

Biomass gasification process modelling approaches

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ABSTRACT

In developed European countries, the number of a small and middle-scale biomass gasification combined heat and power plants as well as syngas production plants has been significantly increased in the last decade mostly due to extensive incentives. However, existing issues regarding syngas quality, process efficiency, emissions and environmental standards are preventing biomass gasification technology to become more economically viable.

To encounter these issues, special attention is given to the development of mathematical models which can contribute to a more efficient plant design, to predict when the process becomes ineffective or harmful or they can be used for control purposes. Mathematical models can range from three-dimensional models that take fluid dynamics and chemical reactions kinetics into consideration, to simpler models where the mass and energy balances are considered over the entire or a part of a gasifier to predict process parameters. The complexity and computational intensiveness of detailed models imposes the need for development of simpler models, either based on first principles or neural networks, which can be used for a fast process parameter prediction and control. The complexity of simpler models can also range from chemical reaction equilibrium based models that take only few most important process reactions into consideration to artificial intelligence system based models or more complex equilibrium or pseudo-equilibrium models where the tar formation is also considered. Due to need for intensive measurements, not many works on artificial intelligence system based biomass gasification models have been reported. Results derived from these kinds of models often vary from author to author.

The work presents an analysis of different biomass gasification modelling aspects that can be used for an on-line process control. After related literature review and measurement data analysis, different modelling approaches for the process parameter prediction will be devised. Models results and possibilities of neural networks to predict process parameters with high speed and accuracy will be analysed. Measurement data for model performance analysis will be derived from biomass gasification plant located at Technical University Dresden.

1. INTRODUCTION

Gasification of biomass is a high-temperature partial oxidation process in which a solid carbon based feedstock is converted into a gaseous mixture (H_2 , CO , CO_2 , CH_4 , light hydrocarbons, tar, char, ash and minor contaminates) called "syngas", using gasifying agents [1]. As the most important process products of gasification, H_2 and CO contain only around 50% of the energy in the gas while the remained energy is contained in CH_4 and higher (aromatic) hydrocarbons [2]. As gasifying agents, air, pure oxygen, steam, carbon dioxide, nitrogen or their mixtures could be used. The utilisation of different gasifying agents results in different gasification process characteristics (gas quality, gas production rate, char and tar production and gas lower heating value).

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Gasification process could be divided into three main stages: drying (100-200 °C), pyrolysis (200–500 °C) and gasification (500–1000 °C) [1,2]. In the drying process the moisture from biomass evaporates and biomass becomes dry. In the pyrolysis stage of the process, the volatile components from biomass are vaporised through various complex reactions. By-products of the pyrolysis stage are char and other inert components that have not been vaporised. In the gasification process, the char is gasified through reactions with the gasifying agent and products of pyrolysis (H_2 and CO). The energy that is needed for this process is produced from combustion of part of the fuel, char and gases. The main reactions during the biomass gasification process [3,4] are shown in Table 1.

Reaction	Chemical reactions	ΔH [kJ/mol]
Primary devolatilisation (pyrolysis)	Biomass $\rightarrow H_2O, CO, CO_2, CH_4, C_2H_4$ and C	
Tar cracking and reforming	Primary tar \rightarrow Secondary tar + $H_2, CO, CO_2, CH_4, C_2H_4$	
Homogenous gas-phase	Secondary tars $\rightarrow C, CO, H_2$	
	$H_2 + 0,5 O_2 \rightarrow H_2O$	- 242
	$CO + 0,5 O_2 \rightarrow CO_2$	- 283
	$CH_4 + 0,5 O_2 \rightarrow CO + 2 H_2$	- 110
	$CH_4 + CO_2 \rightarrow 2 CO + 2 H_2$	+247
	$CH_4 + H_2O \rightarrow CO + 3 H_2$	+206
	$CO + H_2O \rightarrow CO_2 + H_2$	- 40,9
Heterogeneous	$C + O_2 \rightarrow CO_2$	- 393,5
	$C + 0,5 O_2 \rightarrow CO$	- 123,1
	$C + CO_2 \rightarrow 2 CO$	+ 159,9
	$C + H_2O \rightarrow CO + H_2$	+ 118,5
	$C + 2 H_2 \rightarrow CH_4$	- 87,5

Table 1: Main reactions during biomass gasification process

The performance of biomass gasification processes is influenced by large numbers of operation parameters concerning the gasifier and biomass [1], such as fuel and gasification agent flow rate, composition and moisture content of the biomass, geometrical configuration of the gasifier, reaction/residence time, type of gasifying agent, different size of biomass particles (typically from 0.1-0.4 mm for entrained flow gasifiers [1], 0.4-1.5 mm for fluidised bed gasifiers [5] and 5-100 mm for fixed bed gasifiers [6]), gasification temperature (750-1000°C [2, 5]), pressure (1 – 20 bar [5]) and the gasifying agent/biomass ratio.

Gasifiers can be mainly classified as autothermal or allothermal gasifiers [7]. In autothermal gasifiers the reactions of combustion and gasification are performed simultaneously in one single reactor while in allothermal gasifiers, part of reactor that is used for gasification reactions is indirectly heated. Three types of gasifier are used for biomass gasification purposes: fluidised bed; fixed bed; and entrained flow gasifiers (Fig. 1.).

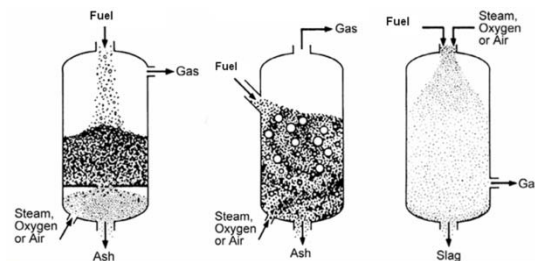


Fig. 1. Simplified scheme of fixed bed (left), fluidised bed (middle) and entrained flow (right) gasifier [8]

The downdraft type of gasifiers are the most manufactured (75%) types of gasifiers in Europe, United States of America and Canada. 20% of all produced gasifiers are fluidised bed gasifiers and the remaining 5% are updraft and other types of gasifiers [9]. Products of gasification are mostly used for separately or combined heat and power generation, liquid fuels production and for chemical production. Biomass gasification seems to have promising potential for electricity and heat cogeneration through conventional or fuel cells based technology.

Mathematical models can be used to explain, predict or simulate the process behaviour and to analyse effects of different process variables on process performance. Mathematical models are essential for process optimisation and control because they can be used to analyse effects of various different operating parameters on process behaviour in reasonable time and with reasonable costs. Nowadays, special attention is given to the biomass gasification process modelling [10] which can contribute to more efficient plant design, emission and syngas generation prediction or plant control in order to optimise the gasification process.

2. MATHEMATICAL MODELS FOR THE BIOMASS GASIFICATION PROCESS

Mathematical modelling is mostly based on the conservation laws of mass, energy and momentum. The complexity of models can range from complex three-dimensional models that take fluid dynamics (CFD models) and chemical reactions into consideration to simpler models where mass and energy balances are considered over the entire gasifier to predict the gas composition.

Kinetic mathematical models are used to describe kinetic mechanisms of the biomass gasification process. They take into consideration various chemical reactions and transfer phenomena among phases [1]. Kinetic models are very useful in detailed description of the biomass conversion during the gasification process, for the gasifier design and process improvement purposes, but due to their computationally intensiveness and long computational time they are still impractical for online process control. Models that do not solve particular processes and chemical reactions in the gasifier and instead consist of overall mass and heat balances for the entire gasifier are called equilibrium models. Equilibrium models are generally based on chemical reaction equilibrium and take into account the second law of thermodynamics for the entire gasification process [1]. Artificial neural networks (ANN) models use a pure mathematical modelling approach which correlates the input and output data to form a mathematical prediction model. ANN is a universal function approximator that has ability to approximate any continuous function to an arbitrary precision even without apriori knowledge on structure of the function that is approximated [11]. A comparison of different modelling approaches is described in Table 2.

Mathematical model approach		Advantages	Disadvantages
<i>Kinetic models</i>		More realistic process description Extensive information regarding process operation Good for gasifier design and improvement purposes	All possible process reactions are not considered Different model reaction coefficients and kinetics constants Dependable on the gasifier design Impractical for online process control
<i>Equilibrium models</i>		Independent from gasifier type and design or specific range of operating conditions Useful in prediction of gasifier performance under various different operational parameters Easy to implement Fast convergence	Describe only stationary gasification process Do not offer insight in gasification process
	<i>Stoichiometric models</i>	Applicable for describing complex reactions in general	Only some reactions are taken into consideration Reaction mechanisms must be clearly defined Equilibrium constants are highly dependable on specific range of process parameters
	<i>Non-stoichiometric models</i>	Simplicity of input data Used to predict the syngas composition	Describe gasification process only in general Lack of detailed process information
	<i>Pseudo-equilibrium models</i>	More realistic equilibrium models	Estimation of methane, carbon and tar in outlet steam is necessary Model is dependable on site specific measurements and type of the gasifier.
<i>Artificial neural networks models</i>		Do not need extensive knowledge regarding process	Depends on large quantity of experimental data Many idealised assumptions
	<i>Hybrid neural network model</i>		Knowledge regarding process is needed

Table 2: Comparison of different modelling approaches [12]

The literature [13-31] offers several comprehensive gasification models that could be used for biomass gasification process control and optimisation. Devised models are mostly equilibrium based models and offer only static process analysis and optimisation. Often, for development of this kind of models, several assumptions have to be made. Many authors in their research analyse different kind of effects on gasification process so it is hard to correlate results derived from their research. Most of the literature is focused on the development of equilibrium models for downdraft fixed bed or fluidised bed gasifiers because these types of gasifier have proven their reliability in a lot of demonstration and test plants and are the most manufactured type of gasifiers in the EU, USA and Canada.

3. EQUILIBRIUM MODELS ANALYSIS

For the biomass gasification process and equilibrium models performance analysis, two different equilibrium modelling approaches have been devised. The equilibrium model without tar calculations is based on Babu et al. [22] methodology while the equilibrium model with tar calculations is based on methodology proposed by Barman et al. [23]. Both models are based on energy and mass conservation laws as well as equilibrium chemical balances calculations. Equilibrium chemical balances of the water gas shift reaction (K_1), methane reaction (K_2) and methane reforming reaction (K_3) have been taken into consideration. Input parameters of both models are biomass composition, biomass moisture content and air input. Output model parameters are syngas composition and process temperature. The syngas is assumed to consist of H_2 , CO , CO_2 , H_2O (vapour), CH_4 , N_2 gases and tar ($CH_{0.83}$). In the equilibrium model with tar calculation, the chemical compound “Acenaphthene” has been used to represent tar in model calculations. The energy that is released or consumed during process reactions is taken from Table 1. The summary of both modelling approaches is presented in Table 3.

	Equilibrium model without tar calculations	Equilibrium model with tar calculations
Mass balance	$CH_xO_y + wH_2O + mO_2 + m \cdot 3.76N_2$ $= x_1H_2 + x_2CO + x_3CO_2 + x_4H_2O + x_5CH_4 + 3.76N_2$	$CH_xO_y + wH_2O + mO_2 + m \cdot 3.76N_2$ $= x_1H_2 + x_2CO + x_3CO_2 + x_4H_2O + x_5CH_4 + 3.76N_2 + x_6CH_{0.83}$
Chemical balance	$K_1 = f(temp) = \frac{H_2 \cdot CO_2}{CO \cdot H_2O}$ $K_2 = f(temp) = \frac{CH_4}{(H_2)^2}$	$K_1 = f(temp) = \frac{H_2 \cdot CO_2}{CO \cdot H_2O}, K_2 = f(temp) = \frac{CH_4}{(H_2)^2},$ $K_3 = f(temp) = \frac{CO \cdot (H_2)^3}{CH_4 \cdot H_2O}$
Energy balance	$Q_{in} + LHV_{biomass} = LHV_{syngas} + Q_{reactions}$	$Q_{in} + LHV_{biomass} = LHV_{syngas} + Q_{reactions}$

Table 3. Summary of two different equilibrium modelling approaches

The modelling scheme is presented on Fig. 2. Both models are based on an iteration approach for the process parameter calculation. First, the initial process temperature and the gas composition are assumed. Based on an initial process temperature assumption, chemical balance constants (kinetic constants) are calculated. Based on mass and chemical balances and model inputs, the new syngas composition is calculated. When difference between previous calculation and current calculation is less than 1%, the iteration circle is stopped and current results are taken as final. After syngas composition calculation, the process temperature is calculated (based on energy balance equations). If the difference between calculated and initial temperature assumption is larger than 1%, calculated temperature is set to become the new initial temperature and the whole calculation-iteration process repeats again.

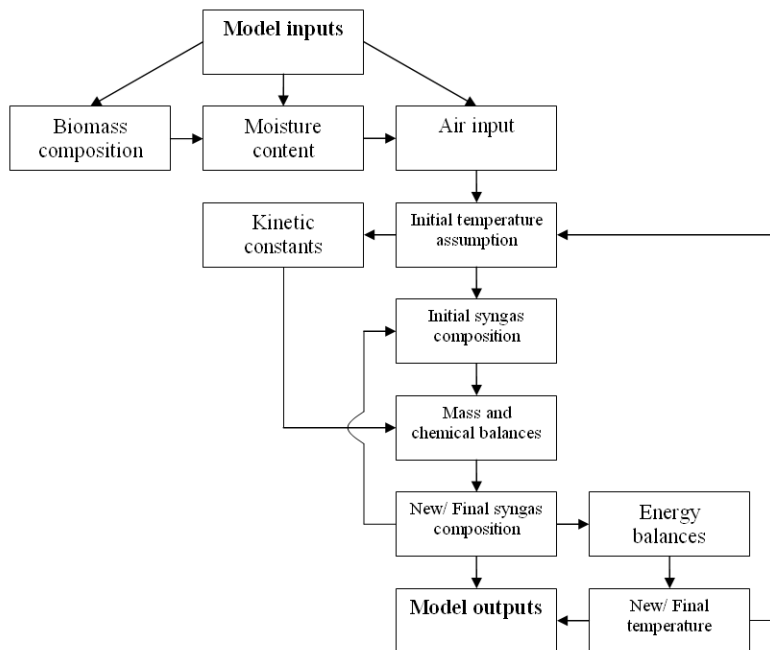


Fig. 2. Modelling scheme - Equilibrium model

Model results can be seen on Fig. 2 and 3. Figure 2 represents results derived from equilibrium model without tar calculations. Results show that with an increase of the moisture content in the biomass together with an increase of the air flow, the process temperature decreases. Due to temperature dependence of different chemical reactions, similar tendency can be seen for H_2 , CO and H_2O syngas composition values. Results derived from the equilibrium model with tar calculations (Fig. 3.) show good correlation with results derived from the Barman et al. [23] research. Results show that the temperature increases with moisture content while with different air flows it remains relative constant. CO values follow the tendency of temperature changes due to strong dependence of the chemical reactions that involve CO with process temperature. Model tar calculations show that the tar is increased with moisture content in biomass and with air flow decrease. Negative tar values are not physically explainable. They are result of modelling approach (equations that define the equilibrium gasification model). Different equilibrium modelling approaches show different results that cannot be compared in some cases. They are comparable with results derived from literature only for specific operating points.

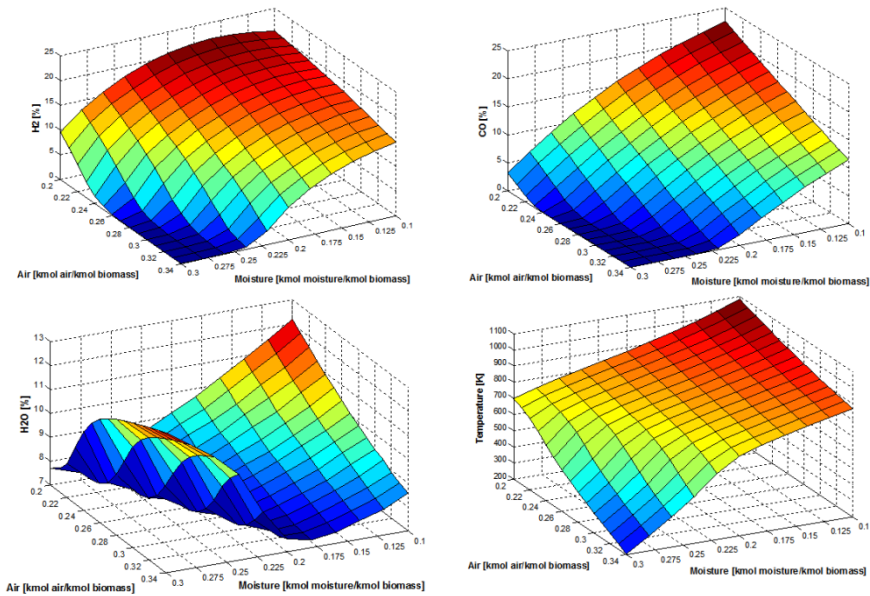


Fig. 3. Results of the equilibrium model without tar calculations

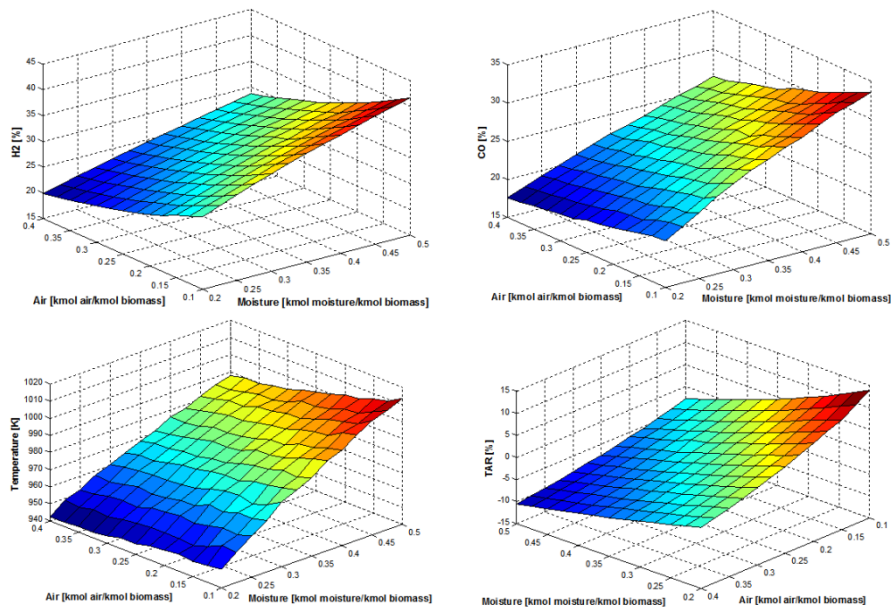


Fig. 4. Results of the equilibrium model with tar calculations

4. NEURAL NETWORK MODEL

For utilizing a neural network model (NNM), the prediction model has to learn/to be trained from observed/measured data. Neural network models require measurements to form input and output data sets for neural network training. With different sets of input and output data as well as different training procedures, results from NNM will differ. NNM are often dependable on site specific measurements. Data for neural network training were extracted from a database attached to 2 biomass gasification facility operated by TU Dresden, Germany with resolution of 30 seconds. One facility (100kW_{th}) is located in Schwarze Pumpe, Germany and the other biomass gasification facility (75kW_{th}) is located in Pirna, Germany. Facility scheme located in Pirna, Germany is presented on Fig. 5.

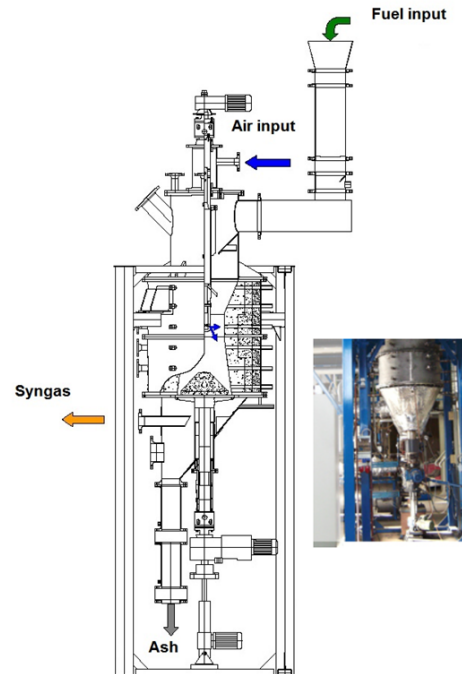


Fig. 5. Experimental biomass gasification facility located in Pirna

In order to devise NNM with acceptable average model prediction error, neural network modelling approach analysis (different input and output sets and training procedures) has to be performed. The example of the comparative analysis of temperature prediction modelling approaches (cases 1-4) for biomass gasification facility located in Schwarze Pumpe is shown in Table 4.

Model inputs				
	Case 1	Case 2	Case 3	Case 4
Fuel flow	total fuel injected (from beginning) [kg]	fuel injected in the last 10 min [kg/10min]	fuel injected in the last 10 min [kg/10min]	fuel injected in the last 10 min [kg/10min]
Air flow	current air flow [m^3/h]	current air flow [m^3/h]	air injected in the last 10 min [$\text{m}^3/10\text{min}$]	air injected in the last 10 min [$\text{m}^3/10\text{min}$]
Related time	time passed from the last fuel injection [min]	time passed from the last fuel injection [min]	time passed from the last fuel injection [min]	time passed from the last fuel injection [min]
Temperature	current temperature [$^{\circ}\text{C}$]	current temperature [$^{\circ}\text{C}$]	current temperature [$^{\circ}\text{C}$]	current temperature [$^{\circ}\text{C}$]
Other	-	-	-	different NN training procedure
Model outputs				
Model output	temperature progression [$^{\circ}\text{C}/\text{min}$]	temperature progression [$^{\circ}\text{C}/\text{min}$]	temperature progression [$^{\circ}\text{C}/\text{min}$]	temperature progression [$^{\circ}\text{C}/\text{min}$]
Average error	10,60 %	52,83 %	14,35 %	7,77 %

Table 4. Comparative analysis of different neural network modelling approaches

Comparative analysis shows that a minimum average model prediction error can be found in the case where the fuel and air injected in the last 10 min together with time passed from the last fuel injection and current outgoing syngas temperature are set to be as input data and temperature progression is set to be as output data.

Similar modelling procedure has been conducted for gasifier located in Pirna, Germany. This gasifier has different operation and design characteristics. Nevertheless, similar modelling approach that has been used for temperature prediction for gasifier located in Schwarze Pumpe has shown good prediction capabilities (in terms of average prediction error).

Different time periods for calculations of injected fuel and air quantities into a gasifier have been used in order to find prediction model with the lowest prediction error. The analysis of influence of time periods on model prediction performance has been shown in Table 5. The lowest average prediction error of NNM for Pirna gasifier is in case when the time period is set to be 25 minutes.

Time period [min]	Average error [%]
10	14,46
15	9,40
20	6,74
25	6,48
30	7,42
35	7,91
40	7,37

Table 5. Analysis of influence of time periods for fuel and air quantities calculation on model prediction error

The similar type of input data sets described from temperature prediction model has been used in order to devise neural network prediction model for the gas composition. Due to measurement characteristics, syngas composition prediction model has been devised for outgoing syngas temperature between 250 - 430 °C. The summary of both models can be found in Table 6.

Model inputs						
	Syngas temperature	Syngas composition (CO, CO ₂ , CH ₄ , H ₂ and O ₂ values)				
Fuel flow	Fuel injected in the last 25 min [kg/25 min]	Fuel injected in the last hour [kg/h]				
Air flow	Air injected in the last 25 min [kg/25 min]	Air injected in the last hour [m ³ /h]				
Related time	Time passed from the last fuel injection [min]	Time passed from the last fuel injection [min]				
Temperature	Current syngas temperature	Syngas temperature				
Number of daily experiments used for NNM training	4	4				
Neural network training method	Gaussian curve membership function	Gaussian curve membership function				
Model boundaries	Modelled syngas temperature: 20 - 450 °C	For syngas temperature: 250 - 430 °C				
Model outputs						
Model output	Temperature progression [°C/min]	Gas content [%]				
Average error / Syngas component prediction error (daily basis)	6,48 %	CO	CO ₂	CH ₄	H ₂	O ₂
		0,01 %	0,05 %	0,12 %	0,45 %	0,97 %

Table 6. The summary of temperature and composition prediction neural network models for gasifier located in Pirna

5. RESULTS

Neural network approximation model (ANFIS) shows good results for the syngas temperature prediction (see Fig. 6.). The error between measured and calculated values is mostly between $\pm 10\%$ which represents good approximation of syngas temperature during plant operation. In some marginal cases the error can reach up to $\pm 25\%$. Neural network prediction model shows good prediction possibilities in terms of the syngas temperature progression prediction during the plant operation with different operating starting points (“cold” start and “warm/preheated” start). Devised model is applicable for syngas temperature prediction range between 20°C and 450°C .

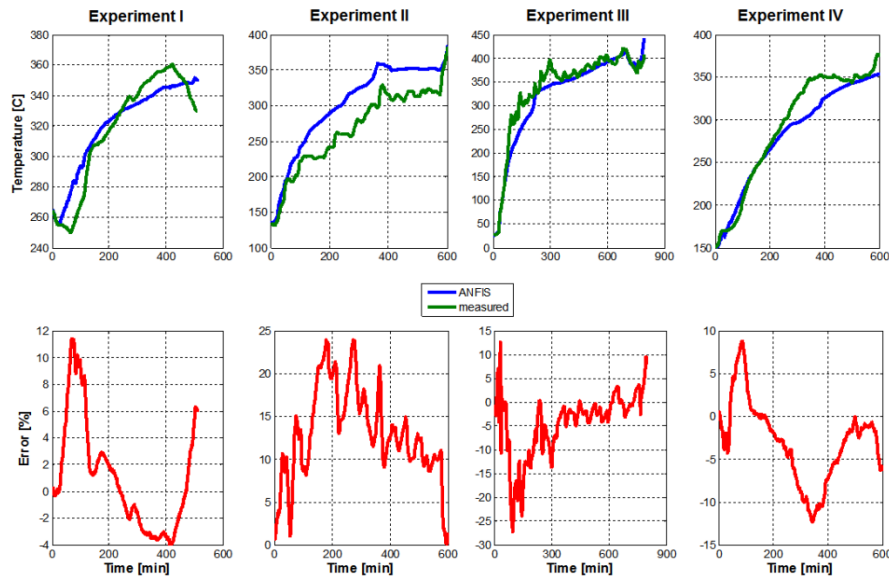


Fig. 6. Results of the neural network model for syngas temperature prediction – Pirna gasifier

In order to verify neural network syngas prediction model devised for Pirna gasifier, additional model prediction test has been performed on new set of measured data. Model prediction has showed good correlation with new input data. Prediction error is mostly between $\pm 10\%$ and in some marginally cases it reaches -25% . The model verification test has been performed for the syngas temperature range between 25°C and 425°C . Pirna NNM verification test results are presented on Fig. 7.

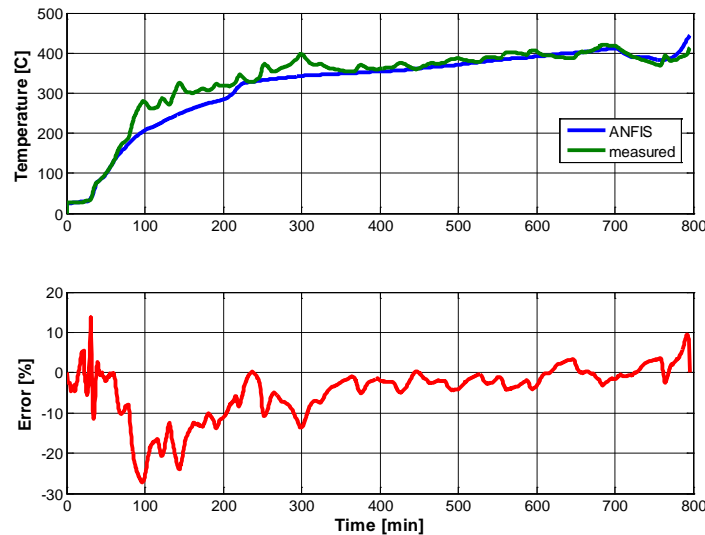


Fig. 7. Neural network model verification test for syngas temperature prediction – Pirna gasifier

Similar to syngas temperature prediction model, syngas composition prediction model has been also analysed. The H_2 neural network prediction model for 4 different experimental sets/measurement campaigns is presented in Fig. 8. Predicted H_2 values and progression of these values during the plant operation is in good correlation with measured data. During the plant operation, H_2 values are mostly between 5-10% of total volume gas composition, with maximum value of 11%.

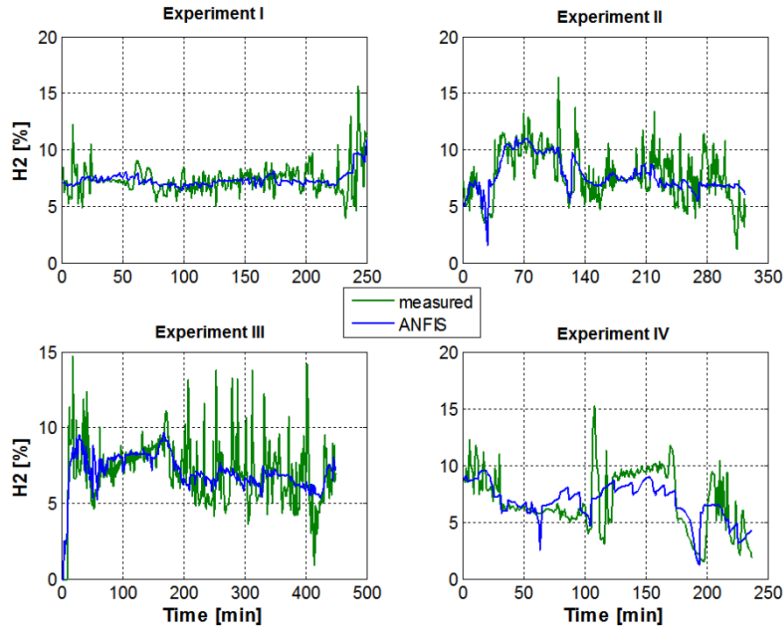


Fig. 8. Results of the neural network model for syngas composition prediction (H_2) – Pirna gasifier

The syngas composition prediction model has been verified on the new set of measured data (Fig. 9.). Although measured H_2 values range significant from minute to minute, neural network model predicts average H_2 values and their progression tendency with reasonable accuracy.

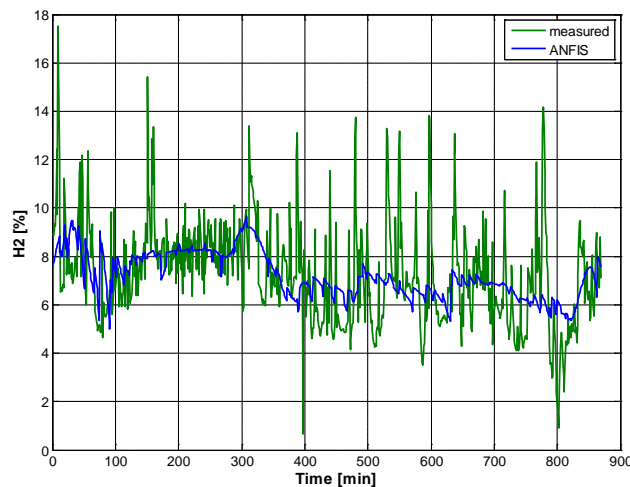


Fig. 9. Neural network model verification test for syngas composition prediction (H_2) – Pirna gasifier

Due to significant differences between minute based measurements of syngas components, prediction model potential to predict averaged syngas composition values has been analysed. Prediction of hourly averaged H_2 values from gasification process is presented in Fig. 10. Neural network prediction model enables good approximation of hourly averaged H_2 values as well as time progression of these values during gasifier operation. Averaged H_2 values are ranging mostly between 6 - 10%.

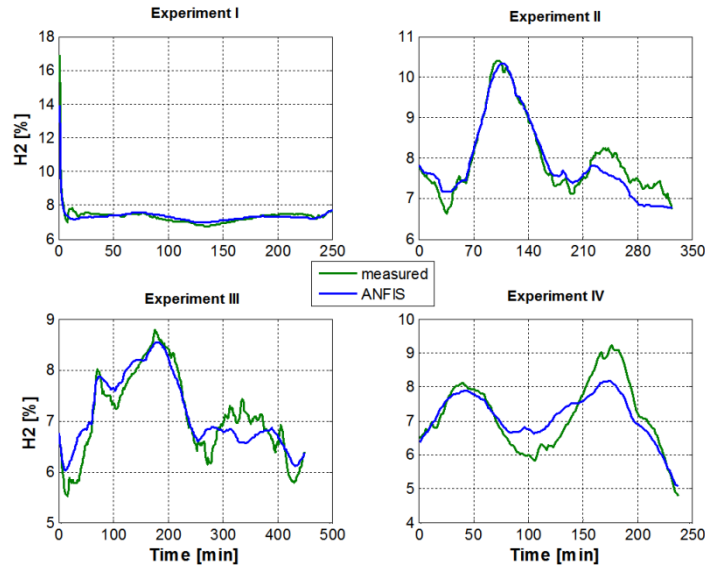


Fig. 10. Results of the neural network model for hourly averaged syngas composition prediction (H₂) – Pirna gasifier

Results of neural network prediction models for other syngas components are presented on Fig. 11 (CH₄), 12 (CO), 13 (CO₂) and 14 (O₂). In all 4 cases, devised NNM shows good syngas composition prediction potential. During the gasifier operation CH₄ values are ranging between 1,5 - 3,5%, CO values between 15 – 25%, CO₂ values between 7 – 13% and O₂ values between 0,5 – 6%. The rest of the syngas composition is composed mostly of nitrogen oxides and higher hydrocarbons (in much smaller amount).

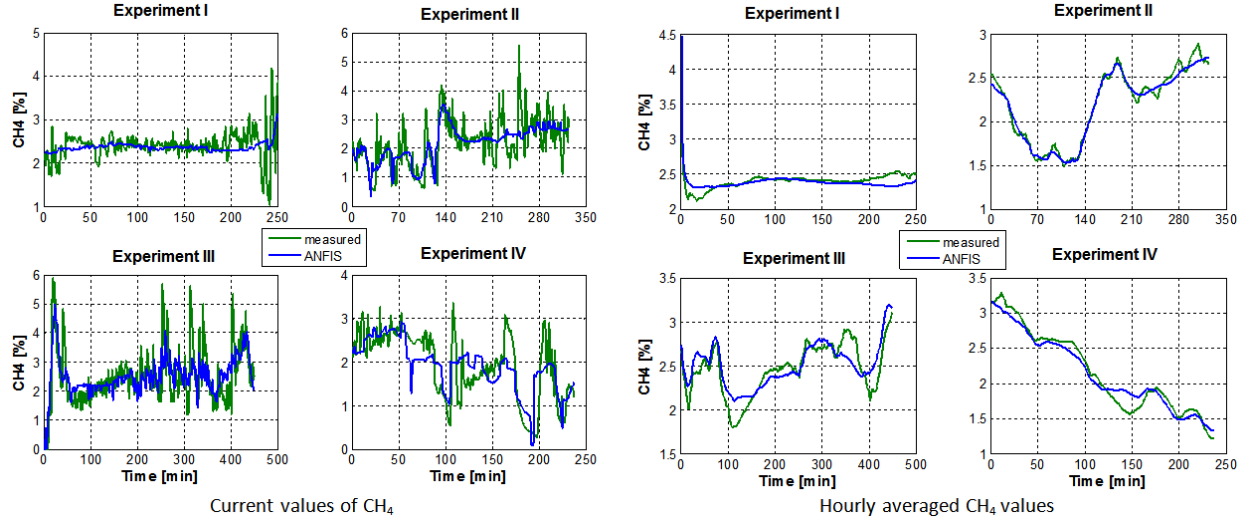


Fig. 11. Results of the neural network model for hourly averaged syngas composition prediction (CH₄) – Pirna gasifier

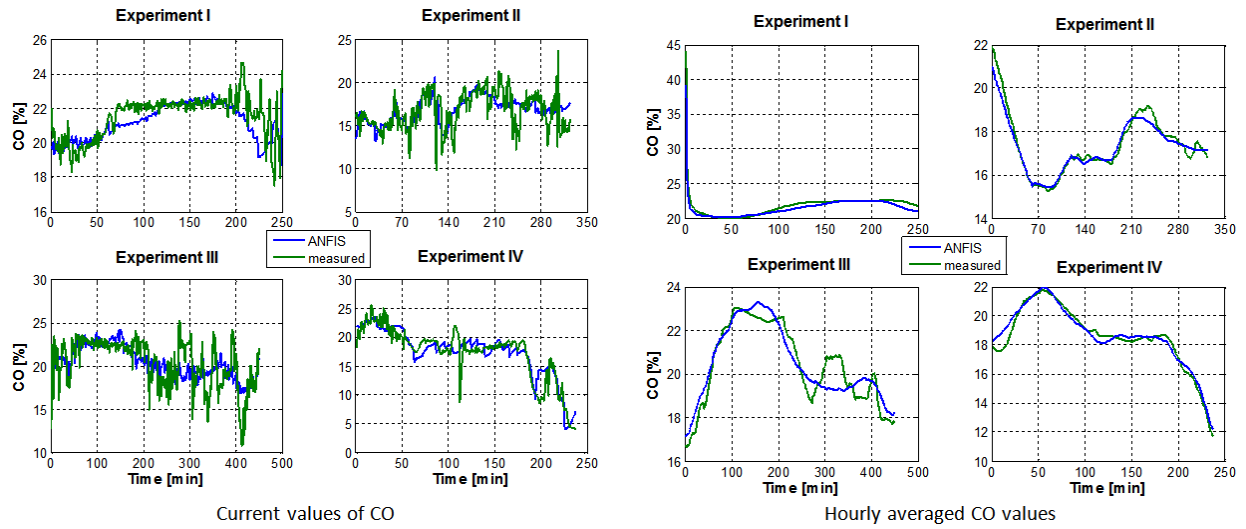


Fig. 12. Results of the neural network model for hourly averaged syngas composition prediction (CO) – Pirna gasifier

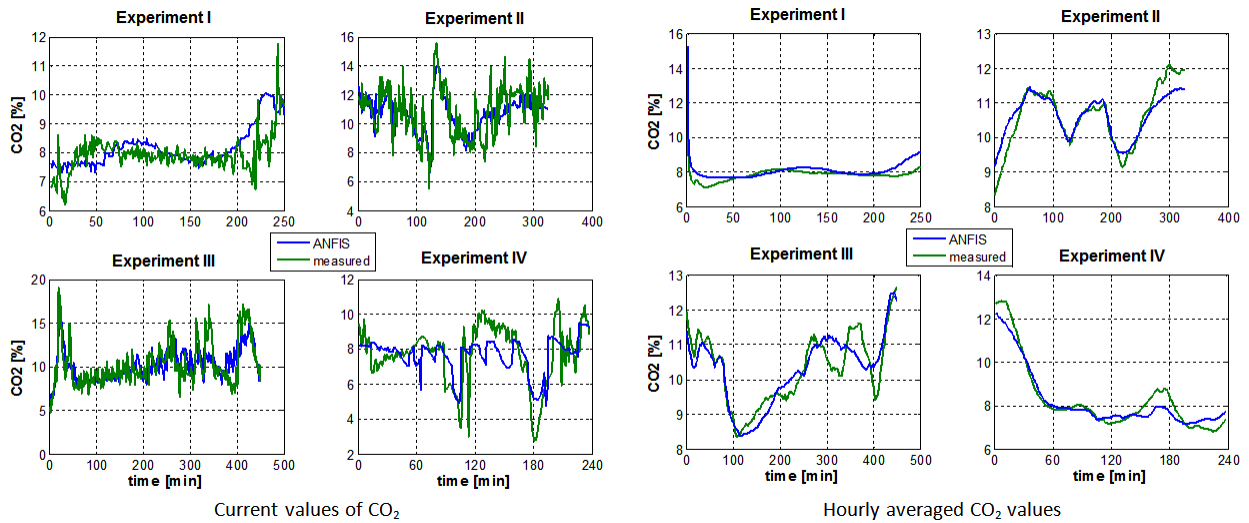


Fig. 13. Results of the neural network model for hourly averaged syngas composition prediction (CO₂) – Pirna gasifier

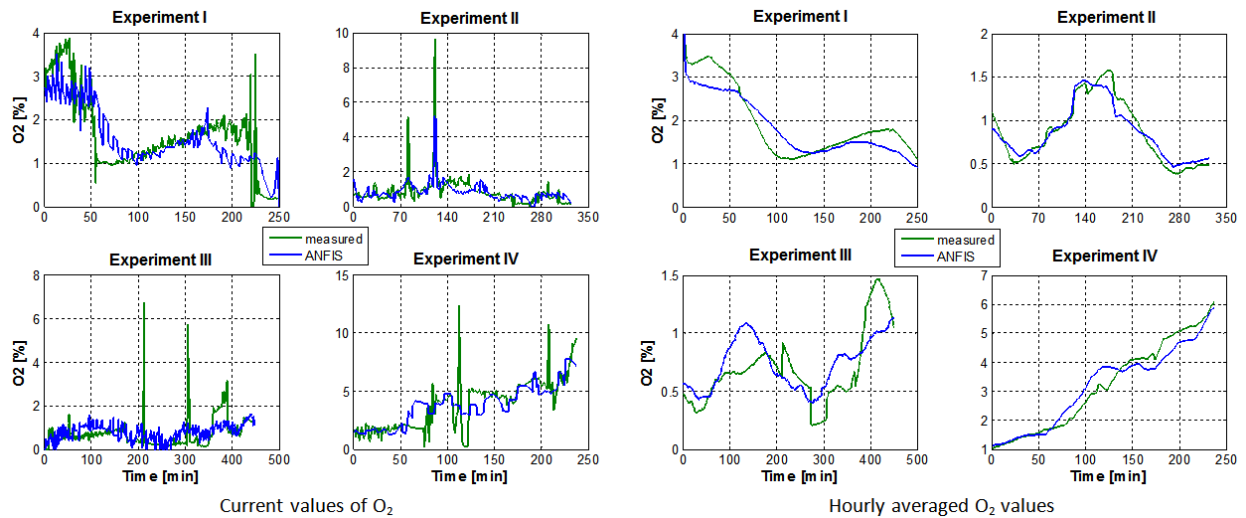


Fig. 14. Results of the neural network model for hourly averaged syngas composition prediction (O₂) – Pirna gasifier

6. CONCLUSION

This paper has analysed the possibilities of different modelling approaches that can be used for an on-line process control to predict biomass gasification process parameters with high speed and accuracy. Biomass gasification is a complex process influenced by large number of operation parameters that still faces some problems regarding environmental standards. In order to improve efficiency and to optimise the process, a plant operation analysis in dependence of various operating conditions is needed. Large scale experiments for these purposes could often be expensive or problematic in terms of safety. Therefore, various mathematical models are utilized to predict the process performance in order to optimise the plant design or process operation in time consuming and financial acceptable way. Devised models often differ in terms of delivered process information and they are often lacking extensive experimental data for verification purposes. After related literature review and measurement data analysis, two different modelling approaches for the process parameter prediction have been devised. Two similar modelling approaches have been used to devise equilibrium biomass gasification models. Results derived from these models differ in terms of calculated parameter values. These kinds of models are suitable for process prediction at specific operation point. In order to describe the process and to predict process parameter values for various operating points, neural network model has been devised. The methodology that has been used for development of neural network prediction model is applicable for different kind of gasifier designs. Devised temperature and syngas composition neural network prediction model has been verified on new set of experimental data and model outputs have been analysed. Neural network models show good correlation with measured data and good capability to predict biomass gasification process parameters with reasonable accuracy and speed.

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