61	0.02	38.69	6278
200	20.5	0.34	11.29	21.82	23.25	0.01	43.63	5494
	400	0.34	11.29	21.82	23.25	0.01	43.63	5494
	600	0.34	11.29	21.82	23.25	0.01	43.63	5494
	800	0.34	11.29	21.82	23.25	0.01	43.63	5494
250	20.5	0.39	12.62	19.03	20.17	6E-05	48.18	4776
	400	0.39	12.62	19.03	20.17	6E-05	48.18	4776
	600	0.39	12.62	19.03	20.17	6E-05	48.18	4776
	800	0.39	12.62	19.03	20.17	6E-05	48.18	4776
300	20.5	0.45	13.81	16.50	17.40	3E-05	52.29	4128
	400	0.45	13.81	16.50	17.40	3E-05	52.29	4128
	600	0.45	13.81	16.50	17.40	3E-05	52.29	4128
	800	0.45	13.81	16.50	17.40	3E-05	52.29	4128
350	20.5	0.50	14.89	14.20	14.89	1.5E-05	56.02	3541
	400	0.50	14.89	14.20	14.89	1.5E-05	56.02	3541
	600	0.50	14.89	14.20	14.89	1.5E-05	56.02	3541
	800	0.50	14.89	14.20	14.89	1.5E-05	56.02	3541
400	20.5	0.56	15.87	12.08	12.60	7E-06	59.45	3005
	400	0.56	15.87	12.08	12.60	7E-06	59.45	3005
	600	0.56	15.87	12.08	12.60	7E-06	59.45	3005
	800	0.56	15.87	12.08	12.60	7E-06	59.45	3005

Table 10. Simulation results for Case 3, sample S1

Chemical equilibrium temperature (°C)	ER	Producer gas composition (mol %, dry basis)					LHV _{dry basis} (kJ/Nm ³)
		CO ₂	H ₂	CO	CH ₄	N ₂	
550	0.29	20.79	15.58	12.46	7.03	44.14	5985
600	0.35	16.79	19.38	15.74	2.43	45.66	5134
650	0.38	14.8	20.52	17.53	0.54	46.61	4797
700	0.39	13.85	20.25	18.6	0.11	47.19	4746
750	0.39	13.19	19.65	19.44	0.02	47.7	4757
800	0.39	12.62	19.03	20.17	0	48.18	4776

Table 11. Literature review (wood gasification - general data) for Aspen Plus model validation; producer gas composition (mol %, dry basis)

Component	Ref.					Aspen Plus results (S1-S12)
	[5]	[20]	[21]	[22]	[11]	
CO ₂	9-15	10.2	10.2	10-15	10-15	16.06-17.64
H ₂	12-20	15.2	15.2	16-20	16-20	17.98-20.33
CO	17-22	22.1	22.1	17-22	17-22	13.71-17.26
CH ₄	2-3	1.7	1.7	2-3	2-3	1.65-2.89
N ₂	50-54	50.8	50.8	50-55	50-55	43.21-48.36
LHV (MJ/Nm ³ , dry basis)						
	5-5.9	5.8	5.8	5-5.86	5-5.86	4.67-5.61

Table 12. Literature review (experimental work and modeling of wood gasification) for Aspen Plus validation; producer gas composition (mol %, dry basis)

Component	Ref.				Aspen Plus results (S1-S12) Model
	[23]	[24]	[24,25]	[24,26]	
	Experiment	Model	Experiment	Experiment	
CO ₂	15.3	9.4-15.3	14-16	9.6-11	16.06-17.64
H ₂	16.5	9.8-16.8	12-16	10-14	17.98-20.33
CO	15.9	18.5-20.3	18-20	18-21	13.71-17.26
CH ₄	2.1	2.4-4.5	2.5	2.5-4.8	1.65-2.89
N ₂	50.2	43-60	45-49	52-54	43.21-48.36
LHV (MJ/Nm ³ , dry basis)					
	4.61-5.02	-	≈4.80-5.28	4.84-5.32	4.67-5.61
ER	0.32-0.37	-	≈0.22-0.31	0.24-0.31	0.32-0.38
Air/Fuel	≈1.78-2	1.4-2.2	1-2	1.4-1.82	1.49-1.81

Table 13. Literature review (experimental work and modelling of wood gasification) for Aspen Plus validation

Component	Ref.				Aspen Plus results (S1-S12) Model
	[23]	[24]	[24,25]	[24,26]	
	Experiment	Model	Experiment	Experiment	
CO ₂	15.3	9.4-15.3	14-16	9.6-11	16.06-17.64
H ₂	16.5	9.8-16.8	12-16	10-14	17.98-20.33
CO	15.9	18.5-20.3	18-20	18-21	13.71-17.26
CH ₄	2.1	2.4-4.5	2.5	2.5-4.8	1.65-2.89
N ₂	50.2	43-60	45-49	52-54	43.21-48.36
LHV (MJ/Nm ³ , dry basis)					
	4.61-5.02	-	≈4.80-5.28	4.84-5.32	4.67-5.61
ER	0.32-0.37	-	≈0.22-0.31	0.24-0.31	0.32-0.38
Air/Fuel	≈1.78-2	1.4-2.2	1-2	1.4-1.82	1.49-1.81

The mathematical model for corn cob gasification process, developed in Engineering Equation Solver (EES) presented in [27], was also used in this study for Aspen Plus model validation. The EES model is also equilibrium model that involves the principle stages of gasification through sub-processes of drying, pyrolysis and gasification. It is a steady state model that is predicting product (CO₂, H₂, CO, CH₄, N₂ and H₂O) distribution trends depending on biomass composition, process temperature and equivalence ratio, and also potential air preheating, steam injection or oxygen enrichment. Modifications of the EES model were made in order to utilize it for wood chips gasification and to minimize differences between Aspen Plus and EES models as much as possible. Since the mole fraction of CH₄ has to be a fixed value, adopted from the literature, the resulting CH₄ value from Aspen Plus is taken into account in EES. It was necessary to vary heat losses in the EES gasifier until ER for all twelve samples did not match with twelve Aspen Plus ER values, Figure 5. Aspen Plus results are in great agreement with the obtained results in

EES, Figures 6-8, and in very good agreement with ranges from Table 8. Heat output in EES gasifier is in a reasonable agreement with the optimal value of gasifier capacity, 250 kW, determined in Aspen Plus.

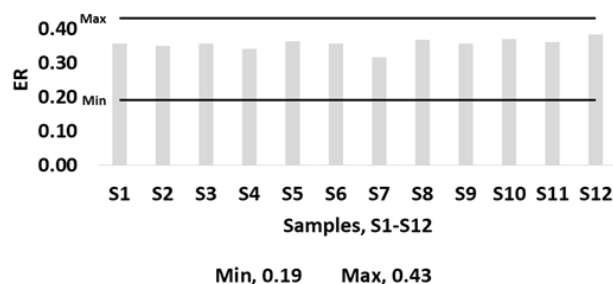


Figure 5. ER for each of the twelve samples S1-S12.

CONCLUSION

In this study, a thermochemical equilibrium model for wood chips downdraft gasification has been presented. Equilibrium composition and LHV of the producer gas are predicted based on the Gibbs energy

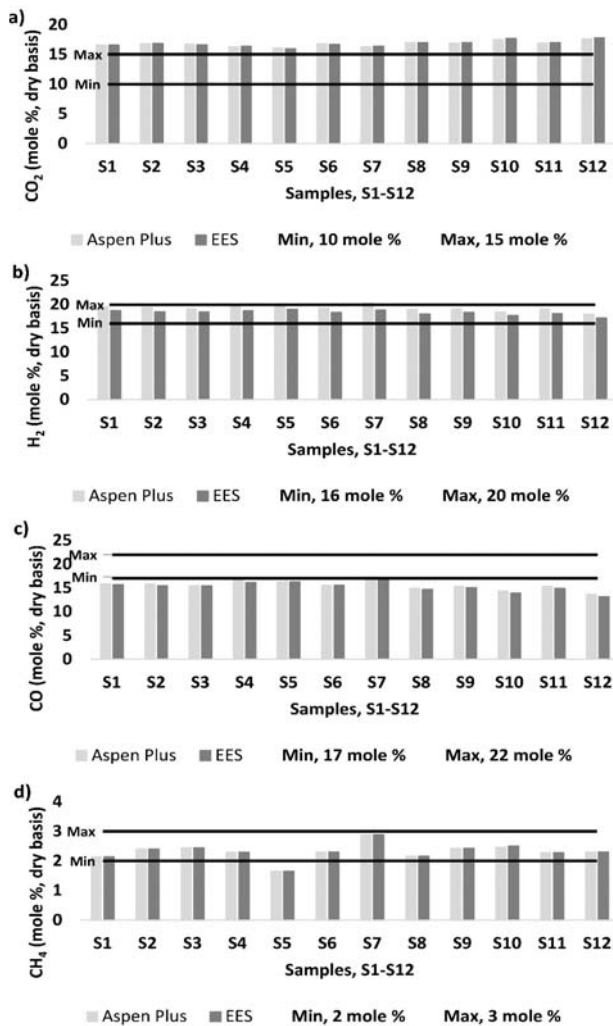


Figure 6. Aspen Plus and EES model predictions of the fractions in producer gas: a) CO₂; b) H₂; c) CO; d) CH₄.

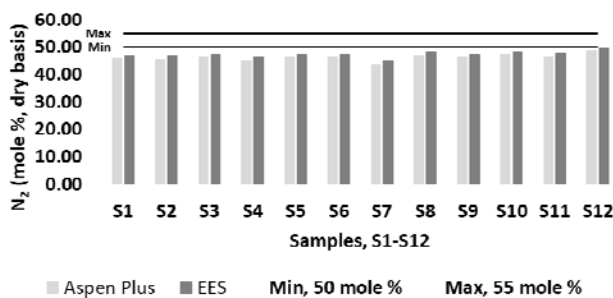


Figure 7. Aspen Plus and EES model predictions of the N₂ fraction in producer gas.

minimization method implemented within the RGibbs reactor in Aspen Plus. There is no influence of outlet temperature in the RYield reactor on the predictions. Chemical equilibrium temperature within the “Restrict chemical equilibrium - specify temperature approach or reactions” gasifier regime controls the whole process. Optimal gasifier capacity and gasification temperature are 250 kW and 600 °C, respectively. This

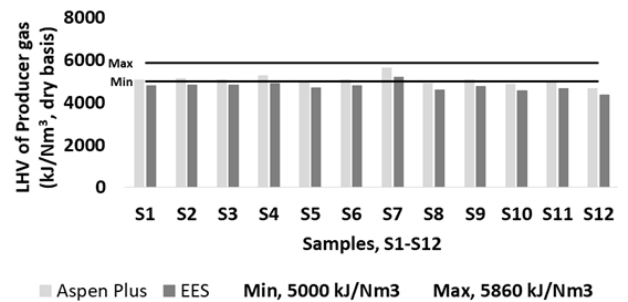


Figure 8. Aspen Plus and EES model predictions of LHV of producer gas.

conclusion is primarily based on model provided outputs, ER, producer gas composition and LHV, and their agreement with the literature. Producer gas composition and LHV are in very good agreement with the literature and in great agreement with the results provided from the modified equilibrium model in Engineering Equation Solver (EES). The presented model can be used for producer gas composition and heating value estimations in similar commercial small-scale systems.

REFERENCES

- [1] D. Bonalumi, Energy Procedia 101 (2016) 432-439
- [2] W. Doherty, A. Reynolds, D. Kennedy, J. Power Sources 277 (2015) 292-303
- [3] D. Neves, H. Thunman, A. Matos, L. Tarelho, A. Gómez-Barea, Prog. Energy Combust. Sci. 37 (2011) 611-630
- [4] A.A.P. Susastriawan, H. Saptoadi, Purnomo, Renew. Sustain. Energy Rev. 76 (2017) 989-1003
- [5] M. Puig-Arnavat, J.C. Bruno, A. Coronas, Renewable Sustainable Energy Rev. 14 (2010) 2841-2851
- [6] J. Brandin, M. Tunér, I. Odenbrand, Small Scale Gasification: Gas Engine CHP for Biofuels, Linnaeus University, Växjö, 2011, p. 21
- [7] C.D. Le, Gasification of Biomass: An Investigation of Key Challenges to Advance Acceptance of the Technology, University of Bath, Bath, 2012, p. 2-7
- [8] J.A. Ruiz, M.C. Juárez, M.P. Morales, P. Muñoz, M.A. Mendivil, Renewable Sustainable Energy Rev. 18 (2013) 174-183
- [9] T.K. Patra, P.N. Sheth, Renew. Sustain. Energy Rev. 50 (2015) 583-593
- [10] J.B. Milligan, Downdraft gasification of biomass, Aston University, Birmingham, 1994, p. 22
- [11] H. Beohar, B. Gupta, V.K. Sethi, M. Pandey, Int. J. Thermal Technol. 2 (2012) 134-140
- [12] P. McKendry, Bioresour. Technol. 83 (2002) 55-63
- [13] M. Čeranić, Uticaj procesnih parametara na pirolizu i gasifikaciju oklaska kukuruza, Univerzitet u Novom Sadu, Novi Sad, 2015, p. 17 (in Serbian)
- [14] ISO/TC 238 - Solid Biofuels

- [15] A.J. Keche, A.P.R. Gaddale, R.G. Tated, *Clean Technol. Environ. Policy* 17 (2015) 465-473
- [16] S.M. Atnaw, S.A. Sulaiman, S. Yusup, *J. Appl. Sci.* 11 (2011) 1913-1920
- [17] C. Panda, *ASPEN Plus Simulation and Experimental Studies on Biomass Gasification*, National Institute of Technology Rourkela, Rourkela, 2012, p. 12
- [18] F. Paviet, F. Chazarenc, M. Tazerout, *Int. J. Chem. React. Eng.* 7 (2009) 1-16
- [19] Z.A. Zainal, A. Rifau, G.A. Quadir, K.N. Seetharamu, *Biomass Bioenergy* 23 (2002) 283-289
- [20] N.L. Panwar, R. Kothari, V.V. Tyagi, *Renew. Sustain. Energy Rev.* 16 (2012) 1801-1816
- [21] T.B. Reed, A. Das, *Handbook of Biomass Downdraft Gasifier Engine Systems*, The Biomass Energy Foundation Press, Colorado, 1988, p. 24
- [22] A.K. Rajvanshi, in *Alternative Energy in Agriculture*, D.Y. Goswami, CRC Press, Greensboro, 1986, p. 83
- [23] Y.-I. Son, S. J. Yoon, Y. K. Kim, J.-G. Lee, *Biomass Bioenergy* 35 (2011) 4215–4220
- [24] C.D. Blasi, *Chem. Eng. Sci.* 55 (2000) 2931-2944
- [25] W.P. Walawender, S.M. Chern, L.T. Fan, in *Fundamentals of Thermochemical Biomass Conversion*, R.P. Overend, T.A. Milne, L.K. Mudge, Springer, Dordrecht, 1985, p. 911
- [26] Y. Wang, C.M. Kinoshita, in *Advances in Thermochemical Biomass Conversion*, Springer, A.V. Bridgwater, Dordrecht, 1993, p. 280
- M.R. Trninić, *Modeling and optimisation of corn cob pyrolysis*, University of Belgrade, Belgrade, 2015, p. 215.

IVANA ČEKOVIĆ¹
 NEBOJŠA MANIĆ²
 DRAGOSLAVA STOJILJKOVIĆ²
 MARTA TRNINIĆ²
 DUŠAN TODOROVIĆ²
 ALEKSANDAR JOVOVIĆ²

¹Inovacioni centar Mašinskog fakulteta,
 Kraljice Marije 16, 11120 Beograd,
 Srbija

²Mašinski fakultet Univerziteta u
 Beogradu, Kraljice Marije 16, 11120
 Beograd, Srbija

NAUČNI RAD

MODELOVANJE PROCESA GASIFIKACIJE DRVNE SEČKE U ASPEN PLUS PAKETU METODOM VIŠESTRUKOG VALIDACIJSKOG PRISTUPA

Termodinamički ravnotežni model razvijen je za proces istosmerne gasifikacije drvne sečke. Stacionarni ASPEN Plus simulator korišćen je za procenu sastava i donje toplotne moći proizvedenog gasa. Razmatrana su tri slučaja, usled različitih pretpostavki uvedenih tokom razvoja matematičkog modela, i svi su detaljno opisani. Eksperimentalni deo realizovan je u manjem komercijalnom CHP postrojenju, pri čemu je uzorkovano dvanaest uzoraka bukove sečke. Koeficijent viška vazduha je u opsegu od 0,32 do 0,38 i odnos vazduh-gorivo od 1,49 do 1,81, za optimalan kapacitet gasifikatora, od 250 kW. Molski udeli CO₂, H₂, CO, CH₄ i N₂ u suvom gasu, su redom 16,06-17,64, 17,98-20,33, 13,71-17,26, 1,65-2,89 i 43,21-48,36. Višestruki validacijski pristup korišćen je za potvrdu modela. Rezultati su u dovoljnoj meri saglasni sa različitim literaturnim izvorima (eksperimenti i modelovanje) i u velikoj meri sa modifikovanim ravnotežnim modelom iz literature razvijenim u Engineering Equation Solver paketu. Odstupanja u rezultatima mogu se objasniti na dva načina. Eksperimenti istosmerne gasifikacije drveta su u određenoj meri različiti i parametri modela se ne mogu u dovoljnoj meri podesiti kako bi se smanjile razlike. Donja toplotna moć proizvedenog gasa kreće se u opsegu od 4,67-5,61 MJ/Nm³.

Ključne reči: ASPEN, istosmerna gasifikacija, eksperiment, modelovanje, višestruki validacijski pristup, drvna sečka.