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MODELING OF ENERGY CROPS GASIFICATION BASED ON EXPERIMENTAL DATA

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Abstract
The paper presents a mathematical model of the selected energy crops gasification. Firstly, the experimental study of the biomass gasification process using fixed-bed reactor was conducted. The highest calorific value was obtained from the gasification of *Miscanthus x giganteus* (3.84 MJ/m^3_n). Based on the experimental results, a model of the gasifier built in Aspen Plus was verified. The developed mathematical model of the gasification system properly reflects the processes occurring in the analyzed gasifier. The relative differences of the lower heating values from the model and experiment did not exceed 1%.

Streszczenie
W artykule zaprezentowano przygotowanie modelu procesu zgazowania roślin energetycznych. Przeprowadzono badania eksperymentalne zgazowania analizowanej biomasy z wykorzystaniem zgazowarki ze złożem stałym. Najwyższą wartość opałową gazu uzyskano ze zgazowania Miskanta olbrzymiego (3.84 MJ/m^3_n). Pozyskane dane eksperymentalne posłużyły do walidacji modelu zbudowanego przy użyciu oprogramowania Aspen Plus. Zbudowany model właściwie odzwierciedla proces zgazowania w analizowanym reaktorze. Względne różnice między wartościami opałowymi gazów ze zbudowanego modelu oraz z eksperymentu nie przekroczyły 1%.

Keywords: **Energy crops; Gasification; Modeling; Experimental research.**

1. INTRODUCTION

In order to contribute to improvement of environment, modern energy systems have to be based on renewable and alternative energy sources. In Poland, where the use of renewable such as solar or geothermal sources is limited, biomass is one the most promising sources of chemical energy. Biomass use is often combined with gasification as one of the interesting technologies of thermochemical conversion of solid fuel into a useful gas [1]. Biomass-derived syngas can be potentially used in power boilers [2-4] or in gas piston engines [5-7] Energy crops are an interesting type of biomass due to its local availability and significant positive impact on the soil [8, 9].

In agroenergetics, three groups of perennial plants are mainly used: trees and shrubs, grasses and perennials [10]. The gasification of energy crops is discussed in the literature, however, the use of *Miscanthus x giganteus* is mainly described [11-20] with attention rarely paid to *Spartina pectinata*, *Sida hermaphrodita* [16]. Lifecycle assessment of *Miscanthus x giganteus* gasification was performed and described in [19]. The authors concluded that gasification, compared with direct combustion and anaerobic digestion, performs best in almost all analyzed categories (global warming potential, non-renewable energy use, acidification, eutrophication and respiratory organics). The only category in which the anaerobic digestion is better is non-renewable energy use. What is more, in the analyses concerning natural gas as a fuel, using *Miscanthus* instead of natural gas to generate electricity reduces non-renewable energy use and global warming.

Gasification process can be a valuable method of energetic utilization of energy crops planted in the areas of wasteland for the purpose of phytoremediation of soil. The resulting process gas, after the removal of impurities, can potentially be used for the production of electricity and heat in a cogeneration system.

There is little research on the gasification of various types of energy crops which should be deeply revised due to high potential of this technology to positively impact the environment. A mathematical model of the gasification process should also be developed for integration with energy system models to provide broad system analysis of possible use of energy crops as a source of energy for combined heat and power plant.

To reach the stated goal, first, experimental research on gasification of the selected plant species in a fixed bed generator using air as a gasifying agent was performed. The model of gas generator was then built and verified based on the measured data.

The modeling of the gasification process, owing to a variety of chemical reactions and the heterogeneity of the process, is not an easy problem. However, numerical models allow multi-criteria analysis and thermodynamic optimization of energy systems to be conducted (considering, e.g., thermodynamic or economic criteria), significantly reducing the risk associated with investment in this type of system. Numerical models allow to determine the performance characteristics of the devices included in the systems as well as those of the whole integrated systems to be determined, considering many significant quantities. In the case of gasification systems, these are, e.g., the type (composition) of fuel, the type of gasifying medium, and the process of purification or cooling of the resulting process gas.

There are two approaches to the construction of gas generator models to be found in the literature. One approach involves the construction of models, which considers the kinetics and dynamics of the gasification process and is mainly based on modeling through CFD (computational fluid dynamics) methods; the second is based on equilibrium models, most often using minimization of the Gibbs function. The main advantages of the latter approach are the much smaller time investment for the construction of the model and realization of the calculations, the lack of a need to know a number of key kinetic parameters of the process and the less time-consuming analysis; however, this approach is more simplified and does not map the complex physicochemical kinetics occurring in the real process [21, 22]. In this study, the second approach was chosen. Regardless of the choice of the modeling method, one of the most important stages of the modeling process is the validation of the model on the basis of real experimental data. This increases the credibility and verification of the correctness of the operation of the built numerical models.

2. EXPERIMENTAL STUDY

The laboratory stand used for energy crops gasification is a laboratory-scale fixed-bed gasification facility. It consists of the reactor (5 kg maximum feedstock) operating with small overpressure. The produced gas passes through a basic gas cleaning apparatus, and the samples are taken to the analysis. The molar fraction of gas composition was measured online using the following analyzers: ABB Uras14, utilizing infrared absorption to measure the concentration of CO and CO_2, Siemens Ultramat 6E, utilizing infrared absorption to measure concentration of CH_4 and Siemens Calomat, utilizing conductivity to measure concentration of H_2. The laboratory stand was described in detail in [23]. The gasification process was conducted for the air excess ratio $\lambda = 0.18$. The scheme of the gasification facility is presented in Figure 1.

The main properties of the gasified biomass are presented in Table 1. The main differences are visible when the phytoremediation potential is concerned, which was described in detail in [8], however it is not significant in this work.

The main results of the experiment are presented in Figures 2 and 3. The highest share of CO and CH_4 was obtained for *Miscanthus x giganteus* which results in the highest LHV of produced gases. The results of the experimental study were discussed in detail in [23].

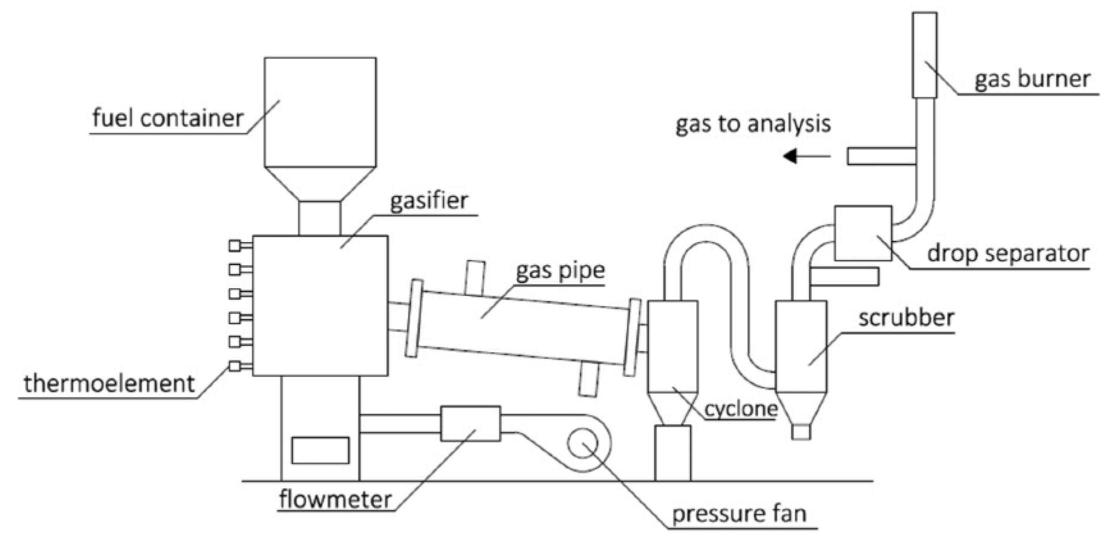

Figure 1.
Scheme of the laboratory stand

Table 1.
Properties of the analyzed energy crops

Quantity	*Miscanthus x giganteus*	*Sida hermaphrodita*	*Panicum virgatum*	*Spartina pectinata*
Ultimate analysis, % (dry basis)				
C	46.6	44.8	45	45.8
H	7.16	7.4	6.9	7.28
N	0.16	0.37	0.55	0.26
S	1.35	1.4	1.43	1.45
O	44.73	46.03	46.12	45.21
Proximate analysis, % (as received)				
ash	1.36	2.6	3.23	3.24
volatiles	75.4	78.8	78.1	77.5
moisture	7.6	9	8.5	8
LHV, MJ/kg	19.45	19	18.35	19.29

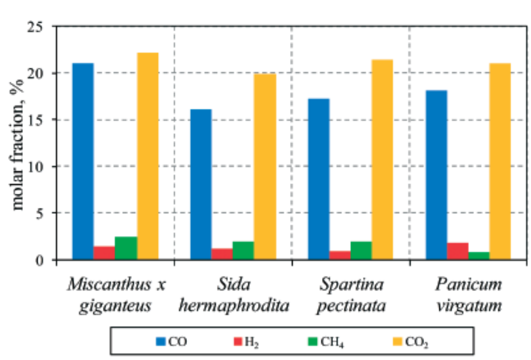

Figure 2.
Molar fraction of main components of the energy crops-derived gases

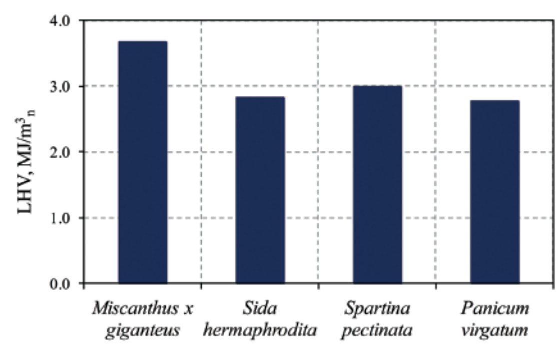

Figure 3.
Lower heating value of the energy crops-derived gases

3. MODEL OF THE GASIFICATION UNIT

For the construction of the model of the gasification unit, Aspen Plus software was used [24]. The main aim of building the model in this study was to reflect the processes occurring in the gas generator, wherein the achievement of the objective was evaluated by comparing the composition and the calorific value of the gas from the model with the values obtained from measurements on the experimental stand. During the analysis, many different structures of the model of the gasification system were considered (from simplified to complex), and the final structure was the result of the minimization of the objective function.

It was assumed in the model that the gasification process is carried out isothermally and in steady-state

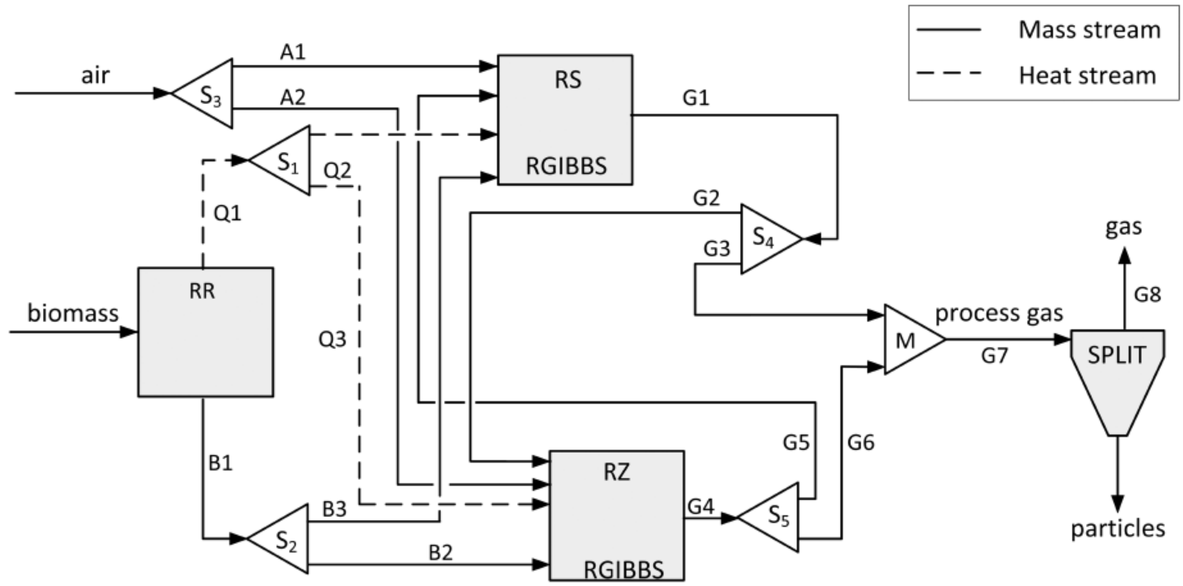

Figure 4.
Schematic diagram of the gasification process model

conditions, and components of a gas in generator are in a thermodynamic equilibrium state. To determine the equilibrium composition of the gas, the model uses minimization of the Gibbs function. A simplified diagram of the model is shown in Fig. 4. Modeling of gasification consists in this case of several stages, aiming to reflect the complexity of the processes proceeding in the real gasifier. Simulation of the decomposition of biomass supplied to the gasifier on elementary components, including carbon, hydrogen, oxygen, sulfur, nitrogen, chlorine and ash, is conducted using the decomposition reactor (RR). This is necessary because the equilibrium reactor RGIBBS (for the modeling of chemical reactions in the gasifier) in the Aspen Plus program calculates products for substrates contained in the database. The RGIBBS reactor considers all components as products and allows a great deal of reactions proceeding in the gasifier to be modelled. In the model, the stream of products (B1) from the balance reactor RR is separated into two streams. Stream B3 is sent to reactor RS, whose aim is to simulate the combustion process (occurring in the combustion zone in a real reactor) in the equilibrium reactor RGIBBS, and the stream B2 directed to reactor RZ, simulating the gasification process (taking place in the gasification zone). The process air is partly supplied to the combustion reactor (stream A1) and partly to the gasification reactor (stream A2). The split fraction of the air, which cannot be determined from the experiment, is the decision variable in the calculations. To the combustion reactor, part of the decomposition products from the reactor RR and part of the products from the gasification process in reactor RS (stream G5) are supplied. The streams are decision variables in the calculations. The case of the gasification reactor is similar. The other streams from reactors RS and RZ (stream G3 and G5) are directed to the collector M. The resulting synthesis gas is a mixture of the products of the two reactors. In the split separator, solid and gas phases are separated. This configuration allows the real processes occurring in the gasifier to be reflected.

Validation of numerical models can be performed based on various indicators of the thermodynamic effectiveness and the parameters and composition of the products obtained. In this paper, the validation of numerical models was based on the comparison of the composition (and simultaneously the Lower Heating Value) of the gas obtained in the experiment with those obtained in the mathematical model. The relative difference of these values was determined.

4. RESULTS OF MODELING

The input data for the proposed models of the gasification process were adopted based on the fuel chemical composition analysis (Table 1) and the results of experimental investigation using laboratory installation (Fig. 1). The main aim of the calculations was the validation of the gasifier model proposed in Section 3. This was realized by the selection of structures and variables in models to obtain the compositions of produced gases similar to those obtained with the experimental rig. The least-square method was adopted. The aim of the analysis (objective function) was to obtain the lowest possible error in the four basic components of the producer gas (nitrogen, carbon oxide, carbon dioxide and methane).

The minimization of the objective function was obtained by changing selected decision variables (denotation according to Fig. 4):

- Air stream air separation ratio in block S3 (directed to the combustion process); γ_{air},
- Fuel stream B1 separation ratio in block S2 (directed to the combustion reactor); γ_{bio},
- Gas from combustion stream G1 separation ratio in block S4; γ_{com},
- Gas from gasification stream G4 separation ratio in block S5; γ_{gas},
- Temperature of gasification process (RZ block); T_{gas},
- Temperature of combustion process (RS block); T_{com}.

For the described variables, the calculation for *Miscanthus x giganteus* was first carried out. The results of the calculations are presented in Table 2.

The molar composition of the producer gas obtained with mathematical modeling of the gasification process and the relative and absolute differences of the experimental and model gas composition are presented in Table 3.

Similar calculations were carried out for other energy crops described in Section 2. The results of those analyses, in the form of relative and absolute differences, are presented in Table 4.

Table 2.
Values of decision variables obtained with gasification modeling

Quantity	Unit	Value of model estimation
γ_{air}	-	0.9219
γ_{bio}	-	0.4901
γ_{com}	-	0.3135
γ_{gas}	-	0.5573
T_{gas}	°C	407.2
T_{com}	°C	1434.2

Table 3.
The results of mathematical modeling for *Miscanthus x giganteus*

Quantity	Experimental value	Model value	Absolute difference	Relative difference, %
CO	0.2104	0.2067	0.0037	1.78
CH_4	0.0245	0.0289	-0.0044	18.15
CO_2	0.2219	0.2154	0.0065	2.91
N2	0.5292	0.5292	0.00	0.00
LHV, MJ/m^3_n	3.68	3.68	0.00	0.00

Table 4.
Absolute (AD) and relative (RD) difference between the results of experiment and modeling of energy crop gasification

Quantity	Sida hermaphrodita		Spartina pectinata		Panicum virgatum	
	AD	RD, %	AD	RD, %	AD	RD, %
CO	-0.0203	-12.59	-0.0108	-6.28	-0.0061	-3.33
CH_4	0.0019	15.28	0.0007	7.60	0.0001	0.40
CO_2	-0.0010	-5.11	-0.0005	-2.57	-0.0003	-3.36
N_2	0.0192	9.65	0.0103	4.80	0.0061	2.91
LHV, MJ/m^3_n	0.01	0.20	0.00	0.09	0.00	0.07

The results show that the gasifier model properly reflects the operation of the laboratory gasification rig, however, it was not possible to reach convergence of the results for all the compounds. Discrepancies between the experimental data and modeling results do not usually overstep a few percent. Difficulty in obtaining better compatibility of the model with the actual measurement results mainly from the accuracy of the fuel composition analysis and number of simplifying assumptions in the numerical model (e.g., temperatures in the gasification process, heat losses, etc.). Nevertheless, the model that was built can be used for further analyses of the gasification process of the analyzed crops. What is more, the model can be a part of an integrated model of energy system fueled with energy crops.

5. SUMMARY

In the first part of the paper the experimental study of energy crops gasification was presented. Firstly, test-bench was briefly described. The laboratory-scale fixed-bed reactor with air as gasifying medium was used. The results of the experimental study consist of the molar compositions of energy crops-derived. Based on these results, a mathematical model of gasifier that was built within the study was verified. It showed a good compatibility with the experimental data.

Gasification of energy crops allows gas to be obtained that can be used to produce heat and electricity. In the carried out analyses, the lower heating value of the obtained gases was in the range of 2.77 MJ/m^3_n (*Panicum virgatum*) to 3.68 MJ/m^3_n (*Miscanthus x giganteus*).

The developed mathematical model of the gasification system properly reflects the processes occurring in the analyzed gasifier and is universal. The resulting relative differences in the composition and heating value of the gas in most cases do not exceed several percent.

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